



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:21 AM GMT

PDB ID : 1KMH  
Title : Crystal Structure of spinach chloroplast F1-ATPase complexed with tentoxin  
Authors : Groth, G.  
Deposited on : 2001-12-16  
Resolution : 3.40 Å(reported)

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

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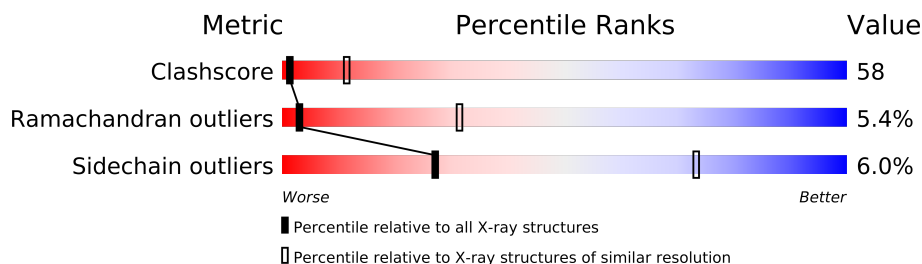
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.40 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	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	507	
2	B	498	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7217 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.

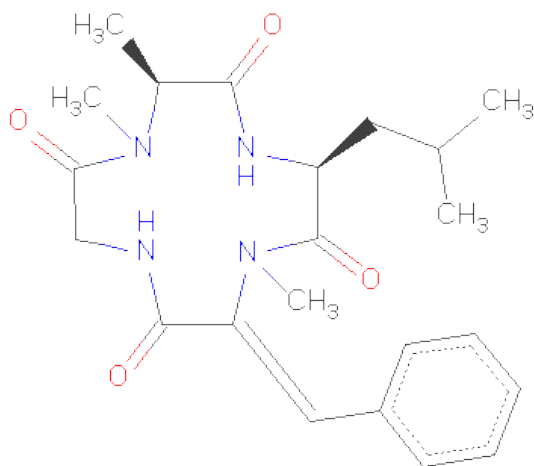
- Molecule 1 is a protein called ATPase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3647	2296	628	710	13			

- Molecule 2 is a protein called ATPase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	467	Total	C	N	O	S	0	0	0
			3540	2234	612	680	14			

- Molecule 3 is TENTOXIN (three-letter code: TTX) (formula:  $C_{22}H_{30}N_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			30	22	4	4		

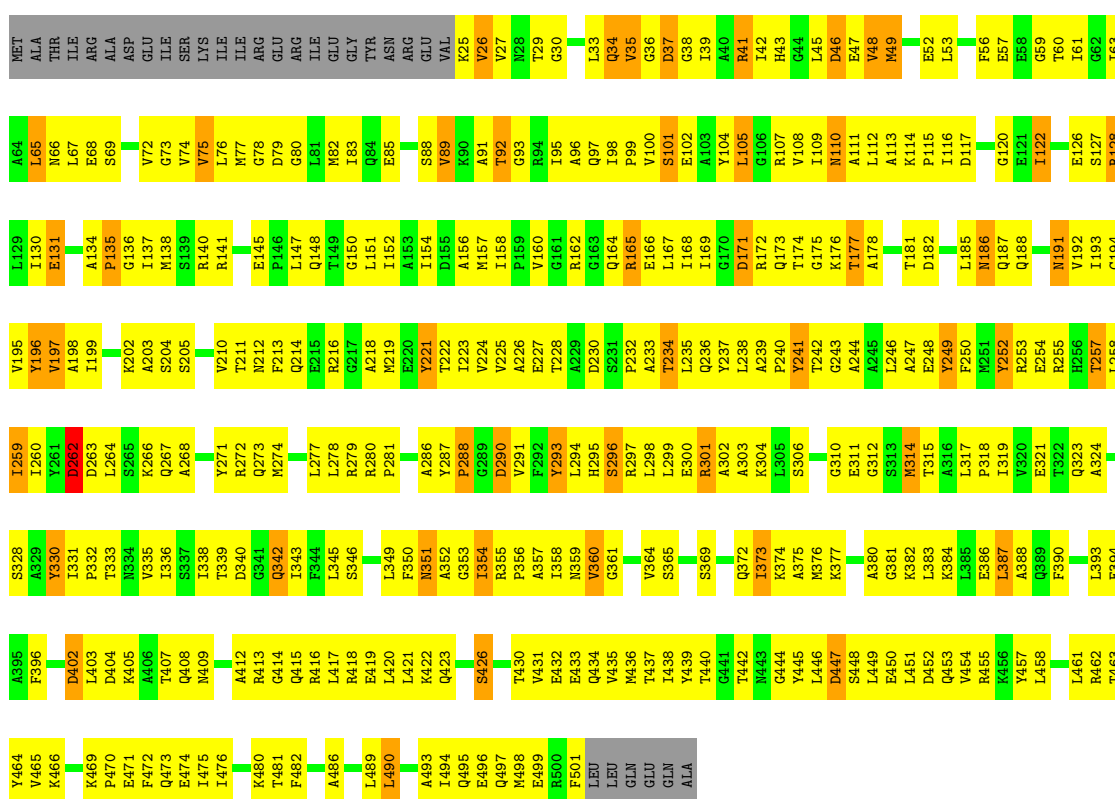
### 3 Residue-property plots

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.

Note EDS was not executed.

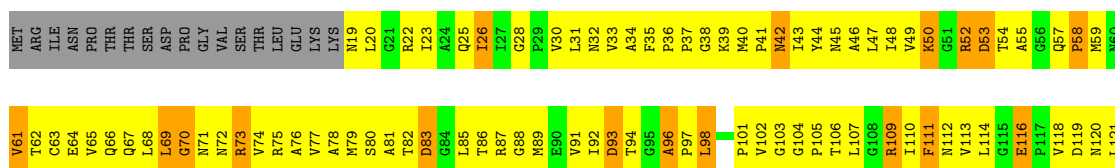
#### • Molecule 1: ATPase alpha subunit

Chain A:



#### • Molecule 2: ATPase beta subunit

Chain B:





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.89Å 146.89Å 381.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.40	Depositor
% Data completeness (in resolution range)	92.5 (6.00-3.40)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.297 , 0.319	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7217	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.13	10/3695 (0.3%)	1.02	11/5002 (0.2%)
2	B	1.16	12/3598 (0.3%)	1.06	16/4883 (0.3%)
All	All	1.15	22/7293 (0.3%)	1.04	27/9885 (0.3%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	ARG	CZ-NH1	9.20	1.45	1.33
1	A	196	TYR	CE2-CZ	-8.64	1.27	1.38
1	A	197	VAL	CB-CG1	8.01	1.69	1.52
1	A	221	TYR	CG-CD2	-7.17	1.29	1.39
2	B	237	GLY	C-O	-6.61	1.13	1.23
2	B	77	VAL	CA-CB	-6.32	1.41	1.54
2	B	80	SER	CB-OG	6.24	1.50	1.42
2	B	28	GLY	C-O	-5.97	1.14	1.23
2	B	244	GLY	C-O	5.95	1.33	1.23
1	A	252	TYR	CG-CD1	-5.92	1.31	1.39
1	A	75	VAL	C-O	-5.89	1.12	1.23
1	A	241	TYR	CG-CD2	-5.78	1.31	1.39
2	B	111	PHE	CE1-CZ	-5.73	1.26	1.37
2	B	232	VAL	CB-CG1	-5.63	1.41	1.52
1	A	293	TYR	CB-CG	-5.55	1.43	1.51
1	A	74	VAL	CB-CG2	-5.50	1.41	1.52
1	A	72	VAL	CA-CB	-5.30	1.43	1.54
1	A	63	ILE	CA-CB	-5.26	1.42	1.54
2	B	96	ALA	C-O	-5.17	1.13	1.23
2	B	109	ARG	CG-CD	-5.16	1.39	1.51
2	B	305	GLU	CD-OE1	5.09	1.31	1.25
2	B	34	ALA	CA-CB	-5.03	1.41	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	73	ARG	NE-CZ-NH2	-12.08	114.26	120.30
2	B	83	ASP	CB-CG-OD2	9.97	127.27	118.30
1	A	117	ASP	CB-CG-OD2	7.85	125.36	118.30
1	A	301	ARG	NE-CZ-NH1	-6.93	116.83	120.30
2	B	333	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	259	ILE	CG1-CB-CG2	-6.43	97.24	111.40
2	B	116	GLU	OE1-CD-OE2	6.30	130.86	123.30
2	B	305	GLU	OE1-CD-OE2	6.17	130.71	123.30
1	A	79	ASP	CB-CG-OD2	6.16	123.85	118.30
2	B	369	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	171	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	290	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	165	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	B	50	LYS	N-CA-C	5.67	126.32	111.00
2	B	93	ASP	CB-CG-OD1	5.63	123.37	118.30
2	B	347	ASP	CB-CG-OD2	5.59	123.33	118.30
2	B	277	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	A	262	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	314	MET	CG-SD-CE	-5.44	91.50	100.20
2	B	73	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	165	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	B	53	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	402	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	273	ASP	CB-CG-OD2	5.13	122.92	118.30
2	B	70	GLY	N-CA-C	-5.13	100.28	113.10
2	B	83	ASP	OD1-CG-OD2	-5.08	113.64	123.30
2	B	26	ILE	CG1-CB-CG2	-5.00	100.39	111.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3647	0	3715	432	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3540	0	3589	423	0
3	B	30	0	29	20	0
All	All	7217	0	7333	844	1

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 58.

