



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:02 PM GMT

PDB ID : 2WSX
Title : CRYSTAL STRUCTURE OF CARNITINE TRANSPORTER FROM ES-
CHERICHIA COLI
Authors : Schulze, S.; Terwisscha Van Scheltinga, A.C.; Kuehlbrandt, W.
Deposited on : 2009-09-10
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>

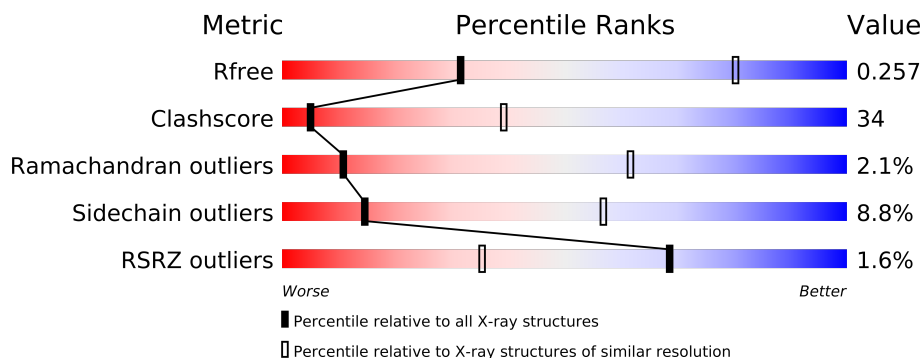
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
R_{free}	66092	1243 (3.70-3.30)
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	504	
1	B	504	
1	C	504	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NM2	A	1505	-	X
2	NM2	B	1504	-	X
2	NM2	B	1505	-	X
2	NM2	C	1504	-	X
2	NM2	C	1505	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11763 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.

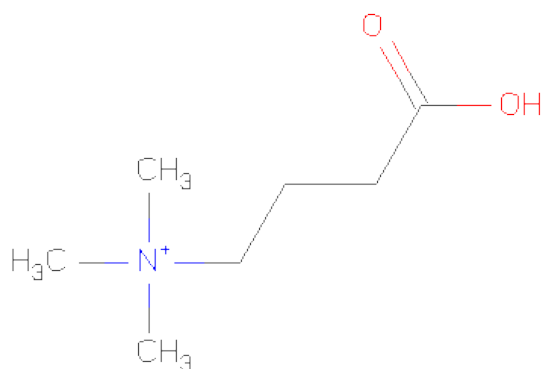
- Molecule 1 is a protein called L-CARNITINE/GAMMA-BUTYROBETAINEN-TIPORTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3901	2624	602	647	28			
1	B	496	Total	C	N	O	S	0	0	0
			3901	2624	602	647	28			
1	C	496	Total	C	N	O	S	0	0	0
			3901	2624	602	647	28			

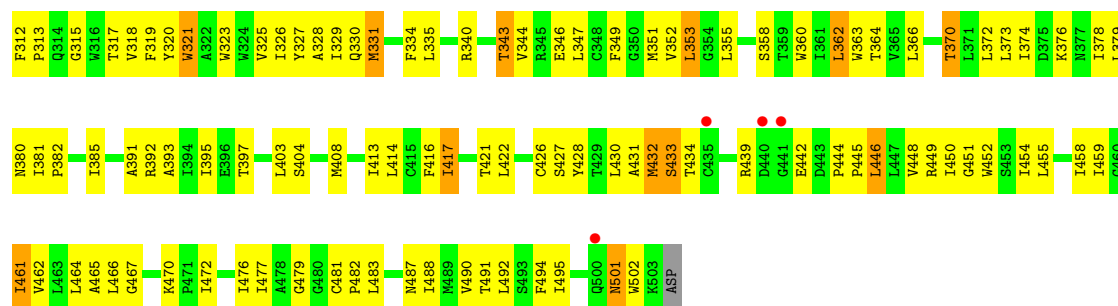
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	GLU	ASN	CONFLICT	UNP P31553
A	254	ALA	GLY	CONFLICT	UNP P31553
A	379	LEU	ILE	CONFLICT	UNP P31553
A	443	ASP	GLU	CONFLICT	UNP P31553
B	81	GLU	ASN	CONFLICT	UNP P31553
B	254	ALA	GLY	CONFLICT	UNP P31553
B	379	LEU	ILE	CONFLICT	UNP P31553
B	443	ASP	GLU	CONFLICT	UNP P31553
C	81	GLU	ASN	CONFLICT	UNP P31553
C	254	ALA	GLY	CONFLICT	UNP P31553
C	379	LEU	ILE	CONFLICT	UNP P31553
C	443	ASP	GLU	CONFLICT	UNP P31553

- Molecule 2 is 3-CARBOXY-N,N,N-TRIMETHYLPROPAN-1-AMINIUM (three-letter code: NM2) (formula: C₇H₁₆NO₂).

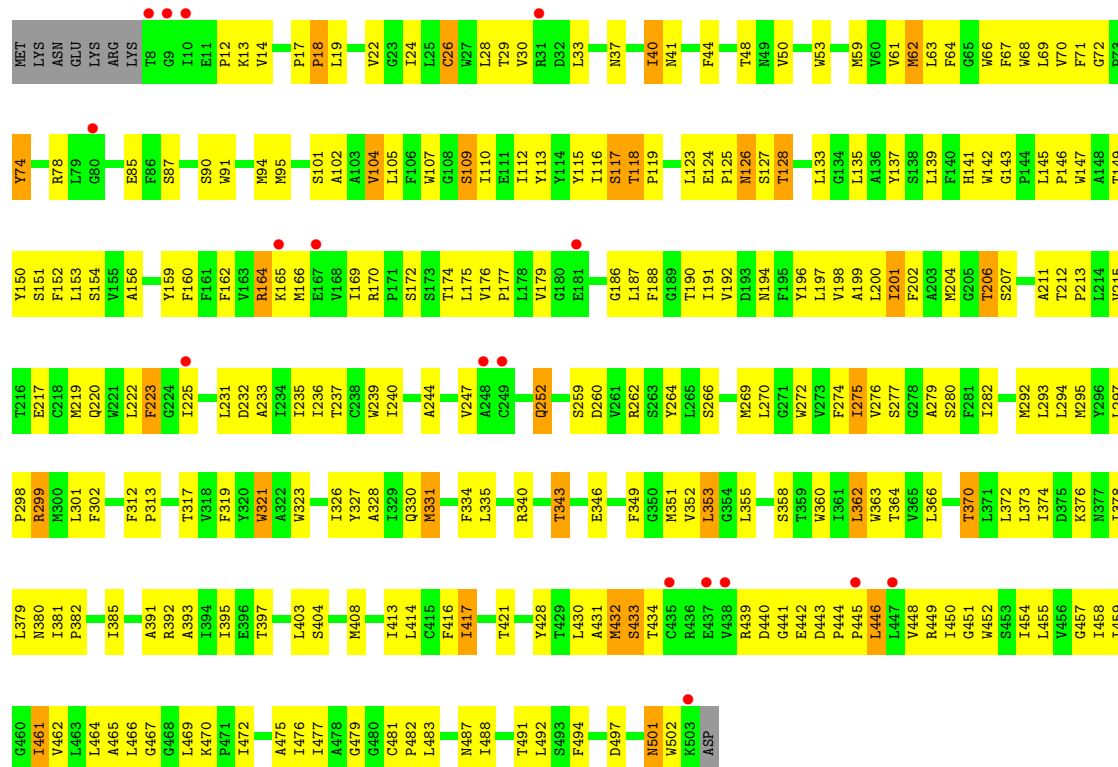


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	7	1	2		
2	A	1	Total	C	N	O	0	0
			10	7	1	2		
2	B	1	Total	C	N	O	0	0
			10	7	1	2		
2	B	1	Total	C	N	O	0	0
			10	7	1	2		
2	C	1	Total	C	N	O	0	0
			10	7	1	2		
2	C	1	Total	C	N	O	0	0
			10	7	1	2		



• Molecule 1: L-CARNITINE/GAMMA-BUTYROBETAINETANTIPORTER

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	124.20Å 124.20Å 154.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.68 – 3.50 24.68 – 3.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.68-3.50) 67.7 (24.68-3.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 3.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.237 , 0.271 0.231 , 0.257	Depositor DCC
R_{free} test set	1231 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	148.5	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 116.6	EDS
Estimated twinning fraction	0.024 for -h,-k,l 0.057 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 24542 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11763	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: NM2

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	0.60	0/4028	0.66	0/5512
1	B	0.54	0/4028	0.66	0/5512
1	C	0.48	0/4028	0.63	0/5512
All	All	0.54	0/12084	0.65	0/16536

There are no bond length outliers.

There are no bond angle outliers.

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	3901	0	3934	266	0
1	B	3901	0	3934	277	0
1	C	3901	0	3934	259	0
2	A	20	0	30	9	0
2	B	20	0	30	8	0
2	C	20	0	30	3	0
All	All	11763	0	11892	793	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 34.

