



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:56 AM GMT

PDB ID : 1JPW
Title : Crystal Structure of a Human Tcf-4 / beta-Catenin Complex
Authors : Poy, F.; Lepourcelet, M.; Shivdasani, R.A.; Eck, M.J.
Deposited on : 2001-08-03
Resolution : 2.50 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>

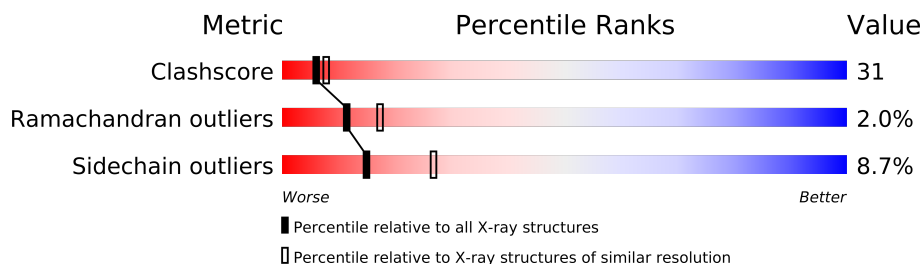
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : 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 2.50 Å.


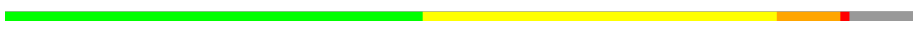




Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	540	
1	B	540	
1	C	540	
2	D	49	
2	E	49	
2	F	49	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12767 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 BETA-CATENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	0	0
			3803	2393	691	693	26			
1	B	502	Total	C	N	O	S	0	0	0
			3803	2393	691	693	26			
1	C	502	Total	C	N	O	S	0	0	0
			3803	2393	691	693	26			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	GLY	LEU	CONFLICT	UNP P35222
A	133	SER	LYS	CONFLICT	UNP P35222
B	132	GLY	LEU	CONFLICT	UNP P35222
B	133	SER	LYS	CONFLICT	UNP P35222
C	132	GLY	LEU	CONFLICT	UNP P35222
C	133	SER	LYS	CONFLICT	UNP P35222

- Molecule 2 is a protein called transcription factor 7-like 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	24	Total	C	N	O	0	0	0
			170	104	26	40			
2	E	24	Total	C	N	O	0	0	0
			170	104	26	40			
2	F	24	Total	C	N	O	0	0	0
			170	104	26	40			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	7	SER	GLY	CONFLICT	UNP Q9NQB0
E	7	SER	GLY	CONFLICT	UNP Q9NQB0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	7	SER	GLY	CONFLICT	UNP Q9NQB0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	290	Total 290	O 290	0	0
3	B	281	Total 281	O 281	0	0
3	C	236	Total 236	O 236	0	0
3	D	19	Total 19	O 19	0	0
3	E	12	Total 12	O 12	0	0
3	F	10	Total 10	O 10	0	0

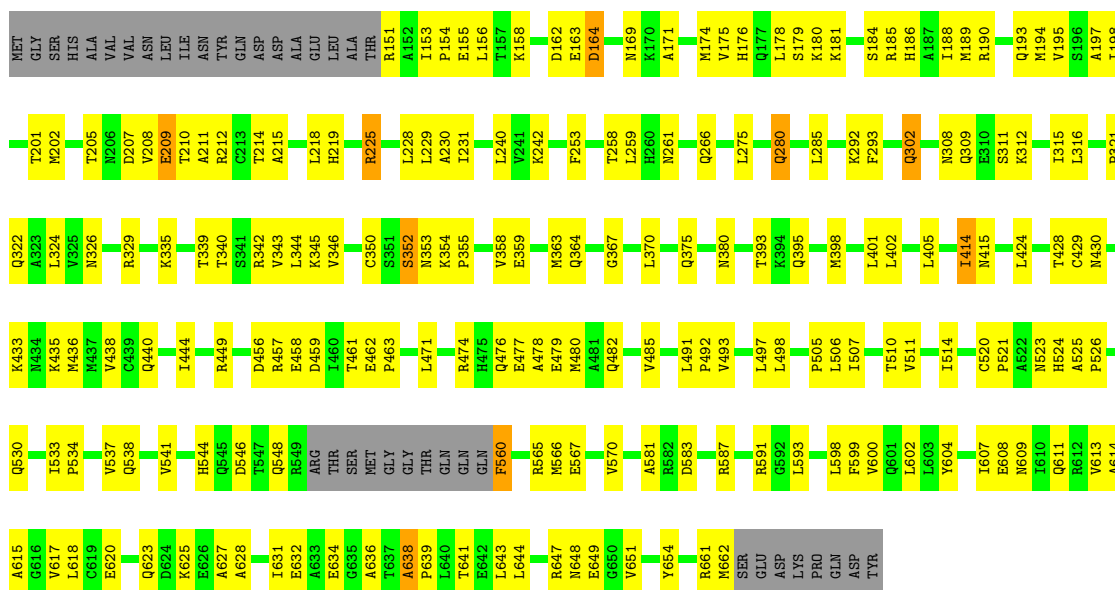
3 Residue-property plots

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.