All (844) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:499:TTX:C7	3:B:499:TTX:H181	1.32	1.57
1:A:274:MET:SD	1:A:274:MET:CE	2.01	1.48
1:A:131:GLU:HG2	1:A:297:ARG:NH1	1.41	1.33
1:A:131:GLU:CG	1:A:297:ARG:NH1	1.92	1.32
3:B:499:TTX:C7	3:B:499:TTX:C18	2.14	1.25
3:B:499:TTX:H73	3:B:499:TTX:C18	1.74	1.17
1:A:131:GLU:CG	1:A:297:ARG:HH12	1.56	1.15
3:B:499:TTX:H72	3:B:499:TTX:C18	1.80	1.09
3:B:499:TTX:H73	3:B:499:TTX:H181	1.14	1.08
3:B:499:TTX:H72	3:B:499:TTX:H181	1.11	1.08
1:A:131:GLU:HG3	1:A:297:ARG:CZ	1.86	1.06
1:A:131:GLU:HG3	1:A:297:ARG:NH1	1.71	1.06
2:B:275:ILE:O	2:B:278:PHE:HB3	1.56	1.03
2:B:243:PRO:HA	2:B:246:ARG:HH21	1.19	1.03
1:A:240:PRO:HB2	1:A:298:LEU:HD21	1.44	1.00
1:A:152:ILE:H	1:A:423:GLN:HE22	1.04	0.99
2:B:19:ASN:HB3	2:B:39:LYS:HD3	1.43	0.99
1:A:39:ILE:HD11	1:A:277:LEU:HB3	1.43	0.99
1:A:131:GLU:CG	1:A:297:ARG:CZ	2.40	0.97
1:A:39:ILE:CD1	1:A:277:LEU:HB3	1.97	0.94
2:B:41:PRO:HG2	2:B:74:VAL:HG11	1.51	0.92
2:B:69:LEU:HD21	2:B:75:ARG:HE	1.34	0.91
2:B:238:GLN:HE21	2:B:238:GLN:HA	1.33	0.90
2:B:46:ALA:O	2:B:94:THR:HG22	1.71	0.88
2:B:222:ILE:HG22	2:B:223:ASN:H	1.38	0.88
1:A:437:THR:HG21	1:A:462:ARG:HH21	1.40	0.87
2:B:251:LEU:HD21	2:B:309:LEU:HD22	1.56	0.86
2:B:185:LEU:HD13	2:B:324:ILE:HG21	1.56	0.86
1:A:240:PRO:CB	1:A:298:LEU:HD21	2.06	0.85
1:A:188:GLN:O	1:A:191:ASN:HB2	1.75	0.85
1:A:152:ILE:H	1:A:423:GLN:NE2	1.73	0.85
2:B:96:ALA:HB1	2:B:97:PRO:HD2	1.59	0.85
1:A:131:GLU:HG2	1:A:297:ARG:HH12	0.72	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:155:VAL:HG22	2:B:431:LEU:HD22	1.59	0.85
2:B:132:ILE:HA	2:B:255:THR:OG1	1.77	0.84
2:B:134:ARG:H	2:B:312:ARG:NH1	1.75	0.84
2:B:246:ARG:HB2	2:B:246:ARG:CZ	2.08	0.84
1:A:152:ILE:N	1:A:423:GLN:HE22	1.77	0.83
1:A:174:THR:HA	1:A:350:PHE:HZ	1.45	0.81
1:A:393:LEU:HD13	1:A:407:THR:HG23	1.60	0.81
2:B:69:LEU:HD12	2:B:73:ARG:HG2	1.62	0.81
2:B:104:GLY:N	2:B:105:PRO:HD2	1.96	0.81
2:B:122:ARG:HB3	2:B:123:PRO:HD2	1.62	0.81
2:B:30:VAL:HG21	2:B:288:LEU:HD22	1.63	0.81
1:A:440:THR:HG22	1:A:446:LEU:HG	1.62	0.80
1:A:373:ILE:HG22	1:A:374:LYS:H	1.46	0.80
1:A:232:PRO:HG2	1:A:235:LEU:HD12	1.63	0.79
1:A:381:GLY:HA2	1:A:384:LYS:HD2	1.64	0.79
2:B:152:GLY:H	2:B:157:ASN:HD21	1.29	0.79
2:B:207:ARG:HH11	2:B:207:ARG:HB3	1.47	0.79
2:B:247:MET:SD	2:B:282:GLY:HA2	2.21	0.79
2:B:390:ARG:HA	2:B:393:GLU:OE1	1.83	0.79
2:B:158:LEU:HD22	2:B:454:THR:HG22	1.65	0.78
2:B:388:ALA:O	2:B:392:LYS:HG3	1.84	0.78
1:A:197:VAL:HG12	1:A:199:ILE:HD11	1.63	0.78
1:A:174:THR:HA	1:A:350:PHE:CZ	2.18	0.78
2:B:105:PRO:HG3	2:B:126:THR:HA	1.64	0.78
2:B:147:SER:O	2:B:374:MET:HE1	1.83	0.78
1:A:264:LEU:HB3	1:A:295:HIS:CE1	2.19	0.78
2:B:41:PRO:HB2	2:B:65:VAL:HG21	1.65	0.78
2:B:302:LEU:HD23	2:B:302:LEU:O	1.83	0.78
1:A:53:LEU:HD11	1:A:96:ALA:HA	1.64	0.78
2:B:285:VAL:O	2:B:289:LEU:HD12	1.84	0.77
2:B:109:ARG:NE	2:B:119:ASP:OD2	2.16	0.77
1:A:68:GLU:HA	2:B:25:GLN:HG2	1.67	0.77
2:B:245:ALA:O	2:B:249:VAL:HG13	1.85	0.77
1:A:445:TYR:HB3	1:A:498:MET:SD	2.24	0.77
1:A:131:GLU:HB3	1:A:297:ARG:HH22	1.49	0.76
1:A:216:ARG:NH1	1:A:426:SER:HB2	2.00	0.76
2:B:389:GLN:O	2:B:393:GLU:HG3	1.84	0.76
2:B:243:PRO:HA	2:B:246:ARG:NH2	1.99	0.76
1:A:65:LEU:HD22	3:B:499:TTX:C18	2.15	0.76
2:B:387:ILE:O	2:B:391:VAL:HG23	1.85	0.76
2:B:429:ARG:HE	2:B:472:GLN:NE2	1.82	0.75
2:B:260:PHE:HB2	2:B:268:VAL:HG21	1.67	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:296:SER:HB2	2:B:239:MET:HB3	1.69	0.75
1:A:354:ILE:HG22	1:A:357:ALA:HA	1.69	0.75
2:B:276:PHE:CD2	2:B:328:TYR:HB3	2.22	0.75
2:B:429:ARG:HE	2:B:472:GLN:HE22	1.35	0.74
1:A:293:TYR:OH	2:B:246:ARG:NH2	2.20	0.74
2:B:275:ILE:HG22	2:B:327:VAL:HG22	1.69	0.74
2:B:310:GLN:HA	2:B:313:ILE:HD12	1.69	0.74
2:B:466:LEU:HB3	2:B:469:LEU:HD12	1.70	0.74
2:B:425:ARG:HD3	2:B:471:GLU:OE2	1.87	0.74
1:A:287:TYR:HB3	1:A:291:VAL:HG21	1.68	0.74
2:B:82:THR:O	2:B:85:LEU:HG	1.86	0.74
2:B:207:ARG:HB3	2:B:207:ARG:NH1	2.01	0.74
2:B:269:LEU:HD22	2:B:322:THR:HB	1.70	0.73
2:B:33:VAL:HG13	2:B:91:VAL:HG21	1.70	0.73
1:A:187:GLN:HE22	1:A:258:LEU:HD22	1.51	0.73
2:B:343:PHE:HA	2:B:346:LEU:HD12	1.68	0.73
1:A:262:ASP:HA	1:A:319:ILE:HD12	1.69	0.73
2:B:41:PRO:CG	2:B:74:VAL:HG11	2.18	0.73
1:A:413:ARG:HA	1:A:416:ARG:HD2	1.70	0.73
1:A:95:ILE:HG12	1:A:95:ILE:O	1.88	0.73
1:A:446:LEU:HA	1:A:449:LEU:HD12	1.69	0.73
1:A:66:ASN:HD22	1:A:68:GLU:CD	1.92	0.72
2:B:160:ALA:HA	2:B:372:SER:HB3	1.71	0.72
1:A:364:VAL:HG12	1:A:365:SER:H	1.51	0.72
2:B:333:ASP:OD2	2:B:335:THR:OG1	2.08	0.72
1:A:293:TYR:CD1	1:A:293:TYR:N	2.53	0.72
1:A:281:PRO:HB2	2:B:287:ALA:HB1	1.70	0.72
2:B:131:PRO:HD2	2:B:134:ARG:HH21	1.55	0.72
1:A:210:VAL:HG13	1:A:219:MET:HE1	1.72	0.72
1:A:187:GLN:OE1	1:A:192:VAL:HB	1.90	0.72
1:A:204:SER:OG	1:A:205:SER:N	2.20	0.72
1:A:158:ILE:HG21	1:A:343:ILE:HG12	1.71	0.71
1:A:461:LEU:CD2	1:A:497:GLN:HB3	2.19	0.71
1:A:49:MET:HG3	1:A:52:GLU:OE1	1.89	0.71
2:B:222:ILE:HG22	2:B:223:ASN:N	2.05	0.71
2:B:310:GLN:NE2	2:B:325:GLN:OE1	2.21	0.71
1:A:138:MET:SD	2:B:119:ASP:C	2.68	0.71
1:A:271:TYR:HD2	1:A:294:LEU:HD11	1.55	0.70
2:B:36:PRO:HD2	2:B:39:LYS:HB2	1.72	0.70
1:A:211:THR:O	1:A:213:PHE:N	2.25	0.70
1:A:247:ALA:HB1	1:A:257:THR:HG21	1.74	0.70
1:A:197:VAL:HG22	1:A:225:VAL:HB	1.71	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:395:LEU:HD21	2:B:428:GLU:HG2	1.73	0.70
2:B:286:SER:HA	2:B:291:ARG:NH1	2.07	0.70
2:B:167:LYS:HB3	2:B:325:GLN:NE2	2.05	0.70
1:A:264:LEU:HB3	1:A:295:HIS:HE1	1.54	0.69
2:B:35:PHE:HB3	2:B:36:PRO:HD2	1.73	0.69
2:B:149:PHE:CD1	2:B:164:ARG:HG2	2.27	0.69
1:A:211:THR:C	1:A:213:PHE:H	1.95	0.69
2:B:398:TYR:HA	2:B:401:LEU:HD12	1.74	0.69
1:A:131:GLU:CB	1:A:297:ARG:HH22	2.05	0.69
1:A:444:GLY:HA2	1:A:447:ASP:OD1	1.92	0.69
1:A:135:PRO:HB2	1:A:140:ARG:HH21	1.58	0.69
1:A:198:ALA:HB3	1:A:226:ALA:HB1	1.73	0.69
1:A:182:ASP:HA	1:A:185:LEU:HD12	1.75	0.69
1:A:162:ARG:NH1	1:A:192:VAL:HG22	2.07	0.69
2:B:82:THR:HB	2:B:85:LEU:HD12	1.75	0.68
1:A:131:GLU:CG	1:A:297:ARG:NH2	2.57	0.68
2:B:19:ASN:O	2:B:92:ILE:HG13	1.93	0.68
2:B:37:PRO:HA	2:B:72:ASN:OD1	1.93	0.68
1:A:350:PHE:HB3	1:A:355:ARG:NH2	2.09	0.68
2:B:118:VAL:HG12	2:B:118:VAL:O	1.92	0.68
2:B:474:PHE:O	2:B:477:VAL:HG22	1.94	0.68
2:B:423:ARG:O	2:B:427:ILE:HG13	1.94	0.68
2:B:264:ASN:O	2:B:266:GLN:N	2.27	0.68
1:A:39:ILE:HD11	1:A:277:LEU:HD13	1.74	0.68
1:A:293:TYR:OH	2:B:246:ARG:CZ	2.42	0.68
1:A:434:GLN:O	1:A:438:ILE:HG12	1.94	0.68
1:A:486:ALA:HA	1:A:489:LEU:HB2	1.76	0.68
1:A:356:PRO:HD2	1:A:423:GLN:H	1.59	0.67
1:A:340:ASP:CG	2:B:207:ARG:HE	1.97	0.67
1:A:198:ALA:HB3	1:A:226:ALA:CB	2.25	0.67
1:A:126:GLU:O	1:A:127:SER:OG	2.13	0.67
1:A:450:GLU:HB2	1:A:453:GLN:OE1	1.94	0.67
1:A:250:PHE:O	1:A:255:ARG:HB2	1.94	0.67
2:B:353:SER:HB3	2:B:356:LEU:HB2	1.76	0.66
2:B:264:ASN:HB2	2:B:266:GLN:HG3	1.75	0.66
1:A:271:TYR:CD2	1:A:294:LEU:HD11	2.30	0.66
1:A:291:VAL:HA	1:A:294:LEU:HD11	1.78	0.66
2:B:148:ILE:HD13	2:B:451:LEU:HD11	1.78	0.66
2:B:25:GLN:HB2	2:B:32:ASN:HD22	1.60	0.66
1:A:293:TYR:CE1	2:B:284:GLU:OE2	2.48	0.66
2:B:104:GLY:N	2:B:105:PRO:CD	2.58	0.66
1:A:131:GLU:CB	1:A:297:ARG:NH2	2.59	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:ILE:HD11	1:A:277:LEU:CB	2.22	0.66
1:A:216:ARG:HH12	1:A:426:SER:HB2	1.58	0.66
2:B:79:MET:SD	2:B:244:GLY:O	2.54	0.66
1:A:197:VAL:HG12	1:A:199:ILE:CD1	2.25	0.66
1:A:187:GLN:NE2	1:A:194:CYS:SG	2.68	0.66
1:A:187:GLN:NE2	1:A:258:LEU:HD22	2.11	0.66