All (793) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:343:THR:HG23	1:B:346:GLU:HB2	1.34	1.08
1:A:343:THR:HG23	1:A:346:GLU:HB2	1.30	1.07
1:B:135:LEU:HD11	1:B:364:THR:HG22	1.32	1.05
1:C:343:THR:HG23	1:C:346:GLU:HB2	1.37	1.04
1:C:135:LEU:HD11	1:C:364:THR:HG22	1.39	1.04
1:A:366:LEU:O	1:A:370:THR:HG23	1.60	1.00
1:C:366:LEU:O	1:C:370:THR:HG23	1.59	1.00
1:A:135:LEU:HD11	1:A:364:THR:HG22	1.42	1.00
1:A:315:GLY:HA3	2:A:1505:NM2:O7	1.63	0.99
1:B:366:LEU:O	1:B:370:THR:HG23	1.67	0.94
1:B:272:TRP:O	1:B:276:VAL:HG13	1.71	0.91
1:A:272:TRP:O	1:A:276:VAL:HG13	1.72	0.90
1:A:202:PHE:O	1:A:206:THR:HG23	1.72	0.89
1:C:272:TRP:O	1:C:276:VAL:HG13	1.73	0.88
1:C:202:PHE:O	1:C:206:THR:HG23	1.74	0.88
1:C:112:ILE:O	1:C:116:ILE:HG13	1.75	0.87
1:B:323:TRP:CD2	2:B:1504:NM2:H102	2.11	0.86
1:B:40:ILE:HD11	1:B:466:LEU:HD13	1.55	0.85
1:C:323:TRP:CD2	2:C:1504:NM2:H102	2.12	0.85
1:C:479:GLY:O	1:C:482:PRO:HD2	1.78	0.84
1:C:22:VAL:O	1:C:26:CYS:HB2	1.78	0.84
1:B:323:TRP:CG	2:B:1504:NM2:H102	2.12	0.83
1:B:202:PHE:O	1:B:206:THR:HG23	1.79	0.83
1:A:142:TRP:CE2	1:A:363:TRP:CZ2	2.67	0.83
1:C:212:THR:HB	1:C:213:PRO:HD3	1.60	0.82
1:B:479:GLY:O	1:B:482:PRO:HD2	1.79	0.82
1:A:26:CYS:O	1:A:30:VAL:HG23	1.80	0.82
1:A:434:THR:HG21	1:A:452:TRP:HE1	1.45	0.82
1:B:37:ASN:OD1	1:B:466:LEU:HD22	1.79	0.81
1:A:112:ILE:O	1:A:116:ILE:HG13	1.79	0.81
1:B:26:CYS:O	1:B:30:VAL:HG23	1.81	0.81
1:C:26:CYS:O	1:C:30:VAL:HG23	1.81	0.81
1:A:159:TYR:CZ	1:A:164:ARG:HD2	2.16	0.81
1:B:172:SER:HA	1:B:175:LEU:HD12	1.63	0.80
1:B:212:THR:HB	1:B:213:PRO:HD3	1.64	0.80
1:B:112:ILE:O	1:B:116:ILE:HG13	1.82	0.80
1:C:434:THR:HG21	1:C:452:TRP:HE1	1.46	0.79
1:B:159:TYR:CZ	1:B:164:ARG:HD2	2.17	0.79
1:A:479:GLY:O	1:A:482:PRO:HD2	1.81	0.79
1:C:141:HIS:HE1	1:C:317:THR:OG1	1.66	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:451:GLY:O	1:A:454:ILE:HG12	1.83	0.79
1:A:40:ILE:HD11	1:A:466:LEU:HD13	1.65	0.79
1:C:430:LEU:O	1:C:434:THR:HG22	1.83	0.78
1:B:434:THR:HG21	1:B:452:TRP:HE1	1.48	0.78
1:B:430:LEU:O	1:B:434:THR:HG22	1.82	0.78
1:A:430:LEU:O	1:A:434:THR:HG22	1.84	0.78
1:A:272:TRP:O	1:A:275:ILE:HD13	1.84	0.78
1:B:133:LEU:HD13	1:B:133:LEU:O	1.84	0.77
1:C:451:GLY:O	1:C:454:ILE:HG12	1.84	0.77
1:A:439:ARG:HB2	1:A:442:GLU:CD	2.04	0.77
1:C:40:ILE:HD11	1:C:466:LEU:HD13	1.66	0.76
1:A:212:THR:HB	1:A:213:PRO:HD3	1.67	0.76
1:A:194:ASN:O	1:A:198:VAL:HG23	1.86	0.76
1:B:240:ILE:HD13	1:B:454:ILE:HA	1.66	0.76
1:B:22:VAL:O	1:B:26:CYS:HB2	1.86	0.76
1:A:63:LEU:HD22	1:A:145:LEU:HD21	1.68	0.76
1:A:222:LEU:HB2	1:A:223:PHE:CD1	2.20	0.75
1:C:272:TRP:O	1:C:275:ILE:HD13	1.87	0.75
1:A:37:ASN:OD1	1:A:466:LEU:HD22	1.86	0.75
1:C:222:LEU:HB2	1:C:223:PHE:CD1	2.22	0.75
1:C:63:LEU:HD22	1:C:145:LEU:HD21	1.69	0.75
1:B:141:HIS:HE1	1:B:317:THR:OG1	1.69	0.75
1:A:343:THR:CG2	1:A:346:GLU:HB2	2.14	0.74
1:A:239:TRP:HH2	1:A:416:PHE:CD1	2.03	0.74
1:A:22:VAL:O	1:A:26:CYS:HB2	1.87	0.74
1:B:299:ARG:HH11	1:B:299:ARG:HG2	1.52	0.74
1:C:159:TYR:CZ	1:C:164:ARG:HD2	2.22	0.74
1:C:13:LYS:HG3	1:C:14:VAL:HG23	1.70	0.74
1:B:343:THR:CG2	1:B:346:GLU:HB2	2.17	0.74
1:B:239:TRP:HH2	1:B:416:PHE:CD1	2.05	0.74
1:A:172:SER:HA	1:A:175:LEU:HD12	1.70	0.73
1:A:141:HIS:HE1	1:A:317:THR:OG1	1.71	0.73
1:B:222:LEU:HB2	1:B:223:PHE:CD1	2.23	0.73
1:C:37:ASN:OD1	1:C:466:LEU:HD22	1.89	0.73
1:C:240:ILE:HD13	1:C:454:ILE:HA	1.70	0.73
1:B:439:ARG:HB2	1:B:442:GLU:CD	2.09	0.73
1:C:299:ARG:HG2	1:C:299:ARG:HH11	1.53	0.73
1:A:434:THR:HG21	1:A:452:TRP:NE1	2.03	0.73
1:C:194:ASN:O	1:C:198:VAL:HG23	1.88	0.72
1:C:439:ARG:HB2	1:C:442:GLU:CD	2.09	0.72
1:B:13:LYS:HG3	1:B:14:VAL:HG23	1.71	0.72
1:C:370:THR:O	1:C:374:ILE:HG13	1.90	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:239:TRP:HH2	1:C:416:PHE:CD1	2.07	0.72
1:B:194:ASN:O	1:B:198:VAL:HG23	1.90	0.72
1:C:22:VAL:HG13	1:C:459:ILE:HD11	1.71	0.72
1:A:323:TRP:NE1	1:A:327:TYR:HE1	1.88	0.72
1:B:63:LEU:HD22	1:B:145:LEU:HD21	1.72	0.71
1:A:13:LYS:HG3	1:A:14:VAL:HG23	1.71	0.71
1:B:197:LEU:O	1:B:201:ILE:HG12	1.90	0.71
1:C:434:THR:HG21	1:C:452:TRP:NE1	2.04	0.71
1:A:12:PRO:HD2	1:A:13:LYS:H	1.54	0.71
1:B:40:ILE:CD1	1:B:466:LEU:HD13	2.21	0.71
1:A:240:ILE:HD13	1:A:454:ILE:HA	1.71	0.71
1:C:133:LEU:O	1:C:133:LEU:HD13	1.90	0.71
1:A:299:ARG:HH11	1:A:299:ARG:HG2	1.54	0.71
1:C:172:SER:HA	1:C:175:LEU:HD12	1.72	0.70
1:A:222:LEU:HB2	1:A:223:PHE:HD1	1.56	0.70
1:B:451:GLY:O	1:B:454:ILE:HG12	1.92	0.70
1:A:320:TYR:O	1:A:323:TRP:N	2.25	0.70
1:A:217:GLU:HB3	1:A:395:ILE:HG13	1.74	0.70
1:C:323:TRP:NE1	1:C:327:TYR:HE1	1.89	0.70
1:B:272:TRP:O	1:B:275:ILE:HD13	1.92	0.69
1:B:434:THR:HG21	1:B:452:TRP:NE1	2.07	0.69
1:B:240:ILE:CD1	1:B:454:ILE:HA	2.22	0.69
1:B:222:LEU:HB2	1:B:223:PHE:HD1	1.56	0.69
1:C:197:LEU:O	1:C:201:ILE:HG12	1.92	0.69
1:A:176:VAL:HB	1:A:177:PRO:HD3	1.75	0.69
1:B:68:TRP:O	1:B:72:GLY:HA3	1.91	0.69
1:C:222:LEU:HB2	1:C:223:PHE:HD1	1.56	0.69
1:B:104:VAL:HG22	1:B:363:TRP:CH2	2.27	0.69
1:C:143:GLY:HA2	1:C:360:TRP:HE1	1.57	0.69
1:C:104:VAL:HG22	1:C:363:TRP:CH2	2.28	0.68
1:B:370:THR:O	1:B:374:ILE:HG13	1.92	0.68
1:B:299:ARG:HD3	1:C:292:MET:HE3	1.74	0.68
1:A:68:TRP:O	1:A:72:GLY:HA3	1.93	0.68
1:B:323:TRP:CG	2:B:1504:NM2:C10	2.76	0.68
1:B:323:TRP:NE1	1:B:327:TYR:HE1	1.90	0.68
1:A:320:TYR:O	1:A:321:TRP:C	2.32	0.68
1:C:68:TRP:O	1:C:72:GLY:HA3	1.93	0.68
1:A:26:CYS:SG	1:A:462:VAL:HG21	2.34	0.67
1:C:428:TYR:CE2	1:C:432:MET:HG3	2.28	0.67
1:A:320:TYR:O	1:A:322:ALA:N	2.28	0.67
1:A:22:VAL:HG13	1:A:459:ILE:HD11	1.76	0.67
1:A:239:TRP:CH2	1:A:416:PHE:CD1	2.83	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:ASP:O	1:A:264:TYR:HD2	1.78	0.67
1:A:197:LEU:O	1:A:201:ILE:HG12	1.95	0.66
1:B:428:TYR:CE2	1:B:432:MET:HG3	2.30	0.66
1:B:22:VAL:HG13	1:B:459:ILE:HD11	1.76	0.66
1:C:240:ILE:HG21	1:C:454:ILE:HG22	1.78	0.66
1:A:413:ILE:HG22	1:A:417:ILE:HD13	1.77	0.65
1:C:323:TRP:CG	2:C:1504:NM2:H102	2.30	0.65
1:B:170:ARG:HD2	1:B:433:SER:O	1.95	0.65
1:A:143:GLY:HA2	1:A:360:TRP:HE1	1.62	0.65
1:B:12:PRO:HD2	1:B:13:LYS:H	1.61	0.65
1:A:446:LEU:O	1:A:450:ILE:HG13	1.95	0.65
1:C:12:PRO:HD2	1:C:13:LYS:H	1.62	0.65
1:A:299:ARG:HD3	1:B:292:MET:HE3	1.78	0.65
1:A:370:THR:O	1:A:374:ILE:HG13	1.96	0.65
1:C:204:MET:O	1:C:207:SER:OG	2.15	0.65
1:A:240:ILE:CD1	1:A:454:ILE:HA	2.27	0.65
1:B:236:ILE:O	1:B:240:ILE:HG13	1.96	0.65
1:C:143:GLY:HA2	1:C:360:TRP:NE1	2.11	0.64
1:A:428:TYR:CE2	1:A:432:MET:HG3	2.32	0.64
1:C:297:LEU:HB3	1:C:298:PRO:HD3	1.79	0.64
1:A:133:LEU:O	1:A:133:LEU:HD13	1.97	0.64
1:C:343:THR:CG2	1:C:346:GLU:HB2	2.22	0.64
1:A:142:TRP:HZ3	2:A:1504:NM2:H82C	1.62	0.64
1:B:240:ILE:HG21	1:B:454:ILE:HG22	1.78	0.64
1:B:236:ILE:HD12	1:B:461:ILE:HG12	1.79	0.64
1:C:260:ASP:O	1:C:264:TYR:HD2	1.80	0.64
1:A:204:MET:HE3	1:A:430:LEU:HD11	1.78	0.64
1:C:187:LEU:HD23	1:C:187:LEU:H	1.61	0.64
1:B:217:GLU:HB3	1:B:395:ILE:HG13	1.78	0.64
1:A:240:ILE:HG21	1:A:454:ILE:HG22	1.79	0.64
1:C:236:ILE:O	1:C:240:ILE:HG13	1.98	0.63
1:C:413:ILE:HG22	1:C:417:ILE:HD13	1.79	0.63
1:A:87:SER:OG	1:A:90:SER:HB2	1.98	0.63
1:A:458:ILE:O	1:A:462:VAL:HG23	1.99	0.63