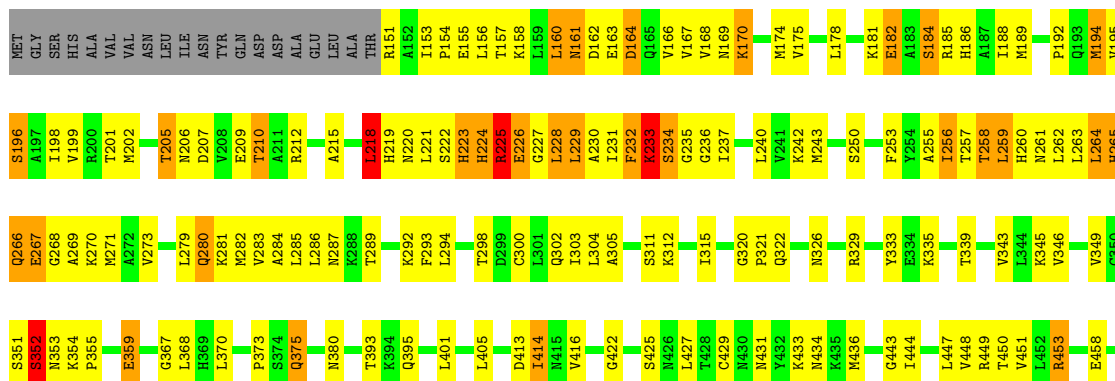
• Molecule 1: BETA-CATENIN

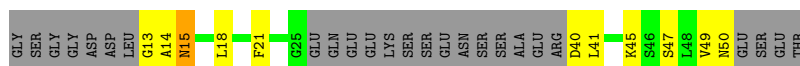
Chain A:



• Molecule 1: BETA-CATENIN

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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	376.53Å 92.65Å 49.25Å 90.00° 95.98° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	86.0 (25.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.304 , 0.390	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12767	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/3857	0.68	0/5238
1	B	0.36	0/3857	0.67	6/5238 (0.1%)
1	C	0.32	0/3857	0.63	4/5238 (0.1%)
2	D	0.41	0/169	0.57	0/226
2	E	0.38	0/169	0.56	0/226
2	F	0.41	0/169	0.57	0/226
All	All	0.37	0/12078	0.65	10/16392 (0.1%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ARG	CG-CD-NE	-10.66	89.42	111.80
1	B	225	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	B	225	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	C	225	ARG	N-CA-C	6.19	127.70	111.00
1	C	218	LEU	CA-CB-CG	6.03	129.16	115.30
1	B	225	ARG	N-CA-C	5.69	126.37	111.00
1	B	218	LEU	CA-CB-CG	5.38	127.67	115.30
1	B	226	GLU	N-CA-C	-5.37	96.52	111.00
1	C	226	GLU	N-CA-C	-5.29	96.70	111.00
1	C	228	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	225	ARG	Sidechain
1	B	560	PHE	Sidechain
1	C	560	PHE	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3803	0	3929	192	0
1	B	3803	0	3929	266	0
1	C	3803	0	3929	273	1
2	D	170	0	151	20	0
2	E	170	0	151	10	0
2	F	170	0	151	12	0
3	A	290	0	0	36	0
3	B	281	0	0	63	0
3	C	236	0	0	46	0
3	D	19	0	0	2	0
3	E	12	0	0	2	0
3	F	10	0	0	1	0
All	All	12767	0	12240	746	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 31.

All (746) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:225:ARG:HH21	1:C:225:ARG:CB	1.22	1.52
1:C:225:ARG:NH2	1:C:225:ARG:HB3	1.34	1.42
1:A:280:GLN:H	1:A:280:GLN:NE2	1.32	1.25
1:C:414:ILE:HD12	1:C:414:ILE:H	1.06	1.19
1:B:280:GLN:N	1:B:280:GLN:HE21	1.39	1.19
1:B:280:GLN:H	1:B:280:GLN:NE2	1.43	1.15