1:A:381:GLY:O	1:A:384:LYS:HB2	1.95	0.66
1:A:430:THR:HG22	1:A:431:VAL:H	1.60	0.66
2:B:310:GLN:HE22	2:B:325:GLN:CD	1.98	0.66
2:B:107:LEU:HD21	2:B:196:VAL:HG13	1.76	0.66
2:B:104:GLY:O	2:B:107:LEU:HD12	1.96	0.65
2:B:435:PHE:HB2	2:B:438:ALA:HB3	1.78	0.65
1:A:295:HIS:CD2	1:A:335:VAL:HG22	2.31	0.65
1:A:293:TYR:HE1	2:B:284:GLU:OE2	1.80	0.65
1:A:356:PRO:HD2	1:A:423:GLN:N	2.10	0.65
1:A:33:LEU:HD21	1:A:43:HIS:HB2	1.78	0.65
1:A:42:ILE:HG21	1:A:45:LEU:HD12	1.78	0.65
2:B:83:ASP:OD1	3:B:499:TTX:O3	2.15	0.65
2:B:302:LEU:C	2:B:302:LEU:HD23	2.16	0.65
1:A:167:LEU:N	1:A:339:THR:HG21	2.12	0.65
2:B:171:PHE:HZ	2:B:342:THR:HB	1.63	0.64
2:B:178:LYS:O	2:B:181:LEU:HB3	1.98	0.64
2:B:149:PHE:HB2	2:B:162:TYR:O	1.96	0.64
2:B:83:ASP:OD1	3:B:499:TTX:C12	2.45	0.64
1:A:232:PRO:HG2	1:A:235:LEU:CD1	2.28	0.64
2:B:216:MET:CE	2:B:232:VAL:HG21	2.28	0.64
2:B:396:GLN:HE21	2:B:400:GLU:CD	2.00	0.64
2:B:101:PRO:HB2	2:B:126:THR:HG21	1.80	0.64
1:A:160:VAL:HA	1:A:164:GLN:OE1	1.98	0.64
1:A:61:ILE:HG22	1:A:77:MET:SD	2.38	0.64
1:A:65:LEU:HD11	1:A:75:VAL:CG2	2.28	0.63
2:B:286:SER:HA	2:B:291:ARG:HH12	1.63	0.63
1:A:126:GLU:OE2	1:A:253:ARG:NH2	2.31	0.63
1:A:376:MET:SD	1:A:435:VAL:HG22	2.38	0.63
1:A:364:VAL:HG12	1:A:365:SER:N	2.12	0.63
1:A:135:PRO:HB2	1:A:140:ARG:HE	1.62	0.63
2:B:69:LEU:HD22	2:B:75:ARG:HH21	1.63	0.63
2:B:163:ARG:HE	2:B:374:MET:CB	2.11	0.63
1:A:422:LYS:HD3	1:A:455:ARG:HH21	1.62	0.63
2:B:170:LEU:HD22	2:B:181:LEU:HD21	1.79	0.63
1:A:53:LEU:CD1	1:A:96:ALA:HA	2.28	0.63
1:A:138:MET:SD	2:B:120:ASN:N	2.72	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:167:LYS:HB3	2:B:325:GLN:HE21	1.63	0.63
2:B:296:VAL:O	2:B:296:VAL:HG12	1.98	0.63
1:A:462:ARG:HB3	1:A:466:LYS:HE3	1.80	0.63
2:B:410:LEU:O	2:B:418:ARG:CZ	2.47	0.63
1:A:461:LEU:O	1:A:465:VAL:HG23	1.99	0.62
2:B:163:ARG:HE	2:B:374:MET:CG	2.13	0.62
2:B:399:LYS:HA	2:B:402:GLN:HE21	1.65	0.62
1:A:34:GLN:HG3	1:A:41:ARG:HB2	1.81	0.62
1:A:156:ALA:O	1:A:380:ALA:HB1	2.00	0.62
1:A:461:LEU:HD22	1:A:497:GLN:HB3	1.81	0.62
2:B:219:SER:OG	2:B:221:VAL:HG23	2.00	0.62
1:A:194:CYS:O	1:A:222:THR:HA	1.99	0.62
2:B:61:VAL:HG21	2:B:85:LEU:HD21	1.81	0.62
1:A:338:ILE:HG12	2:B:239:MET:HE1	1.82	0.62
1:A:137:ILE:HG21	2:B:110:ILE:HD13	1.82	0.62
1:A:150:GLY:N	1:A:186:ASN:ND2	2.47	0.61
2:B:101:PRO:HA	2:B:129:THR:HA	1.81	0.61
1:A:45:LEU:HB3	1:A:48:VAL:HG13	1.82	0.61
2:B:136:ALA:HB1	2:B:311:GLU:O	2.01	0.61
2:B:149:PHE:HB3	2:B:162:TYR:HB2	1.83	0.61
1:A:263:ASP:H	1:A:319:ILE:HB	1.64	0.61
1:A:67:LEU:O	2:B:87:ARG:HD3	1.99	0.61
2:B:179:THR:O	2:B:182:ILE:HG22	2.01	0.61
2:B:105:PRO:CG	2:B:126:THR:HA	2.31	0.61
2:B:163:ARG:HH21	2:B:374:MET:HG3	1.66	0.61
2:B:245:ALA:O	2:B:249:VAL:CG1	2.49	0.60
1:A:110:ASN:HB2	1:A:114:LYS:O	2.00	0.60
1:A:346:SER:HB3	1:A:359:ASN:HD21	1.66	0.60
2:B:49:VAL:HG22	2:B:91:VAL:HG13	1.83	0.60
2:B:458:PHE:HA	2:B:461:ILE:HD12	1.83	0.60
1:A:359:ASN:O	1:A:361:GLY:N	2.34	0.60
3:B:499:TTX:C7	3:B:499:TTX:C17	2.62	0.60
2:B:378:ARG:O	2:B:379:ILE:HD13	2.01	0.60
2:B:167:LYS:HE2	2:B:325:GLN:HE22	1.67	0.60
2:B:81:ALA:HB1	3:B:499:TTX:H111	1.83	0.60
1:A:100:VAL:HG23	1:A:246:LEU:HD23	1.83	0.60
2:B:42:ASN:HB2	2:B:45:ASN:OD1	2.01	0.60
2:B:203:GLY:HA3	2:B:277:ARG:HB3	1.84	0.60
1:A:66:ASN:HD22	1:A:68:GLU:CG	2.15	0.60
1:A:181:THR:HG23	1:A:213:PHE:CE1	2.36	0.60
1:A:130:ILE:HG23	1:A:241:TYR:HB3	1.84	0.60
2:B:471:GLU:C	2:B:473:ALA:H	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:422:ALA:HB1	2:B:426:LYS:NZ	2.17	0.59
1:A:225:VAL:HG21	1:A:243:GLY:HA2	1.83	0.59
2:B:319:GLY:O	2:B:320:SER:HB2	2.02	0.59
2:B:308:SER:O	2:B:309:LEU:HD23	2.02	0.59
2:B:46:ALA:O	2:B:94:THR:CG2	2.46	0.59
1:A:386:GLU:C	1:A:388:ALA:H	2.06	0.59
2:B:163:ARG:HE	2:B:374:MET:HB2	1.67	0.59
3:B:499:TTX:H73	3:B:499:TTX:C17	2.28	0.59
2:B:38:GLY:O	2:B:40:MET:HG3	2.02	0.59
2:B:121:LEU:O	2:B:122:ARG:HB2	2.03	0.59
1:A:128:ARG:HH12	1:A:252:TYR:HE1	1.51	0.59
1:A:65:LEU:HD22	3:B:499:TTX:C19	2.33	0.59
2:B:397:ARG:O	2:B:401:LEU:HG	2.02	0.59
1:A:351:ASN:C	1:A:353:GLY:H	2.05	0.58
1:A:104:TYR:O	1:A:105:LEU:C	2.41	0.58
1:A:181:THR:HG23	1:A:213:PHE:HE1	1.67	0.58
1:A:258:LEU:C	1:A:259:ILE:HD12	2.24	0.58
1:A:239:ALA:HB3	1:A:240:PRO:CD	2.33	0.58
1:A:296:SER:N	1:A:338:ILE:HD13	2.17	0.58
2:B:156:VAL:O	2:B:158:LEU:N	2.36	0.58
1:A:293:TYR:OH	2:B:246:ARG:NH1	2.37	0.58
1:A:237:TYR:O	1:A:240:PRO:HD2	2.02	0.58
1:A:145:GLU:OE1	1:A:304:LYS:NZ	2.31	0.58
1:A:158:ILE:HD11	1:A:360:VAL:HG13	1.84	0.58
1:A:138:MET:SD	2:B:119:ASP:CA	2.92	0.58
1:A:346:SER:OG	1:A:349:LEU:HB2	2.03	0.58
1:A:249:TYR:O	1:A:253:ARG:HG3	2.04	0.58
2:B:69:LEU:HD21	2:B:75:ARG:HB2	1.85	0.58
1:A:274:MET:CG	1:A:274:MET:CE	2.81	0.57
1:A:233:ALA:C	1:A:235:LEU:H	2.08	0.57
2:B:141:GLN:O	2:B:316:THR:HB	2.05	0.57
1:A:210:VAL:HG13	1:A:219:MET:CE	2.34	0.57
2:B:398:TYR:O	2:B:402:GLN:HG3	2.04	0.57
2:B:240:ASN:N	2:B:240:ASN:HD22	2.02	0.57
2:B:48:ILE:HG22	2:B:92:ILE:CG2	2.35	0.57
2:B:463:SER:OG	2:B:465:GLU:HG3	2.04	0.57
2:B:275:ILE:N	2:B:326:ALA:O	2.30	0.57
2:B:471:GLU:O	2:B:473:ALA:N	2.37	0.57
2:B:64:GLU:CD	2:B:248:ARG:HE	2.08	0.57
1:A:336:ILE:HG23	1:A:342:GLN:HE22	1.69	0.57
1:A:375:ALA:HB2	1:A:480:LYS:O	2.04	0.57
1:A:108:VAL:HA	1:A:224:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:278:PHE:CZ	2:B:309:LEU:HD12	2.40	0.57
1:A:111:ALA:C	1:A:112:LEU:HD23	2.25	0.57
1:A:495:GLN:HA	1:A:498:MET:HE2	1.87	0.57
2:B:196:VAL:HG11	2:B:260:PHE:CE2	2.40	0.57
2:B:285:VAL:O	2:B:289:LEU:CD1	2.52	0.57
2:B:53:ASP:OD1	2:B:58:PRO:HG3	2.04	0.56
1:A:167:LEU:H	1:A:339:THR:HG21	1.68	0.56
1:A:56:PHE:CD1	1:A:89:VAL:CG1	2.88	0.56
1:A:167:LEU:HG	1:A:169:ILE:HG13	1.87	0.56
1:A:233:ALA:O	1:A:235:LEU:N	2.37	0.56
2:B:222:ILE:CG2	2:B:223:ASN:H	2.12	0.56
1:A:433:GLU:OE2	1:A:466:LYS:HE2	2.05	0.56
2:B:85:LEU:HD22	2:B:89:MET:HE1	1.87	0.56
1:A:300:GLU:C	1:A:302:ALA:H	2.08	0.56
2:B:204:GLU:C	2:B:239:MET:HG3	2.26	0.56
2:B:310:GLN:HE22	2:B:325:GLN:NE2	2.03	0.56
1:A:266:LYS:NZ	1:A:321:GLU:OE1	2.38	0.56
1:A:437:THR:HG23	1:A:458:LEU:HD22	1.88	0.56
1:A:254:GLU:HG2	1:A:310:GLY:CA	2.35	0.56
1:A:446:LEU:HA	1:A:449:LEU:CD1	2.36	0.56
2:B:111:PHE:HB2	2:B:235:VAL:HG22	1.86	0.56
1:A:239:ALA:HB3	1:A:240:PRO:HD3	1.86	0.56
1:A:451:LEU:O	1:A:453:GLN:N	2.39	0.56
1:A:259:ILE:HD13	1:A:314:MET:HG3	1.87	0.56
1:A:162:ARG:HA	1:A:315:THR:OG1	2.06	0.56
1:A:148:GLN:HE21	1:A:431:VAL:HG21	1.70	0.56
1:A:472:PHE:O	1:A:476:ILE:HG12	2.06	0.56
2:B:83:ASP:CG	3:B:499:TTX:O3	2.44	0.56
1:A:236:GLN:O	1:A:267:GLN:HG3	2.05	0.56
1:A:431:VAL:O	1:A:434:GLN:HB2	2.06	0.56
2:B:186:ILE:HG23	2:B:190:ALA:HB3	1.88	0.56
2:B:35:PHE:HB3	2:B:36:PRO:CD	2.36	0.56
2:B:134:ARG:O	2:B:312:ARG:HD2	2.06	0.56
2:B:195:GLY:O	2:B:231:LYS:HE2	2.06	0.56
2:B:68:LEU:O	2:B:69:LEU:C	2.44	0.55
1:A:287:TYR:CZ	1:A:331:ILE:HD13	2.41	0.55
1:A:419:GLU:HA	1:A:422:LYS:HG3	1.87	0.55
1:A:227:GLU:OE2	1:A:239:ALA:HA	2.06	0.55
2:B:167:LYS:CE	2:B:310:GLN:NE2	2.69	0.55
2:B:237:GLY:HA3	2:B:249:VAL:HG11	1.88	0.55
2:B:280:GLN:O	2:B:284:GLU:HG3	2.06	0.55
1:A:37:ASP:O	1:A:277:LEU:HD13	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:96:ALA:HB1	2:B:97:PRO:CD	2.34	0.55
2:B:148:ILE:HG12	2:B:149:PHE:H	1.71	0.55
1:A:211:THR:C	1:A:213:PHE:N	2.60	0.55
2:B:274:ASN:HA	2:B:326:ALA:O	2.07	0.55
1:A:197:VAL:HA	1:A:225:VAL:O	2.07	0.55
2:B:299:GLN:H	2:B:299:GLN:NE2	2.04	0.55
2:B:240:ASN:N	2:B:240:ASN:ND2	2.55	0.55
1:A:138:MET:SD	2:B:119:ASP:HA	2.47	0.55