1:B:164:ARG:HB2	1:B:166:MET:HG3	1.78	0.63
1:C:240:ILE:CD1	1:C:454:ILE:HA	2.27	0.63
1:C:142:TRP:CE2	1:C:363:TRP:CZ2	2.87	0.63
1:A:204:MET:O	1:A:207:SER:OG	2.17	0.63
1:B:142:TRP:CE2	1:B:363:TRP:CZ2	2.86	0.63
1:B:26:CYS:SG	1:B:462:VAL:HG21	2.39	0.63
1:A:223:PHE:N	1:A:223:PHE:CD1	2.68	0.62
1:A:40:ILE:CD1	1:A:466:LEU:HD13	2.28	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:326:ILE:HD11	1:B:479:GLY:HA3	1.80	0.62
1:B:335:LEU:CD1	1:B:351:MET:HE1	2.29	0.62
1:A:236:ILE:O	1:A:240:ILE:HG13	1.99	0.62
1:A:297:LEU:HB3	1:A:298:PRO:HD3	1.82	0.62
1:A:187:LEU:H	1:A:187:LEU:HD23	1.65	0.61
1:C:17:PRO:HB2	1:C:18:PRO:HD3	1.82	0.61
1:B:328:ALA:HB3	1:B:487:ASN:HD21	1.65	0.61
1:B:107:TRP:HE1	1:B:323:TRP:HZ3	1.46	0.61
1:C:328:ALA:HB3	1:C:487:ASN:HD21	1.65	0.61
1:B:413:ILE:HG22	1:B:417:ILE:HD13	1.83	0.61
1:B:162:PHE:CD2	1:B:340:ARG:HG3	2.35	0.61
1:A:215:VAL:O	1:A:219:MET:HG3	1.99	0.61
1:C:217:GLU:HB3	1:C:395:ILE:HG13	1.82	0.61
1:A:145:LEU:O	1:A:145:LEU:HD23	1.99	0.61
1:C:162:PHE:CD2	1:C:340:ARG:HG3	2.34	0.61
1:C:26:CYS:SG	1:C:462:VAL:HG21	2.40	0.61
1:C:458:ILE:O	1:C:462:VAL:HG23	2.00	0.61
1:C:446:LEU:O	1:C:450:ILE:HG13	2.01	0.61
1:A:164:ARG:HB2	1:A:166:MET:HG3	1.82	0.61
1:B:59:MET:HG3	1:B:321:TRP:CD1	2.36	0.61
1:B:204:MET:O	1:B:207:SER:OG	2.19	0.61
1:A:64:PHE:O	1:A:67:PHE:HB2	2.01	0.61
1:A:262:ARG:NH1	1:A:421:THR:HG21	2.16	0.61
1:C:164:ARG:CZ	1:C:501:ASN:HD22	2.14	0.61
1:C:239:TRP:CH2	1:C:416:PHE:CD1	2.89	0.61
1:A:159:TYR:OH	1:A:164:ARG:HD2	2.01	0.60
1:B:187:LEU:H	1:B:187:LEU:HD23	1.66	0.60
1:B:239:TRP:CH2	1:B:416:PHE:CD1	2.87	0.60
1:A:87:SER:OG	1:A:90:SER:CB	2.49	0.60
1:A:330:GLN:OE1	1:A:330:GLN:HA	1.99	0.60
1:A:469:LEU:HD12	2:A:1505:NM2:H81C	1.84	0.60
1:A:142:TRP:CD2	1:A:363:TRP:CZ2	2.89	0.60
1:B:22:VAL:HG12	1:B:455:LEU:HD11	1.84	0.60
1:A:373:LEU:HD12	1:A:397:THR:HB	1.83	0.60
1:C:373:LEU:HD12	1:C:397:THR:HB	1.83	0.60
1:C:40:ILE:CD1	1:C:466:LEU:HD13	2.32	0.60
1:B:355:LEU:O	1:B:358:SER:HB3	2.02	0.60
1:C:236:ILE:HD12	1:C:461:ILE:HG12	1.83	0.60
1:C:247:VAL:HG12	1:C:446:LEU:HD11	1.84	0.60
1:B:373:LEU:HD12	1:B:397:THR:HB	1.82	0.60
1:B:124:GLU:O	1:B:127:SER:HB3	2.02	0.60
1:C:455:LEU:HA	1:C:458:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:143:GLY:O	1:C:146:PRO:HD2	2.02	0.60
1:B:143:GLY:HA2	1:B:360:TRP:HE1	1.66	0.60
1:A:162:PHE:CD2	1:A:340:ARG:HG3	2.37	0.60
1:A:455:LEU:HA	1:A:458:ILE:HD12	1.84	0.59
1:A:164:ARG:CZ	1:A:501:ASN:HD22	2.15	0.59
1:C:164:ARG:HB2	1:C:166:MET:HG3	1.83	0.59
1:C:59:MET:HG3	1:C:321:TRP:CD1	2.37	0.59
1:B:372:LEU:O	1:B:376:LYS:HG3	2.02	0.59
1:B:330:GLN:HA	1:B:330:GLN:OE1	2.01	0.59
1:C:66:TRP:O	1:C:70:VAL:HG23	2.02	0.59
1:A:223:PHE:N	1:A:223:PHE:HD1	2.01	0.59
1:B:260:ASP:O	1:B:264:TYR:HD2	1.84	0.59
1:B:391:ALA:O	1:B:395:ILE:HG12	2.01	0.59
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.59
1:A:381:ILE:N	1:A:382:PRO:CD	2.65	0.59
1:B:335:LEU:HD12	1:B:351:MET:HE1	1.85	0.59
1:B:312:PHE:HB3	1:B:313:PRO:HD3	1.83	0.59
1:A:279:ALA:O	1:A:280:SER:C	2.40	0.59
1:C:262:ARG:NH1	1:C:421:THR:HG21	2.17	0.59
1:A:143:GLY:HA2	1:A:360:TRP:NE1	2.17	0.58
1:B:297:LEU:HB3	1:B:298:PRO:HD3	1.84	0.58
1:B:446:LEU:O	1:B:450:ILE:HG13	2.03	0.58
1:A:196:TYR:OH	1:A:330:GLN:NE2	2.36	0.58
1:A:252:GLN:H	1:A:252:GLN:HE21	1.50	0.58
1:B:323:TRP:CD1	2:B:1504:NM2:H102	2.38	0.58
1:C:326:ILE:HD11	1:C:479:GLY:HA3	1.84	0.58
1:C:87:SER:OG	1:C:90:SER:HB2	2.02	0.58
1:C:204:MET:HE3	1:C:430:LEU:HD11	1.85	0.58
1:A:335:LEU:CD1	1:A:351:MET:HE1	2.33	0.58
1:C:299:ARG:HH11	1:C:299:ARG:CG	2.16	0.58
1:B:143:GLY:HA2	1:B:360:TRP:NE1	2.19	0.58
1:C:124:GLU:O	1:C:127:SER:HB3	2.03	0.58
1:A:142:TRP:HZ3	2:A:1504:NM2:C8	2.16	0.58
1:A:170:ARG:HD2	1:A:433:SER:O	2.04	0.58
1:A:59:MET:HG3	1:A:321:TRP:CD1	2.39	0.58
1:C:330:GLN:HA	1:C:330:GLN:OE1	2.03	0.58
1:C:107:TRP:HE1	1:C:323:TRP:HZ3	1.51	0.57
1:C:483:LEU:HD22	1:C:483:LEU:N	2.18	0.57
1:B:247:VAL:HG12	1:B:446:LEU:HD11	1.85	0.57
1:C:372:LEU:O	1:C:376:LYS:HG3	2.04	0.57
1:A:142:TRP:CE2	1:A:363:TRP:HZ2	2.19	0.57
1:C:196:TYR:OH	1:C:330:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:VAL:HG12	1:B:62:MET:N	2.18	0.57
1:B:233:ALA:HB2	1:B:461:ILE:HG21	1.87	0.57
1:C:64:PHE:O	1:C:67:PHE:HB2	2.05	0.57
1:B:483:LEU:N	1:B:483:LEU:HD22	2.20	0.57
1:C:223:PHE:N	1:C:223:PHE:CD1	2.72	0.57
1:C:381:ILE:N	1:C:382:PRO:CD	2.68	0.57
1:B:40:ILE:HD11	1:B:466:LEU:CD1	2.32	0.57
1:A:331:MET:SD	2:A:1504:NM2:O4	2.62	0.57
1:B:164:ARG:CZ	1:B:501:ASN:HD22	2.18	0.57
1:A:142:TRP:CZ2	1:A:363:TRP:HZ2	2.23	0.57
1:A:66:TRP:O	1:A:70:VAL:HG23	2.03	0.57
1:B:299:ARG:HH11	1:B:299:ARG:CG	2.18	0.56
1:C:355:LEU:O	1:C:358:SER:HB3	2.05	0.56
1:A:22:VAL:HG12	1:A:455:LEU:HD11	1.87	0.56
1:B:44:PHE:CD2	1:B:470:LYS:HE3	2.40	0.56
1:B:87:SER:OG	1:B:90:SER:HB2	2.05	0.56
1:A:343:THR:HG23	1:A:346:GLU:CB	2.20	0.56
1:C:170:ARG:HD2	1:C:433:SER:O	2.05	0.56
1:C:244:ALA:HB2	1:C:450:ILE:HG21	1.87	0.56
1:B:64:PHE:O	1:B:67:PHE:HB2	2.06	0.56
1:B:381:ILE:N	1:B:382:PRO:CD	2.69	0.56
1:A:69:LEU:HD11	1:A:152:PHE:HA	1.88	0.56
1:C:87:SER:OG	1:C:90:SER:CB	2.54	0.56
1:B:379:LEU:N	1:B:379:LEU:HD23	2.21	0.56
1:A:17:PRO:HB2	1:A:18:PRO:HD3	1.88	0.56
1:B:279:ALA:O	1:B:280:SER:C	2.43	0.56
1:B:119:PRO:HB2	1:B:123:LEU:HB2	1.88	0.56
1:C:119:PRO:HB2	1:C:123:LEU:HB2	1.88	0.56
1:B:145:LEU:O	1:B:145:LEU:HD23	2.05	0.56
1:B:323:TRP:CE2	2:B:1504:NM2:H102	2.40	0.56
1:A:61:VAL:HG12	1:A:62:MET:N	2.19	0.56
1:A:124:GLU:O	1:A:127:SER:HB3	2.05	0.56
1:C:483:LEU:CD2	1:C:483:LEU:N	2.69	0.56
1:A:323:TRP:NE1	1:A:327:TYR:CE1	2.73	0.56
1:B:176:VAL:HB	1:B:177:PRO:HD3	1.88	0.55
1:A:159:TYR:CE1	1:A:164:ARG:HD2	2.42	0.55
1:B:244:ALA:CB	1:B:450:ILE:HD13	2.36	0.55
1:B:215:VAL:O	1:B:219:MET:HG3	2.06	0.55
1:A:107:TRP:HE1	1:A:323:TRP:HZ3	1.54	0.55
1:B:223:PHE:N	1:B:223:PHE:CD1	2.74	0.55
1:B:211:ALA:O	1:B:215:VAL:HG23	2.07	0.55
1:C:176:VAL:HB	1:C:177:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:252:GLN:HE21	1:C:252:GLN:H	1.54	0.55
1:A:299:ARG:HH11	1:A:299:ARG:CG	2.17	0.55
1:C:379:LEU:HD23	1:C:379:LEU:H	1.71	0.55
1:B:252:GLN:HE21	1:B:252:GLN:H	1.53	0.55
1:C:483:LEU:CD2	1:C:483:LEU:H	2.19	0.55
1:A:204:MET:SD	1:A:426:CYS:HB3	2.47	0.55
1:B:200:LEU:HG	1:B:204:MET:CE	2.37	0.55
1:B:200:LEU:HG	1:B:204:MET:HE2	1.89	0.55
1:B:143:GLY:O	1:B:146:PRO:HD2	2.07	0.55
1:C:259:SER:O	1:C:262:ARG:HB3	2.07	0.55
1:A:331:MET:O	1:A:334:PHE:N	2.39	0.55
1:A:259:SER:O	1:A:262:ARG:HB3	2.07	0.55
1:A:328:ALA:HB3	1:A:487:ASN:HD21	1.71	0.55
1:B:483:LEU:N	1:B:483:LEU:CD2	2.69	0.55
1:B:14:VAL:HG21	1:B:170:ARG:CZ	2.37	0.55
1:A:187:LEU:O	1:A:191:ILE:HG13	2.06	0.55
1:A:236:ILE:HD12	1:A:461:ILE:HG12	1.89	0.55
1:B:156:ALA:HB1	1:B:494:PHE:HB2	1.89	0.55
1:B:159:TYR:OH	1:B:164:ARG:HD2	2.05	0.54
1:A:461:ILE:O	1:A:465:ALA:N	2.34	0.54
1:B:187:LEU:O	1:B:191:ILE:HG13	2.08	0.54
1:A:44:PHE:CD2	1:A:470:LYS:HE3	2.42	0.54
1:C:275:ILE:H	1:C:275:ILE:HD13	1.73	0.54
1:B:156:ALA:HA	1:B:494:PHE:CD1	2.41	0.54
1:A:95:MET:HE3	1:A:335:LEU:HD22	1.90	0.54
1:C:428:TYR:CD2	1:C:432:MET:HG3	2.43	0.54
1:A:220:GLN:HB2	1:A:225:ILE:O	2.08	0.54