1:A:196:TYR:CZ	1:A:262:ASP:OD2	2.60	0.55
1:A:340:ASP:OD1	2:B:207:ARG:NE	2.31	0.55
1:A:493:ALA:HB1	1:A:497:GLN:NE2	2.21	0.55
2:B:327:VAL:HG21	2:B:342:THR:HG21	1.89	0.54
1:A:101:SER:OG	1:A:102:GLU:N	2.39	0.54
2:B:299:GLN:H	2:B:299:GLN:HE21	1.54	0.54
1:A:241:TYR:HE1	1:A:267:GLN:HE22	1.55	0.54
1:A:387:LEU:HD13	1:A:421:LEU:HD11	1.90	0.54
2:B:269:LEU:HD12	2:B:271:PHE:CZ	2.41	0.54
2:B:103:GLY:C	2:B:105:PRO:HD2	2.27	0.54
2:B:158:LEU:HD22	2:B:454:THR:CG2	2.36	0.54
2:B:146:LEU:HD13	2:B:163:ARG:NH2	2.21	0.54
1:A:47:GLU:O	1:A:48:VAL:C	2.44	0.54
1:A:210:VAL:O	1:A:214:GLN:HG3	2.06	0.54
1:A:216:ARG:CZ	1:A:426:SER:HB2	2.37	0.54
1:A:193:ILE:N	1:A:193:ILE:HD12	2.23	0.54
2:B:270:LEU:HD22	2:B:313:ILE:HG23	1.89	0.54
1:A:387:LEU:HD21	1:A:417:LEU:HB2	1.89	0.54
1:A:496:GLU:O	1:A:499:GLU:HB2	2.08	0.54
1:A:111:ALA:HB2	1:A:227:GLU:CG	2.38	0.54
1:A:39:ILE:HD11	1:A:277:LEU:CD1	2.38	0.54
2:B:255:THR:HA	2:B:258:GLU:HG2	1.88	0.54
1:A:244:ALA:O	1:A:248:GLU:HG3	2.08	0.54
1:A:375:ALA:HB2	1:A:481:THR:HA	1.88	0.54
1:A:152:ILE:HG22	1:A:421:LEU:HD23	1.90	0.54
1:A:199:ILE:HD12	1:A:199:ILE:N	2.22	0.54
1:A:210:VAL:HG22	1:A:224:VAL:HG21	1.89	0.54
1:A:196:TYR:CE1	1:A:262:ASP:OD2	2.61	0.54
2:B:182:ILE:O	2:B:186:ILE:HG13	2.07	0.54
2:B:275:ILE:O	2:B:275:ILE:HG13	2.08	0.53
2:B:52:ARG:HD2	2:B:61:VAL:HG23	1.89	0.53
1:A:111:ALA:HB2	1:A:227:GLU:CD	2.28	0.53
2:B:368:LEU:HD12	2:B:399:LYS:HD3	1.91	0.53
2:B:171:PHE:CZ	2:B:342:THR:HB	2.43	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:470:PRO:HG2	2:B:473:ALA:HB2	1.90	0.53
2:B:300:PRO:HG2	2:B:301:THR:HG23	1.90	0.53
2:B:183:MET:CE	2:B:212:LEU:HB2	2.38	0.53
2:B:45:ASN:O	2:B:65:VAL:HG23	2.08	0.53
2:B:362:TYR:HA	2:B:363:PRO:C	2.29	0.53
2:B:351:VAL:HB	2:B:369:ASP:O	2.09	0.53
1:A:430:THR:HG22	1:A:431:VAL:N	2.24	0.53
1:A:131:GLU:HG2	1:A:297:ARG:CZ	2.21	0.53
1:A:115:PRO:HG3	1:A:120:GLY:O	2.09	0.53
1:A:451:LEU:C	1:A:453:GLN:H	2.11	0.53
2:B:278:PHE:HZ	2:B:309:LEU:HD12	1.74	0.53
1:A:182:ASP:O	1:A:185:LEU:HB2	2.08	0.53
1:A:302:ALA:HA	1:A:314:MET:HE2	1.90	0.53
1:A:65:LEU:HB2	1:A:280:ARG:HH22	1.74	0.53
1:A:390:PHE:O	1:A:394:GLU:HG3	2.08	0.53
1:A:457:TYR:O	1:A:461:LEU:HG	2.09	0.53
2:B:429:ARG:HD2	2:B:471:GLU:HB3	1.90	0.53
2:B:201:GLY:O	2:B:249:VAL:HG21	2.08	0.53
1:A:412:ALA:HB1	1:A:416:ARG:NH2	2.24	0.53
2:B:106:THR:O	2:B:111:PHE:HE1	1.92	0.53
2:B:183:MET:HE1	2:B:212:LEU:HB2	1.90	0.53
2:B:171:PHE:HZ	2:B:342:THR:CB	2.22	0.52
2:B:396:GLN:NE2	2:B:400:GLU:CD	2.62	0.52
2:B:361:ILE:N	2:B:361:ILE:HD12	2.24	0.52
2:B:260:PHE:HB2	2:B:268:VAL:CG2	2.38	0.52
1:A:359:ASN:C	1:A:361:GLY:H	2.12	0.52
1:A:122:ILE:H	1:A:122:ILE:HD13	1.73	0.52
1:A:350:PHE:HB3	1:A:355:ARG:CZ	2.39	0.52
2:B:209:GLY:HA2	2:B:236:TYR:OH	2.09	0.52
1:A:386:GLU:O	1:A:388:ALA:N	2.42	0.52
1:A:387:LEU:CD1	1:A:421:LEU:HD11	2.39	0.52
2:B:473:ALA:O	2:B:483:ALA:HA	2.09	0.52
2:B:264:ASN:O	2:B:265:GLU:C	2.46	0.52
1:A:195:VAL:HG12	1:A:197:VAL:HG23	1.91	0.52
2:B:107:LEU:HA	2:B:232:VAL:O	2.09	0.52
1:A:66:ASN:HB2	1:A:73:GLY:HA3	1.92	0.52
1:A:419:GLU:OE1	1:A:451:LEU:HA	2.10	0.52
1:A:422:LYS:C	1:A:423:GLN:HG3	2.30	0.52
2:B:19:ASN:O	2:B:92:ILE:HA	2.09	0.52
2:B:270:LEU:CD2	2:B:313:ILE:HG23	2.40	0.52
1:A:291:VAL:HA	1:A:294:LEU:CD1	2.40	0.52
1:A:259:ILE:N	1:A:259:ILE:HD12	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:246:ARG:HB2	2:B:246:ARG:NH1	2.25	0.52
2:B:274:ASN:H	2:B:326:ALA:HB3	1.73	0.52
2:B:122:ARG:HB3	2:B:123:PRO:CD	2.37	0.52
2:B:113:VAL:HG22	2:B:249:VAL:HG12	1.90	0.52
1:A:164:GLN:O	1:A:315:THR:HG23	2.10	0.52
1:A:57:GLU:C	1:A:59:GLY:H	2.13	0.52
1:A:466:LYS:HA	1:A:473:GLN:OE1	2.10	0.52
2:B:52:ARG:HD2	2:B:61:VAL:CG2	2.40	0.52
2:B:198:VAL:HG22	2:B:233:ALA:HB3	1.91	0.52
1:A:262:ASP:O	1:A:263:ASP:HB2	2.09	0.52
1:A:431:VAL:O	1:A:435:VAL:HG23	2.09	0.52
2:B:144:THR:O	2:B:146:LEU:HG	2.09	0.52
2:B:189:ILE:O	2:B:193:HIS:HB2	2.10	0.52
1:A:141:ARG:HG3	1:A:306:SER:HA	1.92	0.52
1:A:338:ILE:HA	2:B:239:MET:HE1	1.91	0.51
1:A:258:LEU:HA	1:A:315:THR:O	2.11	0.51
1:A:331:ILE:HG22	1:A:332:PRO:N	2.23	0.51
2:B:165:GLY:CA	2:B:315:SER:HB3	2.41	0.51
2:B:202:VAL:HB	2:B:274:ASN:O	2.10	0.51
2:B:19:ASN:O	2:B:20:LEU:HD23	2.09	0.51
1:A:52:GLU:OE2	1:A:91:ALA:HB1	2.10	0.51
2:B:109:ARG:HE	2:B:119:ASP:CG	2.11	0.51
1:A:359:ASN:C	1:A:361:GLY:N	2.64	0.51
1:A:288:PRO:HG2	1:A:291:VAL:HG22	1.90	0.51
2:B:184:GLU:OE2	2:B:435:PHE:HA	2.11	0.51
1:A:237:TYR:O	1:A:267:GLN:NE2	2.43	0.51
1:A:158:ILE:HD12	1:A:158:ILE:N	2.25	0.51
1:A:498:MET:HA	1:A:501:PHE:HD1	1.74	0.51
2:B:299:GLN:HB2	2:B:300:PRO:HD2	1.91	0.51
2:B:63:CYS:SG	2:B:78:ALA:HA	2.50	0.51
2:B:255:THR:HA	2:B:258:GLU:OE2	2.10	0.51
2:B:167:LYS:HG2	2:B:323:SER:OG	2.10	0.51
2:B:167:LYS:HE2	2:B:325:GLN:NE2	2.26	0.51
1:A:187:GLN:OE1	1:A:194:CYS:SG	2.69	0.51
1:A:273:GLN:O	1:A:277:LEU:HG	2.10	0.51
2:B:207:ARG:O	2:B:209:GLY:N	2.44	0.51
1:A:440:THR:CG2	1:A:446:LEU:HG	2.37	0.51
2:B:429:ARG:C	2:B:431:LEU:N	2.63	0.51
1:A:36:GLY:O	1:A:37:ASP:CB	2.58	0.51
1:A:219:MET:HG2	1:A:219:MET:O	2.11	0.51
1:A:272:ARG:HG3	1:A:286:ALA:O	2.11	0.51
1:A:193:ILE:HD11	1:A:255:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:ILE:HG23	1:A:225:VAL:HA	1.92	0.51
1:A:419:GLU:HG2	1:A:422:LYS:HE3	1.93	0.51
2:B:163:ARG:NE	2:B:374:MET:HB2	2.25	0.51
1:A:248:GLU:OE2	1:A:301:ARG:HB3	2.11	0.51
1:A:76:LEU:HD11	1:A:83:ILE:HG13	1.92	0.51
2:B:176:VAL:HG23	2:B:352:LEU:HD23	1.92	0.51
1:A:254:GLU:HG2	1:A:310:GLY:HA3	1.94	0.50
2:B:112:ASN:HB3	2:B:114:LEU:H	1.76	0.50
1:A:166:GLU:O	1:A:317:LEU:HA	2.12	0.50
2:B:276:PHE:CG	2:B:328:TYR:HB3	2.46	0.50
2:B:302:LEU:C	2:B:302:LEU:CD2	2.79	0.50
2:B:106:THR:HA	2:B:111:PHE:HZ	1.76	0.50
1:A:471:GLU:O	1:A:475:ILE:HG12	2.11	0.50
2:B:377:PRO:HD3	2:B:385:TYR:CE2	2.45	0.50
1:A:152:ILE:HG23	1:A:438:ILE:HD11	1.92	0.50
1:A:300:GLU:C	1:A:302:ALA:N	2.65	0.50
1:A:197:VAL:CG1	1:A:199:ILE:HD11	2.36	0.50
2:B:134:ARG:H	2:B:312:ARG:HH12	1.53	0.50
1:A:278:LEU:O	1:A:279:ARG:HB2	2.11	0.50
2:B:203:GLY:O	2:B:277:ARG:HG3	2.12	0.50
2:B:243:PRO:HB3	2:B:284:GLU:OE1	2.12	0.50
1:A:493:ALA:HB1	1:A:497:GLN:HE22	1.76	0.50
1:A:259:ILE:HD13	1:A:314:MET:CG	2.41	0.50
1:A:165:ARG:HG2	1:A:299:LEU:O	2.12	0.50
1:A:166:GLU:OE1	1:A:166:GLU:HA	2.11	0.50
2:B:251:LEU:HD21	2:B:309:LEU:HD13	1.93	0.50
2:B:423:ARG:HA	2:B:426:LYS:HD2	1.93	0.50
2:B:410:LEU:O	2:B:418:ARG:NH2	2.45	0.50
1:A:65:LEU:CD1	1:A:278:LEU:CD1	2.90	0.50
1:A:166:GLU:O	1:A:318:PRO:HD2	2.12	0.50
1:A:157:MET:SD	1:A:360:VAL:HG11	2.51	0.50
1:A:436:MET:O	1:A:439:TYR:HB3	2.11	0.50
1:A:210:VAL:O	1:A:219:MET:HE3	2.12	0.50
2:B:238:GLN:HE21	2:B:238:GLN:CA	2.08	0.50
2:B:255:THR:O	2:B:258:GLU:HG2	2.12	0.50
1:A:100:VAL:O	1:A:101:SER:HB3	2.10	0.50
2:B:148:ILE:HA	2:B:374:MET:CE	2.42	0.50
1:A:351:ASN:O	1:A:353:GLY:N	2.45	0.50
1:A:39:ILE:HD13	1:A:277:LEU:HB3	1.89	0.49
2:B:110:ILE:HB	2:B:119:ASP:HB3	1.94	0.49
1:A:345:LEU:CD2	1:A:358:ILE:HD13	2.42	0.49
1:A:131:GLU:CD	3:B:499:TTX:H42	2.33	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:275:ILE:CG2	2:B:327:VAL:HG22	2.41	0.49
1:A:210:VAL:O	1:A:210:VAL:CG1	2.60	0.49
1:A:339:THR:HG22	1:A:340:ASP:N	2.26	0.49
2:B:235:VAL:HG11	2:B:252:THR:CG2	2.43	0.49
2:B:48:ILE:O	2:B:92:ILE:HG22	2.13	0.49
1:A:33:LEU:CD2	1:A:43:HIS:HB2	2.43	0.49
1:A:47:GLU:O	1:A:48:VAL:O	2.30	0.49
1:A:57:GLU:OE2	1:A:88:SER:N	2.33	0.49
1:A:260:ILE:HA	1:A:317:LEU:O	2.13	0.49