1:B:439:ARG:HD2	1:B:442:GLU:OE2	2.08	0.54
1:B:259:SER:O	1:B:262:ARG:HB3	2.06	0.54
1:B:323:TRP:NE1	1:B:327:TYR:CE1	2.74	0.54
1:C:279:ALA:O	1:C:280:SER:C	2.46	0.54
1:B:455:LEU:HA	1:B:458:ILE:HD12	1.90	0.54
1:C:323:TRP:CG	2:C:1504:NM2:C10	2.90	0.54
1:A:247:VAL:HG12	1:A:446:LEU:HD11	1.88	0.54
1:B:262:ARG:NH1	1:B:421:THR:HG21	2.23	0.54
1:C:461:ILE:O	1:C:465:ALA:N	2.36	0.53
1:B:66:TRP:O	1:B:70:VAL:HG23	2.09	0.53
1:B:232:ASP:O	1:B:236:ILE:HG13	2.08	0.53
1:C:244:ALA:CB	1:C:450:ILE:HD13	2.37	0.53
1:A:115:TYR:CE2	1:A:137:TYR:HB3	2.44	0.53
1:C:152:PHE:CE2	1:C:491:THR:HG23	2.44	0.53
1:B:483:LEU:CD2	1:B:483:LEU:H	2.21	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:439:ARG:HD2	1:A:442:GLU:OE2	2.07	0.53
1:C:14:VAL:HG21	1:C:170:ARG:CZ	2.38	0.53
1:A:391:ALA:O	1:A:395:ILE:HG12	2.08	0.53
1:C:223:PHE:N	1:C:223:PHE:HD1	2.06	0.53
1:C:61:VAL:HG12	1:C:62:MET:N	2.22	0.53
1:B:17:PRO:HB2	1:B:18:PRO:HD3	1.88	0.53
1:C:159:TYR:OH	1:C:164:ARG:HD2	2.09	0.53
1:B:244:ALA:HB2	1:B:450:ILE:HG21	1.91	0.53
1:A:74:TYR:CD2	1:A:74:TYR:N	2.76	0.53
1:C:323:TRP:NE1	1:C:327:TYR:CE1	2.75	0.53
1:C:139:LEU:HD22	1:C:360:TRP:CD2	2.44	0.53
1:B:127:SER:O	1:B:128:THR:C	2.46	0.53
1:A:156:ALA:HB1	1:A:494:PHE:HB2	1.91	0.53
1:C:22:VAL:HG12	1:C:455:LEU:HD11	1.91	0.53
1:A:275:ILE:HD13	1:A:275:ILE:H	1.74	0.53
1:A:373:LEU:HD13	1:A:379:LEU:HD21	1.91	0.53
1:A:379:LEU:H	1:A:379:LEU:HD23	1.73	0.53
1:A:152:PHE:CD2	1:A:491:THR:HG23	2.43	0.53
1:C:135:LEU:CD1	1:C:364:THR:HG22	2.27	0.53
1:C:476:ILE:HG22	1:C:477:ILE:N	2.23	0.53
1:B:126:ASN:OD1	1:B:126:ASN:N	2.42	0.53
1:A:127:SER:O	1:A:128:THR:C	2.47	0.53
1:A:274:PHE:CE1	1:A:282:ILE:HG21	2.44	0.53
1:B:335:LEU:HD13	1:B:351:MET:CE	2.39	0.52
1:B:331:MET:O	1:B:334:PHE:N	2.41	0.52
1:C:74:TYR:CD2	1:C:74:TYR:N	2.77	0.52
1:C:156:ALA:HB1	1:C:494:PHE:HB2	1.90	0.52
1:C:233:ALA:HB2	1:C:461:ILE:HG21	1.91	0.52
1:C:95:MET:CE	1:C:335:LEU:HD22	2.39	0.52
1:A:101:SER:OG	1:A:102:ALA:N	2.43	0.52
1:A:234:ILE:O	1:A:237:THR:OG1	2.26	0.52
1:B:87:SER:OG	1:B:90:SER:CB	2.57	0.52
1:B:458:ILE:O	1:B:462:VAL:HG23	2.10	0.52
1:A:373:LEU:HB3	1:A:379:LEU:HD21	1.92	0.52
1:A:393:ALA:O	1:A:397:THR:HG23	2.10	0.52
1:A:381:ILE:O	1:A:385:ILE:HG13	2.09	0.52
1:A:95:MET:CE	1:A:335:LEU:HD22	2.39	0.52
1:C:156:ALA:HA	1:C:494:PHE:CD1	2.45	0.52
1:C:219:MET:HE1	1:C:231:LEU:HD11	1.92	0.52
1:C:44:PHE:CD2	1:C:470:LYS:HE3	2.45	0.52
1:C:196:TYR:C	1:C:196:TYR:CD1	2.83	0.52
1:C:215:VAL:O	1:C:219:MET:HG3	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:380:ASN:OD1	1:B:382:PRO:HD2	2.10	0.52
1:A:321:TRP:O	1:A:325:VAL:HG23	2.10	0.52
1:B:71:PHE:CD2	1:B:71:PHE:N	2.78	0.52
1:B:428:TYR:CD2	1:B:432:MET:HG3	2.45	0.51
1:C:70:VAL:HG11	1:C:349:PHE:CZ	2.46	0.51
1:C:101:SER:OG	1:C:102:ALA:N	2.42	0.51
1:A:199:ALA:CB	1:A:483:LEU:HD21	2.40	0.51
1:A:211:ALA:O	1:A:215:VAL:HG23	2.10	0.51
1:B:74:TYR:N	1:B:74:TYR:CD2	2.77	0.51
1:A:222:LEU:HB2	1:A:223:PHE:CE1	2.46	0.51
1:A:355:LEU:O	1:A:358:SER:HB3	2.11	0.51
1:C:391:ALA:O	1:C:395:ILE:HG12	2.11	0.51
1:C:44:PHE:CE2	1:C:470:LYS:HE3	2.46	0.51
1:C:472:ILE:O	1:C:475:ALA:HB3	2.10	0.51
1:B:150:TYR:CZ	1:B:328:ALA:HA	2.46	0.51
1:B:90:SER:O	1:B:94:MET:HG3	2.11	0.51
1:C:145:LEU:O	1:C:145:LEU:HD23	2.10	0.51
1:B:461:ILE:HA	1:B:464:LEU:HB2	1.93	0.51
1:A:90:SER:O	1:A:94:MET:HG3	2.11	0.51
1:A:233:ALA:HB2	1:A:461:ILE:HG21	1.93	0.51
1:A:239:TRP:CH2	1:A:416:PHE:CE1	2.99	0.51
1:A:12:PRO:CD	1:A:13:LYS:H	2.22	0.51
1:C:187:LEU:O	1:C:191:ILE:HG13	2.11	0.51
1:C:152:PHE:CD2	1:C:491:THR:HG23	2.46	0.50
1:C:199:ALA:CB	1:C:483:LEU:HD21	2.41	0.50
1:A:428:TYR:CD2	1:A:432:MET:HG3	2.46	0.50
1:A:44:PHE:CE2	1:A:470:LYS:HE3	2.46	0.50
1:A:48:THR:CG2	1:A:477:ILE:HD13	2.42	0.50
1:B:13:LYS:HB2	1:B:190:THR:HG21	1.93	0.50
1:B:334:PHE:C	1:B:334:PHE:CD1	2.83	0.50
1:B:188:PHE:O	1:B:192:VAL:HG23	2.12	0.50
1:A:119:PRO:HB2	1:A:123:LEU:HB2	1.92	0.50
1:C:135:LEU:HD11	1:C:364:THR:CG2	2.28	0.50
1:C:349:PHE:O	1:C:353:LEU:HD12	2.12	0.50
1:A:461:ILE:HA	1:A:464:LEU:HB2	1.94	0.50
1:B:239:TRP:CH2	1:B:416:PHE:CE1	3.00	0.50
1:C:446:LEU:HD12	1:C:450:ILE:HD11	1.93	0.50
1:C:379:LEU:N	1:C:379:LEU:HD23	2.27	0.50
1:B:152:PHE:CE2	1:B:491:THR:HG23	2.47	0.50
1:B:159:TYR:CE1	1:B:164:ARG:HD2	2.47	0.50
1:C:41:ASN:HD22	1:C:41:ASN:N	2.09	0.50
1:A:126:ASN:N	1:A:126:ASN:OD1	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:315:GLY:HA3	2:B:1505:NM2:O7	2.12	0.50
1:C:48:THR:CG2	1:C:477:ILE:HD13	2.42	0.50
1:A:164:ARG:NH1	1:A:501:ASN:HD22	2.10	0.50
1:C:164:ARG:NH1	1:C:501:ASN:HD22	2.10	0.50
1:C:373:LEU:HB3	1:C:379:LEU:HD21	1.93	0.50
1:B:244:ALA:HB1	1:B:450:ILE:HD13	1.92	0.50
1:A:335:LEU:HD13	1:A:351:MET:HE1	1.92	0.50
1:A:347:LEU:O	1:A:351:MET:HG2	2.11	0.50
1:B:115:TYR:OH	1:B:141:HIS:HD2	1.95	0.50
1:A:152:PHE:CE2	1:A:491:THR:HG23	2.47	0.50
1:C:69:LEU:HD11	1:C:152:PHE:HA	1.94	0.50
1:A:446:LEU:HD12	1:A:450:ILE:HD11	1.94	0.49
1:C:334:PHE:CD1	1:C:334:PHE:C	2.85	0.49
1:B:223:PHE:HD1	1:B:223:PHE:N	2.09	0.49
1:A:244:ALA:CB	1:A:450:ILE:HD13	2.41	0.49
1:B:274:PHE:CE2	1:B:279:ALA:HB2	2.47	0.49
1:C:126:ASN:OD1	1:C:126:ASN:N	2.45	0.49
1:C:343:THR:HG23	1:C:346:GLU:CB	2.27	0.49
1:B:276:VAL:CG2	1:B:277:SER:N	2.75	0.49
1:C:213:PRO:O	1:C:217:GLU:HB2	2.12	0.49
1:A:483:LEU:N	1:A:483:LEU:CD2	2.75	0.49
1:A:483:LEU:HD22	1:A:483:LEU:N	2.28	0.49
1:A:213:PRO:O	1:A:217:GLU:HB2	2.13	0.49
1:C:147:TRP:CE2	1:C:355:LEU:HB3	2.48	0.49
1:B:44:PHE:CE2	1:B:470:LYS:HE3	2.47	0.49
1:B:196:TYR:OH	1:B:330:GLN:NE2	2.46	0.49
1:B:381:ILE:O	1:B:385:ILE:HG13	2.13	0.49
1:C:461:ILE:HA	1:C:464:LEU:HB2	1.94	0.49
1:B:476:ILE:HG22	1:B:477:ILE:N	2.28	0.49
1:A:41:ASN:HD22	1:A:41:ASN:N	2.10	0.49
1:B:95:MET:HE3	1:B:335:LEU:HD22	1.95	0.49
1:C:74:TYR:HD2	1:C:74:TYR:N	2.11	0.49
1:B:74:TYR:N	1:B:74:TYR:HD2	2.11	0.49
1:C:109:SER:O	1:C:370:THR:HG21	2.13	0.49
1:B:323:TRP:CD1	2:B:1504:NM2:C10	2.96	0.49
1:A:323:TRP:CD2	2:A:1504:NM2:H102	2.48	0.49
1:A:61:VAL:O	1:A:64:PHE:N	2.46	0.49
1:C:146:PRO:O	1:C:149:THR:OG1	2.28	0.49
1:B:196:TYR:C	1:B:196:TYR:CD1	2.86	0.49
1:C:159:TYR:CE1	1:C:164:ARG:HD2	2.48	0.48
1:B:145:LEU:HB3	1:B:146:PRO:HD3	1.94	0.48
1:B:139:LEU:HD22	1:B:360:TRP:CD2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:312:PHE:HB3	1:C:313:PRO:HD3	1.94	0.48
1:A:138:SER:HB3	1:A:363:TRP:CD1	2.48	0.48
1:C:127:SER:O	1:C:128:THR:C	2.52	0.48
1:C:479:GLY:O	1:C:483:LEU:HD23	2.13	0.48
1:C:299:ARG:CG	1:C:299:ARG:NH1	2.76	0.48
1:C:188:PHE:O	1:C:192:VAL:HG23	2.13	0.48
1:C:145:LEU:HB3	1:C:146:PRO:HD3	1.95	0.48
1:C:13:LYS:HB2	1:C:190:THR:HG21	1.94	0.48
1:A:379:LEU:HD23	1:A:379:LEU:N	2.28	0.48
1:B:323:TRP:HE1	1:B:327:TYR:HE1	1.58	0.48
1:C:323:TRP:HE1	1:C:327:TYR:HE1	1.60	0.48
1:A:293:LEU:O	1:A:297:LEU:HB2	2.14	0.48
1:B:461:ILE:O	1:B:465:ALA:N	2.36	0.48
1:B:69:LEU:HD11	1:B:152:PHE:HA	1.96	0.48
1:B:321:TRP:CE3	1:B:321:TRP:HA	2.49	0.48
1:C:24:ILE:HG22	1:C:28:LEU:CD1	2.44	0.48
1:C:276:VAL:CG2	1:C:277:SER:N	2.77	0.48
1:C:244:ALA:HB1	1:C:450:ILE:HD13	1.94	0.48
1:B:70:VAL:HG12	1:B:71:PHE:CD2	2.48	0.48