2:B:279:VAL:O	2:B:282:GLY:N	2.42	0.49
2:B:197:SER:O	2:B:232:VAL:HA	2.12	0.49
1:A:263:ASP:HA	1:A:319:ILE:O	2.13	0.49
1:A:56:PHE:CE1	1:A:89:VAL:HG11	2.48	0.49
1:A:240:PRO:HB2	1:A:298:LEU:CD2	2.29	0.48
2:B:94:THR:HG23	2:B:96:ALA:H	1.78	0.48
2:B:251:LEU:CD2	2:B:309:LEU:HD22	2.37	0.48
1:A:35:VAL:HG11	1:A:83:ILE:HB	1.94	0.48
1:A:386:GLU:OE2	1:A:442:THR:HG23	2.14	0.48
2:B:475:TYR:CE1	2:B:476:LEU:HG	2.48	0.48
2:B:75:ARG:CG	2:B:76:ALA:N	2.76	0.48
1:A:440:THR:HG23	1:A:494:ILE:HG21	1.96	0.48
2:B:196:VAL:HG11	2:B:260:PHE:CD2	2.49	0.48
2:B:216:MET:HE1	2:B:232:VAL:HG21	1.94	0.48
1:A:95:ILE:O	1:A:95:ILE:HG23	2.12	0.48
2:B:69:LEU:CD2	2:B:75:ARG:HH21	2.26	0.48
1:A:498:MET:HA	1:A:501:PHE:CD1	2.48	0.48
2:B:391:VAL:HG13	2:B:427:ILE:CG2	2.44	0.48
2:B:139:PHE:O	2:B:142:LEU:HD12	2.14	0.48
1:A:295:HIS:C	1:A:297:ARG:N	2.67	0.48
2:B:422:ALA:HB1	2:B:426:LYS:HZ1	1.79	0.48
2:B:186:ILE:HA	2:B:190:ALA:HB3	1.96	0.48
1:A:295:HIS:C	1:A:297:ARG:H	2.17	0.48
1:A:69:SER:HB3	2:B:25:GLN:HE21	1.79	0.48
2:B:286:SER:HB2	2:B:299:GLN:HB3	1.95	0.48
2:B:207:ARG:CB	2:B:207:ARG:NH1	2.75	0.48
2:B:85:LEU:CD2	2:B:89:MET:HE1	2.43	0.48
1:A:405:LYS:HA	1:A:408:GLN:HG3	1.96	0.48
2:B:251:LEU:HD21	2:B:309:LEU:CD2	2.34	0.47
2:B:276:PHE:C	2:B:278:PHE:H	2.18	0.47
2:B:42:ASN:ND2	2:B:45:ASN:ND2	2.62	0.47
2:B:31:LEU:O	2:B:76:ALA:N	2.47	0.47
2:B:247:MET:O	2:B:248:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:411:ASP:C	2:B:418:ARG:HH22	2.17	0.47
1:A:36:GLY:O	1:A:37:ASP:HB2	2.14	0.47
2:B:149:PHE:HB3	2:B:162:TYR:CB	2.44	0.47
1:A:396:PHE:N	1:A:396:PHE:CD1	2.82	0.47
2:B:413:LEU:HD22	2:B:417:ASP:HB3	1.96	0.47
1:A:218:ALA:HA	1:A:221:TYR:CE2	2.49	0.47
2:B:381:GLY:O	2:B:385:TYR:HB2	2.15	0.47
1:A:80:GLY:C	1:A:82:MET:N	2.68	0.47
2:B:207:ARG:O	2:B:208:GLU:C	2.52	0.47
1:A:383:LEU:HD12	1:A:417:LEU:HD13	1.96	0.47
2:B:47:LEU:HD23	2:B:93:ASP:HA	1.97	0.47
1:A:463:THR:HA	1:A:466:LYS:HD2	1.96	0.47
2:B:168:ILE:O	2:B:325:GLN:HG3	2.14	0.47
3:B:499:TTX:H21	3:B:499:TTX:H71	1.96	0.47
2:B:333:ASP:OD1	2:B:335:THR:OG1	2.33	0.47
1:A:439:TYR:CD1	1:A:490:LEU:HD13	2.49	0.47
2:B:26:ILE:HD12	2:B:26:ILE:N	2.30	0.47
1:A:33:LEU:HB2	1:A:41:ARG:O	2.14	0.47
1:A:223:ILE:N	1:A:223:ILE:HD12	2.30	0.47
2:B:19:ASN:CB	2:B:39:LYS:HD3	2.31	0.47
1:A:432:GLU:OE2	1:A:473:GLN:O	2.32	0.47
2:B:386:GLU:OE1	2:B:390:ARG:NH2	2.48	0.47
2:B:163:ARG:HG2	2:B:374:MET:SD	2.54	0.47
2:B:62:THR:O	2:B:79:MET:HG2	2.15	0.47
2:B:391:VAL:HG13	2:B:427:ILE:HG21	1.96	0.47
2:B:264:ASN:C	2:B:266:GLN:N	2.68	0.47
1:A:65:LEU:CD1	1:A:278:LEU:HD11	2.45	0.47
1:A:135:PRO:HB2	1:A:140:ARG:NH2	2.28	0.47
2:B:184:GLU:HB2	2:B:435:PHE:CD2	2.50	0.47
1:A:238:LEU:O	1:A:239:ALA:C	2.51	0.46
1:A:430:THR:O	1:A:434:GLN:HG3	2.14	0.46
1:A:242:THR:O	1:A:244:ALA:N	2.48	0.46
1:A:349:LEU:O	1:A:354:ILE:HB	2.15	0.46
1:A:469:LYS:N	1:A:470:PRO:CD	2.78	0.46
3:B:499:TTX:H72	3:B:499:TTX:C17	2.35	0.46
2:B:361:ILE:HD12	2:B:361:ILE:H	1.80	0.46
1:A:197:VAL:HG21	1:A:243:GLY:HA3	1.98	0.46
2:B:466:LEU:HD13	2:B:480:ILE:HD11	1.97	0.46
1:A:33:LEU:CG	1:A:43:HIS:HB2	2.45	0.46
1:A:27:VAL:HG13	1:A:47:GLU:HG3	1.96	0.46
2:B:86:THR:HG22	2:B:87:ARG:N	2.30	0.46
1:A:176:LYS:HG2	1:A:345:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:499:TTX:C6	3:B:499:TTX:HN41	2.28	0.46
1:A:233:ALA:C	1:A:235:LEU:N	2.69	0.46
1:A:165:ARG:NH2	2:B:205:ARG:HD3	2.30	0.46
1:A:454:VAL:O	1:A:457:TYR:HB2	2.15	0.46
1:A:323:GLN:O	1:A:324:ALA:HB3	2.16	0.46
1:A:151:LEU:HA	1:A:423:GLN:HE22	1.81	0.46
1:A:199:ILE:HG13	1:A:239:ALA:CB	2.46	0.46
1:A:356:PRO:CD	1:A:423:GLN:H	2.25	0.46
1:A:417:LEU:O	1:A:421:LEU:HG	2.16	0.46
1:A:457:TYR:HA	1:A:501:PHE:CZ	2.51	0.46
2:B:148:ILE:HG12	2:B:149:PHE:N	2.30	0.46
1:A:272:ARG:HD2	1:A:286:ALA:HB3	1.97	0.46
1:A:264:LEU:HD11	1:A:318:PRO:HB2	1.96	0.46
2:B:429:ARG:C	2:B:431:LEU:H	2.17	0.46
1:A:91:ALA:O	1:A:93:GLY:N	2.49	0.46
1:A:351:ASN:C	1:A:353:GLY:N	2.69	0.46
2:B:298:TYR:CE1	2:B:338:ALA:HB2	2.51	0.46
1:A:65:LEU:HD11	1:A:278:LEU:HD11	1.98	0.46
1:A:158:ILE:HG21	1:A:343:ILE:CG1	2.44	0.46
1:A:128:ARG:HH11	1:A:248:GLU:HB2	1.81	0.46
2:B:227:ILE:O	2:B:227:ILE:HG22	2.16	0.46
1:A:167:LEU:HD12	1:A:168:ILE:H	1.81	0.45
2:B:163:ARG:HG2	2:B:374:MET:HB2	1.99	0.45
2:B:186:ILE:CG2	2:B:190:ALA:HB3	2.46	0.45
2:B:19:ASN:ND2	2:B:93:ASP:OD2	2.49	0.45
1:A:281:PRO:CB	2:B:287:ALA:HB1	2.41	0.45
2:B:238:GLN:NE2	2:B:238:GLN:HA	2.16	0.45
1:A:486:ALA:O	1:A:490:LEU:HB2	2.16	0.45
2:B:247:MET:C	2:B:248:ARG:HG2	2.36	0.45
2:B:161:PRO:HD2	2:B:375:LEU:HG	1.97	0.45
2:B:66:GLN:O	2:B:67:GLN:HG2	2.15	0.45
2:B:148:ILE:HA	2:B:374:MET:HE1	1.97	0.45
1:A:259:ILE:HD13	1:A:314:MET:SD	2.56	0.45
2:B:402:GLN:O	2:B:404:ILE:N	2.49	0.45
1:A:240:PRO:CG	1:A:298:LEU:HD21	2.47	0.45
2:B:222:ILE:CG2	2:B:223:ASN:N	2.74	0.45
1:A:211:THR:O	1:A:214:GLN:N	2.45	0.45
1:A:154:ILE:O	1:A:158:ILE:O	2.35	0.45
2:B:107:LEU:HD23	2:B:232:VAL:N	2.32	0.45
1:A:25:LYS:C	1:A:27:VAL:H	2.20	0.45
2:B:413:LEU:O	2:B:418:ARG:NE	2.42	0.45
2:B:223:ASN:OD1	2:B:228:ALA:HA	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:310:GLN:HE22	2:B:325:GLN:HE22	1.65	0.45
2:B:160:ALA:CA	2:B:372:SER:HB3	2.43	0.45
1:A:128:ARG:HH11	1:A:248:GLU:CB	2.29	0.45
2:B:434:PRO:HD3	2:B:476:LEU:HD22	1.99	0.45
2:B:329:VAL:HG11	2:B:334:LEU:HD23	1.99	0.45
1:A:111:ALA:O	1:A:112:LEU:HD23	2.17	0.45
1:A:418:ARG:O	1:A:422:LYS:HG3	2.17	0.45
2:B:33:VAL:CG1	2:B:91:VAL:HG21	2.43	0.45
2:B:430:PHE:HD1	2:B:474:PHE:HB3	1.82	0.45
2:B:315:SER:HA	2:B:320:SER:HA	1.97	0.45
2:B:261:ARG:HD3	2:B:321:ILE:HG12	1.99	0.45
1:A:165:ARG:NH2	1:A:338:ILE:O	2.49	0.45
1:A:167:LEU:HD21	1:A:169:ILE:HD11	1.97	0.45
2:B:204:GLU:O	2:B:238:GLN:NE2	2.50	0.45
2:B:83:ASP:CG	3:B:499:TTX:C12	2.85	0.45
1:A:415:GLN:O	1:A:451:LEU:HD22	2.17	0.45
2:B:480:ILE:O	2:B:483:ALA:HB3	2.17	0.45
1:A:29:THR:HA	1:A:89:VAL:O	2.16	0.45
1:A:418:ARG:O	1:A:421:LEU:HB2	2.17	0.45
2:B:350:THR:O	2:B:352:LEU:HD13	2.17	0.45
1:A:387:LEU:HA	1:A:390:PHE:CD1	2.52	0.44
1:A:65:LEU:CD2	3:B:499:TTX:C19	2.95	0.44
2:B:98:LEU:O	2:B:132:ILE:HG12	2.18	0.44
1:A:130:ILE:HD13	1:A:238:LEU:HD13	1.98	0.44
1:A:151:LEU:HB3	1:A:154:ILE:HD13	1.99	0.44
1:A:490:LEU:O	1:A:493:ALA:HB3	2.17	0.44
1:A:26:VAL:HG12	1:A:26:VAL:O	2.17	0.44
2:B:107:LEU:HD23	2:B:232:VAL:C	2.37	0.44
2:B:377:PRO:HD3	2:B:385:TYR:CD2	2.53	0.44
1:A:78:GLY:HA2	1:A:232:PRO:HG3	1.98	0.44
1:A:394:GLU:CD	1:A:418:ARG:HH21	2.21	0.44
2:B:216:MET:HE3	2:B:232:VAL:HG21	1.96	0.44
1:A:56:PHE:CG	1:A:83:ILE:HD12	2.52	0.44
2:B:66:GLN:O	2:B:67:GLN:CG	2.65	0.44
1:A:202:LYS:O	1:A:203:ALA:C	2.54	0.44
2:B:204:GLU:O	2:B:239:MET:HG3	2.17	0.44
2:B:271:PHE:HE1	2:B:324:ILE:HD12	1.82	0.44
1:A:210:VAL:HG12	1:A:210:VAL:O	2.17	0.44
1:A:56:PHE:HD2	1:A:60:THR:O	2.01	0.44
2:B:199:PHE:CZ	2:B:273:ASP:HB2	2.53	0.44
1:A:264:LEU:HD11	1:A:318:PRO:CB	2.48	0.44
2:B:203:GLY:HA3	2:B:277:ARG:CB	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:241:GLU:HB2	2:B:246:ARG:HD3	2.00	0.44
1:A:38:GLY:O	1:A:76:LEU:HB2	2.17	0.44
1:A:494:ILE:O	1:A:498:MET:HG3	2.17	0.44
2:B:401:LEU:O	2:B:404:ILE:HB	2.18	0.44
1:A:27:VAL:CG1	1:A:47:GLU:HG3	2.48	0.44
2:B:112:ASN:ND2	2:B:116:GLU:OE1	2.50	0.44
1:A:241:TYR:HE1	1:A:267:GLN:NE2	2.14	0.44
2:B:167:LYS:HZ1	2:B:310:GLN:CD	2.20	0.44
1:A:174:THR:HG23	1:A:350:PHE:CZ	2.53	0.44
1:A:56:PHE:CD1	1:A:89:VAL:HG13	2.53	0.44
1:A:310:GLY:O	1:A:311:GLU:HB2	2.18	0.44
1:A:310:GLY:C	1:A:312:GLY:H	2.20	0.44
2:B:132:ILE:HG22	2:B:251:LEU:O	2.17	0.43
2:B:341:THR:O	2:B:342:THR:C	2.55	0.43
1:A:486:ALA:O	1:A:490:LEU:N	2.51	0.43
2:B:168:ILE:HB	2:B:324:ILE:HA	2.00	0.43
2:B:23:ILE:HG21	2:B:26:ILE:HD11	1.99	0.43
2:B:235:VAL:HG11	2:B:252:THR:HG21	2.00	0.43
1:A:99:PRO:HD2	1:A:113:ALA:HB3	2.00	0.43
2:B:153:ILE:HA	2:B:433:GLN:OE1	2.18	0.43
1:A:39:ILE:HG21	1:A:278:LEU:HD23	2.00	0.43
2:B:460:LEU:HD12	2:B:480:ILE:HG12	1.99	0.43
2:B:299:GLN:HG3	2:B:301:THR:OG1	2.18	0.43
1:A:76:LEU:O	1:A:234:THR:CB	2.66	0.43
1:A:30:GLY:O	1:A:88:SER:HA	2.17	0.43
1:A:176:LYS:CG	1:A:345:LEU:HD12	2.48	0.43
2:B:43:ILE:HG22	2:B:44:TYR:CD1	2.53	0.43
2:B:73:ARG:HB2	2:B:73:ARG:HE	1.43	0.43
2:B:167:LYS:CE	2:B:325:GLN:HE22	2.31	0.43
2:B:156:VAL:C	2:B:158:LEU:H	2.20	0.43
2:B:106:THR:HA	2:B:111:PHE:CZ	2.53	0.43
2:B:203:GLY:CA	2:B:246:ARG:HG2	2.49	0.43
1:A:112:LEU:HD23	1:A:112:LEU:N	2.32	0.43
2:B:410:LEU:HA	2:B:413:LEU:HD12	2.00	0.43
2:B:135:SER:O	2:B:136:ALA:O	2.36	0.43
1:A:264:LEU:CD1	1:A:318:PRO:HB2	2.49	0.43
1:A:136:GLY:O	1:A:140:ARG:HG3	2.18	0.43
1:A:134:ALA:HB1	1:A:301:ARG:HA	2.00	0.43
2:B:167:LYS:HD2	2:B:313:ILE:O	2.19	0.43
2:B:414:SER:O	2:B:418:ARG:HG3	2.19	0.43
1:A:107:ARG:NH2	1:A:115:PRO:HB3	2.34	0.43
1:A:97:GLN:O	1:A:98:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:ILE:HA	1:A:99:PRO:HD3	1.86	0.43
2:B:206:THR:O	2:B:209:GLY:N	2.47	0.43
2:B:128:THR:HG22	2:B:129:THR:N	2.33	0.43
2:B:186:ILE:HA	2:B:190:ALA:CB	2.48	0.43
1:A:76:LEU:O	1:A:234:THR:HB	2.19	0.43
1:A:404:ASP:O	1:A:408:GLN:HG3	2.19	0.43
1:A:438:ILE:HG22	1:A:442:THR:OG1	2.19	0.43
2:B:42:ASN:ND2	2:B:45:ASN:HD21	2.17	0.43
2:B:367:PRO:HB3	2:B:431:LEU:HD13	2.00	0.43
2:B:374:MET:C	2:B:376:GLN:H	2.22	0.43
2:B:430:PHE:CD2	2:B:461:ILE:HD11	2.53	0.43
2:B:43:ILE:O	2:B:44:TYR:HB2	2.18	0.43
2:B:276:PHE:C	2:B:278:PHE:N	2.72	0.43
2:B:271:PHE:CE1	2:B:324:ILE:HD12	2.53	0.43
2:B:121:LEU:O	2:B:122:ARG:CB	2.65	0.43
2:B:30:VAL:CG2	2:B:288:LEU:HD22	2.39	0.43
1:A:91:ALA:O	1:A:92:THR:C	2.57	0.43
2:B:35:PHE:CE1	2:B:41:PRO:HG3	2.54	0.43
2:B:269:LEU:HD22	2:B:322:THR:CB	2.46	0.43
1:A:174:THR:O	1:A:174:THR:HG22	2.18	0.43
2:B:387:ILE:HG23	2:B:462:LEU:HD11	2.01	0.43
1:A:175:GLY:O	1:A:178:ALA:HB3	2.19	0.43
1:A:109:ILE:CG2	1:A:225:VAL:HA	2.49	0.42
1:A:382:LYS:O	1:A:386:GLU:HG3	2.19	0.42
1:A:162:ARG:CZ	1:A:192:VAL:HG22	2.49	0.42
1:A:300:GLU:O	1:A:302:ALA:N	2.51	0.42
2:B:86:THR:CG2	2:B:87:ARG:N	2.82	0.42
2:B:186:ILE:HG23	2:B:190:ALA:CB	2.49	0.42
1:A:128:ARG:NH1	1:A:248:GLU:HB3	2.34	0.42
1:A:481:THR:HG22	1:A:482:PHE:N	2.34	0.42
1:A:369:SER:HB2	1:A:372:GLN:OE1	2.19	0.42
1:A:440:THR:HA	1:A:494:ILE:HD13	2.00	0.42
2:B:23:ILE:HD11	2:B:49:VAL:HG11	2.02	0.42
1:A:419:GLU:HA	1:A:422:LYS:CD	2.48	0.42
1:A:403:LEU:HD13	1:A:407:THR:HG21	2.01	0.42
2:B:156:VAL:HG12	2:B:157:ASN:N	2.33	0.42
2:B:423:ARG:NH2	2:B:464:GLY:HA3	2.34	0.42
1:A:268:ALA:O	1:A:271:TYR:HB3	2.19	0.42
2:B:22:ARG:HB3	2:B:88:GLY:HA2	2.01	0.42
2:B:138:ALA:N	2:B:141:GLN:OE1	2.40	0.42
1:A:339:THR:CG2	1:A:340:ASP:N	2.82	0.42
1:A:272:ARG:HA	1:A:288:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:LYS:O	1:A:177:THR:C	2.58	0.42
1:A:104:TYR:CE2	1:A:109:ILE:HD12	2.54	0.42
1:A:130:ILE:CG2	1:A:241:TYR:HB3	2.49	0.42
2:B:430:PHE:CD1	2:B:474:PHE:HB3	2.54	0.42
1:A:157:MET:SD	1:A:387:LEU:HD12	2.60	0.42
2:B:69:LEU:HD21	2:B:75:ARG:NE	2.16	0.42
2:B:333:ASP:CG	2:B:335:THR:OG1	2.58	0.42
2:B:180:VAL:HG11	2:B:438:ALA:HB2	2.01	0.42
1:A:122:ILE:HD13	1:A:122:ILE:N	2.35	0.42
1:A:173:GLN:HA	1:A:173:GLN:OE1	2.19	0.42
1:A:227:GLU:OE1	1:A:235:LEU:O	2.38	0.42
1:A:386:GLU:C	1:A:388:ALA:N	2.73	0.42
1:A:419:GLU:HA	1:A:422:LYS:CG	2.49	0.42
2:B:156:VAL:C	2:B:158:LEU:N	2.73	0.42
2:B:109:ARG:CD	2:B:119:ASP:OD2	2.67	0.42
2:B:458:PHE:HA	2:B:461:ILE:CD1	2.47	0.42
1:A:260:ILE:CD1	1:A:317:LEU:HB2	2.49	0.42
1:A:100:VAL:HA	1:A:104:TYR:HE1	1.85	0.42
2:B:70:GLY:O	2:B:71:ASN:CB	2.67	0.42
1:A:373:ILE:HG22	1:A:374:LYS:N	2.23	0.42
1:A:172:ARG:HG2	1:A:172:ARG:H	1.72	0.42
1:A:330:TYR:O	1:A:333:THR:HB	2.20	0.42
1:A:65:LEU:CD1	1:A:278:LEU:HD13	2.50	0.41
1:A:293:TYR:HD1	1:A:293:TYR:N	2.08	0.41
2:B:36:PRO:CD	2:B:39:LYS:HD2	2.50	0.41
1:A:433:GLU:HA	1:A:436:MET:HE2	2.02	0.41
2:B:254:LEU:HD22	2:B:313:ILE:HG12	2.01	0.41
2:B:131:PRO:C	2:B:133:HIS:H	2.22	0.41
1:A:53:LEU:HB2	1:A:92:THR:OG1	2.19	0.41
2:B:367:PRO:HB2	2:B:395:LEU:HD13	2.02	0.41
1:A:373:ILE:O	1:A:377:LYS:HG3	2.20	0.41
2:B:102:VAL:HG12	2:B:256:MET:HG3	2.01	0.41
1:A:167:LEU:HD12	1:A:318:PRO:O	2.20	0.41
2:B:48:ILE:HG22	2:B:92:ILE:HG22	2.00	0.41
2:B:431:LEU:HA	2:B:431:LEU:HD23	1.91	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.84	0.41
2:B:169:GLY:HA3	2:B:346:LEU:HD13	2.02	0.41
2:B:170:LEU:HD13	2:B:181:LEU:CD2	2.50	0.41
2:B:261:ARG:HG2	2:B:262:ASP:OD1	2.20	0.41
1:A:295:HIS:HB2	1:A:338:ILE:CD1	2.50	0.41
2:B:65:VAL:HG13	2:B:74:VAL:HB	2.03	0.41
1:A:490:LEU:HD22	1:A:494:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:457:TYR:HA	1:A:501:PHE:CE2	2.55	0.41
1:A:154:ILE:HD12	1:A:154:ILE:N	2.36	0.41
2:B:72:ASN:O	2:B:73:ARG:HB2	2.20	0.41
2:B:52:ARG:HG2	2:B:53:ASP:N	2.35	0.41
2:B:212:LEU:O	2:B:212:LEU:HG	2.21	0.41
2:B:42:ASN:O	2:B:45:ASN:HB2	2.21	0.41
2:B:471:GLU:C	2:B:473:ALA:N	2.68	0.41
2:B:105:PRO:HG2	2:B:126:THR:HG22	2.03	0.41
1:A:187:GLN:CD	1:A:194:CYS:SG	2.99	0.41
2:B:165:GLY:HA2	2:B:315:SER:HB3	2.02	0.41
1:A:470:PRO:O	1:A:474:GLU:HG3	2.20	0.41
1:A:46:ASP:N	1:A:46:ASP:OD1	2.53	0.41
2:B:251:LEU:CG	2:B:309:LEU:HD13	2.50	0.41
1:A:454:VAL:HA	1:A:457:TYR:CD1	2.56	0.41
2:B:387:ILE:CD1	2:B:459:GLN:HB2	2.51	0.41
2:B:163:ARG:NE	2:B:374:MET:CB	2.81	0.41
1:A:216:ARG:NH2	1:A:426:SER:HB2	2.36	0.41
1:A:271:TYR:OH	1:A:290:ASP:HB2	2.21	0.41
1:A:310:GLY:C	1:A:312:GLY:N	2.74	0.41
1:A:148:GLN:HE21	1:A:431:VAL:CG2	2.34	0.41
2:B:40:MET:O	2:B:41:PRO:C	2.53	0.41
2:B:423:ARG:O	2:B:426:LYS:HB2	2.21	0.41
2:B:259:TYR:HE2	2:B:264:ASN:HD21	1.69	0.41
1:A:67:LEU:HB3	2:B:87:ARG:HE	1.86	0.41
1:A:134:ALA:CB	1:A:301:ARG:HA	2.51	0.41
1:A:417:LEU:HA	1:A:420:LEU:HG	2.03	0.41
2:B:68:LEU:O	2:B:70:GLY:N	2.53	0.41
2:B:419:LEU:HD11	2:B:423:ARG:HE	1.85	0.41
1:A:409:ASN:O	1:A:413:ARG:HG3	2.21	0.41
2:B:402:GLN:C	2:B:404:ILE:N	2.75	0.41
2:B:405:ILE:HG13	2:B:406:ALA:N	2.35	0.41
2:B:276:PHE:CZ	2:B:280:GLN:HB2	2.56	0.40
1:A:214:GLN:C	1:A:216:ARG:N	2.74	0.40
2:B:143:ASP:OD2	2:B:316:THR:C	2.59	0.40
2:B:298:TYR:CZ	2:B:338:ALA:HB2	2.55	0.40
2:B:387:ILE:HA	2:B:390:ARG:HD2	2.02	0.40
1:A:135:PRO:O	1:A:140:ARG:NH2	2.54	0.40
2:B:353:SER:HB3	2:B:356:LEU:HD12	2.02	0.40
2:B:131:PRO:C	2:B:133:HIS:N	2.73	0.40
2:B:50:LYS:HG2	2:B:59:MET:CE	2.51	0.40
2:B:167:LYS:HE3	2:B:310:GLN:O	2.21	0.40
2:B:196:VAL:HG12	2:B:197:SER:N	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108:VAL:HG12	1:A:116:ILE:HD11	2.03	0.40
1:A:302:ALA:O	1:A:303:ALA:HB2	2.22	0.40
1:A:414:GLY:C	1:A:416:ARG:H	2.25	0.40
2:B:161:PRO:HD2	2:B:372:SER:HB3	2.04	0.40
2:B:399:LYS:HA	2:B:402:GLN:NE2	2.35	0.40
1:A:56:PHE:CE2	1:A:76:LEU:HD22	2.56	0.40
1:A:422:LYS:O	1:A:423:GLN:HG3	2.21	0.40
1:A:461:LEU:O	1:A:464:TYR:HB2	2.22	0.40
2:B:269:LEU:HD12	2:B:271:PHE:HZ	1.85	0.40
1:A:181:THR:O	1:A:185:LEU:HD12	2.21	0.40
2:B:404:ILE:O	2:B:408:LEU:HB2	2.22	0.40
2:B:417:ASP:HA	2:B:420:THR:HG23	2.04	0.40
2:B:357:ALA:HB2	2:B:364:ALA:CB	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:499:GLU:OE1	1:A:499:GLU:OE1[4_555]	1.69	0.51