1:B:275:ILE:H	1:B:275:ILE:HD13	1.77	0.48
1:A:372:LEU:O	1:A:376:LYS:HG3	2.14	0.48
1:C:200:LEU:HG	1:C:204:MET:CE	2.43	0.48
1:B:204:MET:HE3	1:B:430:LEU:HD11	1.95	0.48
1:C:381:ILE:O	1:C:385:ILE:HG13	2.14	0.48
1:B:299:ARG:NH1	1:B:299:ARG:CG	2.75	0.47
1:B:428:TYR:C	1:B:428:TYR:CD2	2.86	0.47
1:A:326:ILE:HD11	1:A:479:GLY:HA3	1.96	0.47
1:C:232:ASP:O	1:C:236:ILE:HG13	2.14	0.47
1:A:299:ARG:NH1	1:A:299:ARG:CG	2.76	0.47
1:A:335:LEU:HD13	1:A:351:MET:CE	2.44	0.47
1:B:274:PHE:CE1	1:B:282:ILE:HG21	2.49	0.47
1:A:312:PHE:HB3	1:A:313:PRO:HD3	1.95	0.47
1:A:323:TRP:HE1	1:A:327:TYR:HE1	1.60	0.47
1:B:373:LEU:HB3	1:B:379:LEU:HD21	1.96	0.47
1:B:70:VAL:HG11	1:B:349:PHE:CZ	2.48	0.47
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.96	0.47
1:C:239:TRP:CH2	1:C:416:PHE:CE1	3.02	0.47
1:C:335:LEU:CD1	1:C:351:MET:HE1	2.45	0.47
1:A:283:MET:HE3	1:C:53:TRP:CZ3	2.49	0.47
1:A:14:VAL:HG21	1:A:170:ARG:CZ	2.44	0.47
1:C:428:TYR:CD2	1:C:428:TYR:C	2.87	0.47
1:B:347:LEU:O	1:B:351:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:439:ARG:HB2	1:A:442:GLU:OE1	2.14	0.47
1:A:74:TYR:HD2	1:A:74:TYR:N	2.11	0.47
1:C:272:TRP:HA	1:C:275:ILE:CD1	2.45	0.47
1:B:107:TRP:NE1	1:B:323:TRP:HZ3	2.13	0.47
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.79	0.47
1:A:479:GLY:O	1:A:483:LEU:HD23	2.14	0.47
1:A:139:LEU:HD22	1:A:360:TRP:CD2	2.50	0.47
1:A:262:ARG:HH12	1:A:421:THR:HG21	1.78	0.47
1:C:393:ALA:O	1:C:397:THR:HG23	2.15	0.47
1:C:70:VAL:CG1	1:C:349:PHE:CZ	2.98	0.47
1:B:247:VAL:HG12	1:B:446:LEU:CD1	2.45	0.47
1:B:22:VAL:CG1	1:B:455:LEU:HD11	2.43	0.47
1:A:428:TYR:C	1:A:428:TYR:CD2	2.88	0.47
1:A:443:ASP:HA	1:A:444:PRO:HD3	1.79	0.47
1:B:95:MET:CE	1:B:335:LEU:HD22	2.45	0.47
1:C:90:SER:O	1:C:94:MET:HG3	2.14	0.47
1:C:61:VAL:O	1:C:64:PHE:N	2.48	0.47
1:A:71:PHE:CD2	1:A:71:PHE:N	2.82	0.47
1:B:329:ILE:HD11	1:B:490:VAL:HG21	1.97	0.47
1:B:461:ILE:HG13	1:B:461:ILE:H	1.45	0.46
1:A:334:PHE:C	1:A:334:PHE:CD1	2.88	0.46
1:C:70:VAL:HG12	1:C:71:PHE:CD2	2.51	0.46
1:C:331:MET:O	1:C:334:PHE:N	2.48	0.46
1:A:142:TRP:CZ3	2:A:1504:NM2:H82C	2.48	0.46
1:C:439:ARG:HD2	1:C:442:GLU:OE2	2.14	0.46
1:B:296:TYR:O	1:B:300:MET:HG3	2.16	0.46
1:B:219:MET:HE1	1:B:231:LEU:HD11	1.98	0.46
1:B:48:THR:CG2	1:B:477:ILE:HD13	2.45	0.46
1:A:403:LEU:HD23	1:A:403:LEU:N	2.30	0.46
1:B:101:SER:OG	1:B:102:ALA:N	2.49	0.46
1:B:220:GLN:HB2	1:B:225:ILE:O	2.16	0.46
1:A:323:TRP:CD1	1:A:327:TYR:CE1	3.04	0.46
1:C:247:VAL:HG12	1:C:446:LEU:CD1	2.45	0.46
1:C:274:PHE:CE2	1:C:279:ALA:HB2	2.50	0.46
1:B:152:PHE:CD2	1:B:491:THR:HG23	2.50	0.46
1:A:481:CYS:HB2	1:A:482:PRO:HD3	1.98	0.46
1:A:13:LYS:HB2	1:A:190:THR:HG21	1.97	0.46
1:C:247:VAL:HG12	1:C:446:LEU:HD21	1.97	0.46
1:A:150:TYR:CZ	1:A:328:ALA:HA	2.50	0.46
1:A:160:PHE:CE2	1:A:174:THR:HB	2.50	0.46
1:A:45:SER:O	1:A:49:ASN:HB2	2.15	0.46
1:C:488:ILE:HG22	1:C:492:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:232:ASP:O	1:A:236:ILE:HG13	2.15	0.46
1:C:233:ALA:O	1:C:237:THR:HG23	2.16	0.46
1:A:335:LEU:HD12	1:A:351:MET:HE1	1.97	0.46
1:B:446:LEU:HD12	1:B:450:ILE:HD11	1.97	0.46
1:A:431:ALA:HB1	1:A:448:VAL:HG12	1.97	0.46
1:C:222:LEU:HB2	1:C:223:PHE:CE1	2.49	0.46
1:C:12:PRO:CD	1:C:13:LYS:H	2.28	0.46
1:A:280:SER:HB2	1:C:50:VAL:HG13	1.98	0.46
1:A:376:LYS:CB	1:A:378:ILE:HG13	2.45	0.46
1:A:299:ARG:CD	1:B:292:MET:HE3	2.44	0.45
1:A:484:PHE:O	1:A:488:ILE:HG13	2.16	0.45
1:C:196:TYR:HE1	1:C:200:LEU:HD22	1.81	0.45
1:C:141:HIS:CE1	1:C:317:THR:OG1	2.57	0.45
1:A:395:ILE:HG23	1:A:408:MET:HE1	1.98	0.45
1:B:68:TRP:O	1:B:72:GLY:CA	2.60	0.45
1:B:320:TYR:O	1:B:321:TRP:C	2.54	0.45
1:B:301:LEU:HA	1:B:301:LEU:HD12	1.66	0.45
1:A:196:TYR:CD1	1:A:196:TYR:C	2.89	0.45
1:C:376:LYS:CB	1:C:378:ILE:HG13	2.47	0.45
1:C:105:LEU:HA	1:C:105:LEU:HD23	1.64	0.45
1:A:276:VAL:CG2	1:A:277:SER:N	2.77	0.45
1:A:199:ALA:HB3	1:A:483:LEU:HD21	1.98	0.45
1:A:40:ILE:HD11	1:A:466:LEU:CD1	2.41	0.45
1:B:127:SER:O	1:B:129:GLY:N	2.49	0.45
1:C:262:ARG:HH12	1:C:421:THR:HG21	1.81	0.45
1:A:70:VAL:HG11	1:A:349:PHE:CZ	2.52	0.45
1:C:219:MET:SD	1:C:235:ILE:HD11	2.56	0.45
1:B:491:THR:O	1:B:495:ILE:HG13	2.16	0.45
1:A:272:TRP:HA	1:A:275:ILE:CD1	2.46	0.45
1:A:143:GLY:O	1:A:146:PRO:HD2	2.16	0.45
1:C:143:GLY:CA	1:C:360:TRP:HE1	2.27	0.45
1:C:104:VAL:HG13	1:C:362:LEU:HD11	1.97	0.45
1:C:71:PHE:CD2	1:C:71:PHE:N	2.81	0.45
1:C:110:ILE:O	1:C:113:TYR:HB3	2.17	0.45
1:A:187:LEU:H	1:A:187:LEU:CD2	2.29	0.45
1:B:431:ALA:HB1	1:B:448:VAL:HG12	1.97	0.45
1:C:220:GLN:HB2	1:C:225:ILE:O	2.15	0.45
1:C:19:LEU:CD1	1:C:455:LEU:HD22	2.47	0.45
1:A:362:LEU:O	1:A:363:TRP:C	2.55	0.45
1:A:22:VAL:CG1	1:A:455:LEU:HD11	2.46	0.45
1:B:222:LEU:HB2	1:B:223:PHE:CE1	2.52	0.45
1:B:376:LYS:CB	1:B:378:ILE:HG13	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:PRO:C	1:A:127:SER:H	2.19	0.45
1:C:95:MET:HE3	1:C:335:LEU:HD22	1.99	0.45
1:C:312:PHE:HB3	1:C:313:PRO:CD	2.47	0.45
1:A:33:LEU:N	1:A:33:LEU:HD12	2.32	0.45
1:B:199:ALA:CB	1:B:483:LEU:HD21	2.47	0.45
1:B:104:VAL:HG13	1:B:362:LEU:HD11	1.98	0.45
1:B:335:LEU:HD13	1:B:351:MET:HE1	1.95	0.45
1:A:156:ALA:HA	1:A:494:PHE:CD1	2.52	0.45
1:A:327:TYR:CD1	2:A:1504:NM2:H101	2.51	0.45
1:A:63:LEU:O	1:A:64:PHE:C	2.55	0.45
1:C:187:LEU:HD23	1:C:187:LEU:N	2.31	0.44
1:C:150:TYR:CZ	1:C:328:ALA:HA	2.52	0.44
1:A:488:ILE:HG22	1:A:492:LEU:HD12	1.99	0.44
1:B:269:MET:CE	1:B:269:MET:HA	2.47	0.44
1:A:476:ILE:HG22	1:A:477:ILE:N	2.31	0.44
1:B:395:ILE:CG2	1:B:408:MET:HE1	2.47	0.44
1:B:501:ASN:OD1	1:B:501:ASN:N	2.50	0.44
1:B:299:ARG:HD2	1:B:299:ARG:HA	1.64	0.44
1:A:68:TRP:O	1:A:72:GLY:CA	2.64	0.44
1:B:61:VAL:O	1:B:64:PHE:N	2.49	0.44
1:C:335:LEU:HD12	1:C:351:MET:HE1	1.99	0.44
1:B:225:ILE:HG13	1:B:225:ILE:H	1.65	0.44
1:C:444:PRO:CB	1:C:445:PRO:HD2	2.47	0.44
1:A:419:THR:O	1:A:422:LEU:HB3	2.18	0.44
1:A:296:TYR:O	1:A:300:MET:HG3	2.17	0.44
1:C:293:LEU:O	1:C:297:LEU:HB2	2.17	0.44
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.84	0.44
1:B:403:LEU:HD23	1:B:403:LEU:N	2.33	0.44
1:B:213:PRO:O	1:B:217:GLU:HB2	2.18	0.44
1:A:349:PHE:O	1:A:353:LEU:HD12	2.18	0.44
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.69	0.44
1:A:201:ILE:H	1:A:201:ILE:HG12	1.62	0.44
1:A:244:ALA:HB2	1:A:450:ILE:HG21	1.99	0.44
1:B:187:LEU:H	1:B:187:LEU:CD2	2.31	0.44
1:C:373:LEU:HD13	1:C:379:LEU:HD21	2.00	0.44
1:B:153:LEU:HD21	1:B:491:THR:OG1	2.17	0.44
1:B:422:LEU:HD12	1:B:426:CYS:HG	1.82	0.44
1:B:109:SER:O	1:B:370:THR:HG21	2.18	0.44
1:C:403:LEU:N	1:C:403:LEU:HD23	2.33	0.44
1:A:233:ALA:O	1:A:237:THR:HG23	2.17	0.44
1:B:343:THR:HG23	1:B:346:GLU:CB	2.25	0.44
1:B:479:GLY:O	1:B:483:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:125:PRO:C	1:B:127:SER:H	2.20	0.44
1:C:439:ARG:HB2	1:C:442:GLU:OE1	2.17	0.44
1:B:12:PRO:CD	1:B:13:LYS:H	2.27	0.44
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.82	0.44
1:A:321:TRP:HA	1:A:321:TRP:CE3	2.52	0.43
1:A:395:ILE:CG2	1:A:408:MET:HE1	2.48	0.43
1:B:233:ALA:O	1:B:237:THR:HG23	2.18	0.43
1:B:299:ARG:CD	1:C:292:MET:HE3	2.44	0.43
1:B:444:PRO:CB	1:B:445:PRO:HD2	2.47	0.43
1:A:301:LEU:HA	1:A:301:LEU:HD12	1.63	0.43
1:B:135:LEU:CD1	1:B:364:THR:HG22	2.24	0.43
1:A:138:SER:OG	1:A:363:TRP:HD1	2.01	0.43
1:A:323:TRP:CE2	1:A:476:ILE:HD11	2.53	0.43
1:B:393:ALA:O	1:B:397:THR:HG23	2.18	0.43
1:A:70:VAL:HG12	1:A:71:PHE:CD2	2.53	0.43
1:B:343:THR:O	1:B:344:VAL:C	2.56	0.43
1:A:142:TRP:CD1	1:A:142:TRP:N	2.85	0.43
1:A:107:TRP:NE1	1:A:323:TRP:HZ3	2.16	0.43
1:C:321:TRP:CE3	1:C:321:TRP:HA	2.53	0.43
1:A:17:PRO:O	1:A:21:ILE:HG13	2.17	0.43
1:B:73:PRO:C	1:B:75:ALA:H	2.21	0.43
1:A:109:SER:O	1:A:370:THR:HG21	2.18	0.43
1:C:323:TRP:CE2	1:C:476:ILE:HD11	2.52	0.43
1:A:147:TRP:CE2	1:A:355:LEU:HB3	2.54	0.43
1:C:153:LEU:HD21	1:C:491:THR:OG1	2.17	0.43
1:B:266:SER:HB3	1:B:414:LEU:HD11	2.00	0.43
1:B:481:CYS:HB2	1:B:482:PRO:HD3	2.01	0.43
1:B:395:ILE:HG23	1:B:408:MET:HE1	2.01	0.43
1:B:146:PRO:O	1:B:149:THR:OG1	2.27	0.43
1:A:299:ARG:NH1	1:B:292:MET:HE3	2.34	0.43
1:A:269:MET:HA	1:A:269:MET:CE	2.48	0.43
1:C:33:LEU:HD12	1:C:33:LEU:N	2.34	0.43
1:C:187:LEU:H	1:C:187:LEU:CD2	2.27	0.43
1:B:125:PRO:CB	1:B:126:ASN:OD1	2.66	0.43
1:C:443:ASP:HA	1:C:444:PRO:HD3	1.79	0.43
1:B:105:LEU:HA	1:B:105:LEU:HD23	1.63	0.43
1:C:19:LEU:HD13	1:C:455:LEU:HD22	2.00	0.43
1:C:430:LEU:HD23	1:C:430:LEU:HA	1.85	0.43
1:A:247:VAL:HG12	1:A:446:LEU:HD21	2.01	0.43
1:A:432:MET:HG2	1:A:444:PRO:HG3	2.00	0.43
1:A:110:ILE:O	1:A:113:TYR:HB3	2.18	0.43
1:C:29:THR:HG21	1:C:466:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:139:LEU:HD22	1:C:360:TRP:CE2	2.54	0.43
1:B:351:MET:HB3	1:B:351:MET:HE2	1.91	0.43
1:C:312:PHE:C	1:C:312:PHE:CD2	2.92	0.43
1:C:395:ILE:CG2	1:C:408:MET:HE1	2.48	0.43
1:C:117:SER:OG	1:C:118:THR:HG22	2.19	0.43
1:B:17:PRO:O	1:B:21:ILE:HG13	2.19	0.43
1:A:440:ASP:OD1	1:A:441:GLY:N	2.52	0.43
1:C:199:ALA:HB3	1:C:483:LEU:HD21	2.00	0.43
1:C:115:TYR:OH	1:C:141:HIS:HD2	2.01	0.43
1:B:430:LEU:HD23	1:B:430:LEU:HA	1.80	0.43
1:B:201:ILE:HD13	1:B:430:LEU:HD21	2.01	0.43
1:B:432:MET:HG2	1:B:444:PRO:HG3	2.01	0.43
1:A:187:LEU:N	1:A:187:LEU:HD23	2.32	0.43
1:B:39:VAL:O	1:B:43:VAL:HG23	2.18	0.43
1:C:440:ASP:OD1	1:C:441:GLY:N	2.52	0.43
1:B:432:MET:HE2	1:B:432:MET:HB3	1.95	0.42
1:A:247:VAL:HG12	1:A:446:LEU:CD1	2.49	0.42
1:B:349:PHE:O	1:B:353:LEU:HD12	2.19	0.42
1:B:70:VAL:HG12	1:B:71:PHE:CE2	2.54	0.42
1:B:439:ARG:HB2	1:B:442:GLU:OE1	2.18	0.42
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.71	0.42
1:A:162:PHE:CG	1:A:340:ARG:HG3	2.54	0.42
1:C:125:PRO:C	1:C:127:SER:H	2.21	0.42
1:B:70:VAL:CG1	1:B:349:PHE:CZ	3.03	0.42
1:B:219:MET:SD	1:B:235:ILE:HD11	2.60	0.42
1:C:301:LEU:HB3	1:C:302:PHE:CD2	2.54	0.42
1:B:272:TRP:HA	1:B:275:ILE:CD1	2.49	0.42
1:A:292:MET:HE3	1:C:299:ARG:HD3	2.01	0.42
1:A:127:SER:C	1:A:129:GLY:N	2.73	0.42
1:A:200:LEU:HG	1:A:204:MET:CE	2.49	0.42
1:A:145:LEU:C	1:A:145:LEU:HD23	2.40	0.42
1:B:125:PRO:C	1:B:126:ASN:OD1	2.57	0.42
1:C:22:VAL:CG1	1:C:455:LEU:HD11	2.49	0.42
1:B:164:ARG:NH1	1:B:501:ASN:HD22	2.17	0.42
1:B:142:TRP:CD2	1:B:363:TRP:CZ2	3.07	0.42
1:B:321:TRP:CA	1:B:321:TRP:CE3	3.02	0.42
1:A:127:SER:O	1:A:129:GLY:N	2.52	0.42
1:A:431:ALA:HB2	1:A:449:ARG:HA	2.02	0.42
1:C:431:ALA:HB1	1:C:448:VAL:HG12	2.00	0.42
1:B:270:LEU:HA	1:B:270:LEU:HD23	1.78	0.42
1:A:244:ALA:HB1	1:A:450:ILE:HD13	2.00	0.42
1:B:312:PHE:HB3	1:B:313:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:45:SER:O	1:B:49:ASN:HB2	2.19	0.42
1:C:107:TRP:NE1	1:C:323:TRP:HZ3	2.15	0.42
1:A:13:LYS:HD2	1:A:190:THR:OG1	2.19	0.42
1:C:162:PHE:CG	1:C:340:ARG:HG3	2.53	0.42
1:B:303:TYR:O	1:B:313:PRO:HB3	2.20	0.42
1:C:118:THR:HA	1:C:119:PRO:HD3	1.81	0.42
1:C:270:LEU:HD23	1:C:270:LEU:HA	1.80	0.42
1:A:501:ASN:OD1	1:A:501:ASN:N	2.51	0.42
1:C:143:GLY:C	1:C:146:PRO:HD2	2.40	0.42
1:B:11:GLU:HA	1:B:12:PRO:HD3	1.86	0.42
1:B:13:LYS:HD2	1:B:190:THR:OG1	2.19	0.42
1:B:127:SER:C	1:B:129:GLY:N	2.73	0.42
1:A:39:VAL:O	1:A:42:ALA:HB3	2.20	0.42
1:B:179:VAL:HG23	1:B:183:HIS:HB2	2.02	0.42
1:C:201:ILE:HD13	1:C:430:LEU:HD21	2.02	0.42
1:C:13:LYS:HD2	1:C:190:THR:OG1	2.19	0.42
1:C:351:MET:HG3	1:C:352:VAL:N	2.35	0.42
1:A:323:TRP:CG	2:A:1504:NM2:H102	2.55	0.41
1:B:19:LEU:HD13	1:B:455:LEU:HD22	2.02	0.41
1:B:422:LEU:HD12	1:B:426:CYS:SG	2.60	0.41
1:B:273:VAL:HG12	1:B:273:VAL:O	2.18	0.41
1:C:269:MET:CE	1:C:269:MET:HA	2.50	0.41
1:B:19:LEU:CD1	1:B:455:LEU:HD22	2.50	0.41
1:C:380:ASN:OD1	1:C:382:PRO:HD2	2.21	0.41
1:C:211:ALA:O	1:C:215:VAL:HG23	2.19	0.41
1:A:164:ARG:CB	1:A:166:MET:HG3	2.50	0.41
1:B:301:LEU:HB3	1:B:302:PHE:CD2	2.55	0.41
1:B:488:ILE:HG22	1:B:492:LEU:HD12	2.02	0.41
1:C:26:CYS:SG	1:C:458:ILE:HG22	2.60	0.41
1:B:26:CYS:SG	1:B:458:ILE:HG22	2.61	0.41
1:A:118:THR:HA	1:A:119:PRO:HD3	1.75	0.41
1:A:73:PRO:C	1:A:75:ALA:H	2.24	0.41
1:B:299:ARG:NH1	1:B:299:ARG:HG2	2.27	0.41
1:B:321:TRP:O	1:B:325:VAL:HG23	2.20	0.41
1:A:497:ASP:O	1:A:497:ASP:OD1	2.39	0.41
1:C:481:CYS:HB2	1:C:482:PRO:HD3	2.02	0.41
1:A:104:VAL:HG13	1:A:362:LEU:HD11	2.03	0.41
1:B:201:ILE:H	1:B:201:ILE:HG12	1.62	0.41
1:B:317:THR:HG22	1:B:318:VAL:N	2.35	0.41
1:B:147:TRP:CE2	1:B:355:LEU:HB3	2.55	0.41
1:C:91:TRP:O	1:C:94:MET:HB2	2.20	0.41
1:C:501:ASN:N	1:C:501:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:362:LEU:HB3	1:C:363:TRP:H	1.72	0.41
1:B:431:ALA:CB	1:B:448:VAL:HG12	2.50	0.41
1:C:160:PHE:CE2	1:C:174:THR:HB	2.55	0.41
1:B:446:LEU:HD22	1:B:446:LEU:HA	1.87	0.41
1:A:351:MET:O	1:A:355:LEU:HD12	2.20	0.41
1:B:262:ARG:HH12	1:B:421:THR:HG21	1.86	0.41
1:C:431:ALA:HB2	1:C:449:ARG:HA	2.02	0.41
1:A:200:LEU:HG	1:A:204:MET:HE2	2.02	0.41
1:C:299:ARG:HA	1:C:299:ARG:HD2	1.70	0.41
1:B:187:LEU:N	1:B:187:LEU:HD23	2.35	0.41
1:C:469:LEU:O	1:C:472:ILE:HB	2.21	0.41
1:C:151:SER:HA	1:C:154:SER:HB2	2.02	0.41
1:B:247:VAL:HG12	1:B:446:LEU:HD21	2.02	0.40
1:B:66:TRP:HE3	1:B:67:PHE:CD2	2.39	0.40
1:A:225:ILE:H	1:A:225:ILE:HG13	1.64	0.40
1:A:431:ALA:CB	1:A:448:VAL:HG12	2.51	0.40
1:B:210:LEU:HD23	1:B:210:LEU:HA	1.87	0.40
1:C:457:GLY:O	1:C:461:ILE:HG13	2.21	0.40
1:A:292:MET:HE3	1:C:299:ARG:NH1	2.36	0.40
1:B:91:TRP:O	1:B:94:MET:HB2	2.21	0.40
1:C:266:SER:HB3	1:C:414:LEU:HD11	2.02	0.40
1:C:497:ASP:O	1:C:497:ASP:OD1	2.39	0.40
1:B:327:TYR:CD1	2:B:1504:NM2:H101	2.55	0.40
1:B:351:MET:HG3	1:B:352:VAL:N	2.36	0.40
1:C:373:LEU:CD1	1:C:397:THR:HA	2.52	0.40
1:B:69:LEU:HA	1:B:69:LEU:HD23	1.83	0.40
1:B:431:ALA:HB2	1:B:449:ARG:HA	2.01	0.40
1:B:199:ALA:HB3	1:B:483:LEU:HD21	2.04	0.40
1:C:200:LEU:HG	1:C:204:MET:HE2	2.04	0.40
1:C:457:GLY:O	1:C:461:ILE:CG1	2.70	0.40
1:C:142:TRP:CD2	1:C:363:TRP:CZ2	3.10	0.40
1:C:321:TRP:CE3	1:C:321:TRP:CA	3.05	0.40
1:C:294:LEU:HA	1:C:294:LEU:HD23	1.78	0.40
1:C:323:TRP:CD1	1:C:327:TYR:CE1	3.09	0.40
1:A:139:LEU:HD22	1:A:360:TRP:CE2	2.57	0.40
1:A:292:MET:CE	1:A:296:TYR:HE1	2.35	0.40
1:B:162:PHE:CG	1:B:340:ARG:HG3	2.57	0.40
1:B:293:LEU:O	1:B:297:LEU:HB2	2.22	0.40
1:A:312:PHE:HB3	1:A:313:PRO:CD	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	494/504 (98%)	423 (86%)	61 (12%)	10 (2%)	11	63
1	B	494/504 (98%)	419 (85%)	63 (13%)	12 (2%)	9	59
1	C	494/504 (98%)	421 (85%)	64 (13%)	9 (2%)	13	65
All	All	1482/1512 (98%)	1263 (85%)	188 (13%)	31 (2%)	11	62