## 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	475/507 (94%)	362 (76%)	86 (18%)	27 (6%)	3	30
2	B	465/498 (93%)	365 (78%)	76 (16%)	24 (5%)	3	32
All	All	940/1005 (94%)	727 (77%)	162 (17%)	51 (5%)	3	31

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	SER
1	A	212	ASN
1	A	447	ASP

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Mol	Chain	Res	Type
2	B	265	GLU
2	B	343	PHE
1	A	48	VAL
1	A	85	GLU
1	A	92	THR
1	A	110	ASN
1	A	171	ASP
1	A	330	TYR
1	A	352	ALA
1	A	354	ILE
1	A	360	VAL
1	A	387	LEU
1	A	448	SER
2	B	55	ALA
2	B	157	ASN
2	B	208	GLU
2	B	286	SER
2	B	472	GLN
1	A	37	ASP
1	A	105	LEU
1	A	186	ASN
1	A	234	THR
1	A	262	ASP
1	A	296	SER
1	A	351	ASN
1	A	452	ASP
2	B	54	THR
2	B	69	LEU
2	B	239	MET
2	B	402	GLN
2	B	403	ASP
2	B	451	LEU
1	A	26	VAL
1	A	288	PRO
2	B	122	ARG
2	B	154	LYS
2	B	156	VAL
2	B	240	ASN
1	A	328	SER
1	A	402	ASP
2	B	52	ARG
2	B	345	HIS