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	LYS
1	A	321	TRP
1	B	40	ILE
1	B	165	LYS
1	C	40	ILE
1	C	165	LYS
1	A	40	ILE
1	A	282	ILE
1	A	320	TYR
1	A	362	LEU
1	B	62	MET
1	B	128	THR
1	B	362	LEU
1	B	467	GLY
1	C	362	LEU
1	A	62	MET
1	A	128	THR
1	A	467	GLY
1	B	282	ILE
1	B	309	LYS
1	C	62	MET
1	C	282	ILE
1	C	467	GLY
1	A	18	PRO
1	B	18	PRO

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Mol	Chain	Res	Type
1	C	18	PRO
1	B	472	ILE
1	C	128	THR
1	B	52	GLY
1	B	186	GLY
1	C	186	GLY

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	410/425 (96%)	373 (91%)	37 (9%)	14	55
1	B	410/425 (96%)	374 (91%)	36 (9%)	14	57
1	C	410/425 (96%)	375 (92%)	35 (8%)	15	58
All	All	1230/1275 (96%)	1122 (91%)	108 (9%)	14	57

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	CYS
1	A	78	ARG
1	A	85	GLU
1	A	104	VAL
1	A	109	SER
1	A	117	SER
1	A	118	THR
1	A	126	ASN
1	A	137	TYR
1	A	142	TRP
1	A	164	ARG
1	A	169	ILE
1	A	179	VAL
1	A	201	ILE
1	A	206	THR
1	A	223	PHE
1	A	252	GLN