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Mol	Chain	Res	Type
1	A	373	ILE
2	B	136	ALA
2	B	296	VAL
2	B	175	GLY
2	B	61	VAL
2	B	455	ILE

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/414 (94%)	367 (95%)	21 (5%)	31	77
2	B	381/410 (93%)	356 (93%)	25 (7%)	24	70
All	All	769/824 (93%)	723 (94%)	46 (6%)	27	73

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	35	VAL
1	A	41	ARG
1	A	46	ASP
1	A	49	MET
1	A	65	LEU
1	A	89	VAL
1	A	122	ILE
1	A	128	ARG
1	A	131	GLU
1	A	135	PRO
1	A	147	LEU
1	A	177	THR
1	A	191	ASN
1	A	228	THR
1	A	230	ASP
1	A	249	TYR
1	A	257	THR
1	A	342	GLN

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Mol	Chain	Res	Type
1	A	426	SER
1	A	490	LEU
2	B	42	ASN
2	B	57	GLN
2	B	58	PRO
2	B	98	LEU
2	B	129	THR
2	B	140	THR
2	B	149	PHE
2	B	187	ASN
2	B	238	GLN
2	B	240	ASN
2	B	246	ARG
2	B	248	ARG
2	B	249	VAL
2	B	269	LEU
2	B	274	ASN
2	B	288	LEU
2	B	299	GLN
2	B	308	SER
2	B	310	GLN
2	B	316	THR
2	B	325	GLN
2	B	352	LEU
2	B	395	LEU
2	B	417	ASP
2	B	481	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	70	ASN
1	A	148	GLN
1	A	186	ASN
1	A	295	HIS
1	A	359	ASN
1	A	409	ASN
1	A	423	GLN
1	A	497	GLN
2	B	19	ASN
2	B	25	GLN

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Mol	Chain	Res	Type
2	B	42	ASN
2	B	60	ASN
2	B	187	ASN
2	B	238	GLN
2	B	240	ASN
2	B	264	ASN
2	B	299	GLN
2	B	310	GLN
2	B	325	GLN
2	B	396	GLN
2	B	402	GLN
2	B	459	GLN
2	B	472	GLN

### 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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	TTX	B	499	2	31,31,31	3.21	8 (25%)	43,43,43	3.89	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTX	B	499	2	-	0/45/45/45	0/1/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	499	TTX	O1-C6	11.38	1.43	1.22
3	B	499	TTX	C15-C14	-8.11	1.33	1.50
3	B	499	TTX	C6-N1	5.34	1.45	1.35
3	B	499	TTX	C5-C6	5.07	1.64	1.53
3	B	499	TTX	C7-N1	-3.99	1.38	1.47
3	B	499	TTX	C12-N3	-3.71	1.29	1.35
3	B	499	TTX	C9-N3	-2.88	1.42	1.47
3	B	499	TTX	C15-N1	-2.45	1.34	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	499	TTX	C5-C6-N1	-14.89	91.91	118.84
3	B	499	TTX	C7-N1-C6	-14.23	95.53	118.82
3	B	499	TTX	C4-C5-C6	6.94	121.72	109.37
3	B	499	TTX	C6-N1-C15	6.66	141.30	123.69
3	B	499	TTX	C13-N4-C14	5.38	130.12	121.02
3	B	499	TTX	C9-C8-N2	3.63	122.07	115.52
3	B	499	TTX	C11-N3-C12	-3.09	114.64	121.97
3	B	499	TTX	C6-C5-N2	-3.02	101.68	108.76
3	B	499	TTX	C18-C17-C16	2.80	130.78	121.21
3	B	499	TTX	C15-C14-N4	2.17	121.72	117.60
3	B	499	TTX	C7-N1-C15	2.12	120.04	117.27
3	B	499	TTX	C21-C22-C17	2.02	123.24	120.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.