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Mol	Chain	Res	Type
1	A	275	ILE
1	A	276	VAL
1	A	295	MET
1	A	299	ARG
1	A	319	PHE
1	A	321	TRP
1	A	331	MET
1	A	343	THR
1	A	370	THR
1	A	392	ARG
1	A	403	LEU
1	A	404	SER
1	A	417	ILE
1	A	427	SER
1	A	432	MET
1	A	433	SER
1	A	446	LEU
1	A	461	ILE
1	A	501	ASN
1	A	502	TRP
1	B	26	CYS
1	B	78	ARG
1	B	85	GLU
1	B	104	VAL
1	B	109	SER
1	B	117	SER
1	B	118	THR
1	B	126	ASN
1	B	137	TYR
1	B	164	ARG
1	B	169	ILE
1	B	179	VAL
1	B	201	ILE
1	B	206	THR
1	B	218	CYS
1	B	223	PHE
1	B	252	GLN
1	B	275	ILE
1	B	295	MET
1	B	299	ARG
1	B	319	PHE
1	B	321	TRP

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Mol	Chain	Res	Type
1	B	331	MET
1	B	343	THR
1	B	353	LEU
1	B	370	THR
1	B	392	ARG
1	B	404	SER
1	B	417	ILE
1	B	427	SER
1	B	432	MET
1	B	433	SER
1	B	446	LEU
1	B	461	ILE
1	B	501	ASN
1	B	502	TRP
1	C	26	CYS
1	C	74	TYR
1	C	78	ARG
1	C	85	GLU
1	C	104	VAL
1	C	109	SER
1	C	117	SER
1	C	118	THR
1	C	126	ASN
1	C	137	TYR
1	C	164	ARG
1	C	169	ILE
1	C	179	VAL
1	C	201	ILE
1	C	206	THR
1	C	223	PHE
1	C	252	GLN
1	C	275	ILE
1	C	295	MET
1	C	299	ARG
1	C	319	PHE
1	C	321	TRP
1	C	331	MET
1	C	343	THR
1	C	353	LEU
1	C	370	THR
1	C	392	ARG
1	C	404	SER

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Mol	Chain	Res	Type
1	C	417	ILE
1	C	432	MET
1	C	433	SER
1	C	446	LEU
1	C	461	ILE
1	C	501	ASN
1	C	502	TRP

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

Mol	Chain	Res	Type
1	A	41	ASN
1	A	141	HIS
1	A	252	GLN
1	A	330	GLN
1	A	487	ASN
1	B	41	ASN
1	B	141	HIS
1	B	252	GLN
1	B	330	GLN
1	B	487	ASN
1	C	41	ASN
1	C	141	HIS
1	C	252	GLN
1	C	330	GLN
1	C	487	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NM2	A	1504	-	9,9,9	0.93	0	12,12,12	0.81	0
2	NM2	A	1505	-	9,9,9	0.96	0	12,12,12	0.96	1 (8%)
2	NM2	B	1504	-	9,9,9	0.87	0	12,12,12	0.87	0
2	NM2	B	1505	-	9,9,9	0.88	0	12,12,12	0.87	0
2	NM2	C	1504	-	9,9,9	0.88	0	12,12,12	0.87	0
2	NM2	C	1505	-	9,9,9	0.88	0	12,12,12	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NM2	A	1504	-	-	0/7/7/7	0/0/0/0
2	NM2	A	1505	-	-	0/7/7/7	0/0/0/0
2	NM2	B	1504	-	-	0/7/7/7	0/0/0/0
2	NM2	B	1505	-	-	0/7/7/7	0/0/0/0
2	NM2	C	1504	-	-	0/7/7/7	0/0/0/0
2	NM2	C	1505	-	-	0/7/7/7	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1505	NM2	C3-C6-C5	-2.18	108.56	114.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	496/504 (98%)	-0.24	1 (0%) 93 80	86, 124, 188, 351	0
1	B	496/504 (98%)	-0.12	6 (1%) 75 42	91, 152, 236, 365	0
1	C	496/504 (98%)	0.00	17 (3%) 43 19	100, 177, 268, 359	0
All	All	1488/1512 (98%)	-0.12	24 (1%) 68 35	86, 149, 247, 365	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	THR	10.7
1	C	9	GLY	8.2
1	C	165	LYS	5.3
1	B	440	ASP	4.9
1	C	249	CYS	4.7
1	C	31	ARG	4.0
1	C	167	GLU	4.0
1	A	8	THR	3.6
1	C	437	GLU	3.4
1	C	503	LYS	3.2
1	B	441	GLY	3.2
1	C	447	LEU	3.1
1	C	438	VAL	2.9
1	C	80	GLY	2.7
1	C	10	ILE	2.7
1	C	181	GLU	2.7
1	C	445	PRO	2.6
1	B	500	GLN	2.4
1	B	435	CYS	2.4
1	C	435	CYS	2.3
1	B	81	GLU	2.3
1	C	248	ALA	2.2
1	B	181	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	225	ILE	2.1

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
2	NM2	C	1504	10/10	0.46	8.45	180,180,180,180	0
2	NM2	B	1505	10/10	0.36	4.94	213,213,213,213	0
2	NM2	C	1505	10/10	0.47	4.67	200,200,200,200	0
2	NM2	A	1505	10/10	0.28	3.30	168,168,168,168	0
2	NM2	B	1504	10/10	0.36	3.28	152,152,152,152	0
2	NM2	A	1504	10/10	0.20	0.03	127,127,127,127	0

6.5 Other polymers ⓘ

There are no such residues in this entry.