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:225:ARG:HG3	1:B:226:GLU:H	1.08	1.10
1:B:414:ILE:H	1:B:414:ILE:HD13	1.00	1.09
1:C:228:LEU:HD22	1:C:228:LEU:H	1.16	1.09
1:B:225:ARG:NH1	1:B:225:ARG:HG2	1.43	1.06
1:B:225:ARG:NH1	1:B:225:ARG:CG	2.20	1.05
1:B:225:ARG:HG3	1:B:226:GLU:N	1.67	1.04
1:B:225:ARG:CG	1:B:226:GLU:N	2.15	1.04
1:C:225:ARG:HH21	1:C:225:ARG:CG	1.70	1.03
1:B:225:ARG:HH11	1:B:225:ARG:HG2	0.96	1.02
1:B:474:ARG:HB3	1:B:474:ARG:HH11	1.26	0.98
1:A:280:GLN:N	1:A:280:GLN:HE21	1.61	0.97
1:A:280:GLN:H	1:A:280:GLN:HE21	0.99	0.96
1:C:225:ARG:C	1:C:225:ARG:HD2	1.84	0.96
1:B:202:MET:HE3	1:B:218:LEU:HD23	1.47	0.96
1:C:474:ARG:HB3	1:C:474:ARG:HH11	1.29	0.95
1:A:618:LEU:HD21	3:A:947:HOH:O	1.65	0.95
1:A:280:GLN:N	1:A:280:GLN:NE2	2.15	0.95
1:A:591:ARG:HD3	1:A:627:ALA:HB2	1.48	0.94
1:C:280:GLN:HE21	1:C:314:ILE:HG21	1.32	0.93
1:C:267:GLU:O	1:C:269:ALA:N	2.02	0.92
3:C:785:HOH:O	2:F:13:GLY:HA3	1.69	0.92
1:B:414:ILE:CD1	1:B:414:ILE:H	1.80	0.92
1:B:267:GLU:O	1:B:269:ALA:N	2.03	0.91
1:C:414:ILE:CD1	1:C:414:ILE:H	1.82	0.91
1:B:414:ILE:N	1:B:414:ILE:HD13	1.84	0.91
1:C:280:GLN:NE2	1:C:314:ILE:HG21	1.86	0.91
1:C:326:ASN:HD22	1:C:329:ARG:HH21	1.15	0.90
1:B:228:LEU:HD13	1:B:265:HIS:CD2	2.07	0.89
1:B:225:ARG:CG	1:B:226:GLU:H	1.78	0.89
1:A:253:PHE:HB3	3:D:73:HOH:O	1.72	0.88
1:C:228:LEU:HD12	1:C:265:HIS:CD2	2.08	0.88
1:C:228:LEU:CD2	1:C:228:LEU:H	1.86	0.88
1:C:225:ARG:HD2	1:C:226:GLU:N	1.88	0.87
1:A:154:PRO:O	1:A:158:LYS:HG3	1.74	0.87
1:C:618:LEU:HA	3:C:799:HOH:O	1.74	0.87
1:B:479:GLU:HG2	3:B:769:HOH:O	1.75	0.86
1:C:155:GLU:O	1:C:158:LYS:HG2	1.75	0.86
1:C:414:ILE:N	1:C:414:ILE:HD12	1.91	0.86
1:B:326:ASN:HD22	1:B:329:ARG:HH21	1.18	0.86
1:C:225:ARG:NH2	1:C:225:ARG:CB	2.07	0.86
1:B:538:GLN:HB3	3:B:936:HOH:O	1.74	0.85
1:B:236:GLY:O	1:B:240:LEU:HG	1.76	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:225:ARG:HB2	1:B:225:ARG:CZ	2.05	0.85
1:A:599:PHE:HB2	3:A:947:HOH:O	1.75	0.84
1:B:228:LEU:HD13	1:B:265:HIS:HD2	1.39	0.84
1:A:202:MET:HE1	1:A:218:LEU:HD21	1.60	0.84
1:C:225:ARG:HH21	1:C:225:ARG:HB3	0.68	0.83
1:B:185:ARG:HE	1:B:220:ASN:HB3	1.42	0.83
1:C:573:CYS:HB2	3:C:760:HOH:O	1.78	0.82
1:A:153:ILE:HB	1:A:154:PRO:HD3	1.61	0.82
1:C:471:LEU:HB2	3:C:788:HOH:O	1.80	0.81
1:C:620:GLU:O	1:C:623:GLN:HG3	1.79	0.81
1:A:326:ASN:HD22	1:A:329:ARG:HH21	1.27	0.80
1:C:185:ARG:HE	1:C:220:ASN:HB3	1.46	0.80
1:B:223:HIS:CD2	1:B:223:HIS:H	1.99	0.80
1:A:478:ALA:O	1:A:482:GLN:HG3	1.81	0.80
1:C:228:LEU:CD1	1:C:265:HIS:CD2	2.65	0.79
1:B:164:ASP:HB3	3:B:873:HOH:O	1.82	0.79
1:A:525:ALA:HB3	1:A:526:PRO:HD3	1.64	0.79
1:C:312:LYS:HE3	1:C:346:VAL:HG12	1.65	0.79
1:B:166:VAL:HB	3:B:873:HOH:O	1.84	0.78
1:C:354:LYS:HB2	1:C:355:PRO:HD3	1.65	0.78
1:B:326:ASN:HD22	1:B:329:ARG:NH2	1.82	0.77
1:B:198:ILE:HG22	3:B:803:HOH:O	1.84	0.77
1:C:225:ARG:CG	1:C:225:ARG:NH2	2.35	0.77
1:C:225:ARG:C	1:C:227:GLY:N	2.33	0.77
1:C:326:ASN:HD22	1:C:329:ARG:NH2	1.81	0.77
1:C:236:GLY:O	1:C:240:LEU:HG	1.84	0.76
1:A:292:LYS:HG2	2:D:44:VAL:HG13	1.67	0.76
1:B:312:LYS:HE3	1:B:346:VAL:HG12	1.67	0.76
1:B:186:HIS:HA	1:B:189:MET:HE3	1.67	0.76
1:C:351:SER:O	1:C:352:SER:HB2	1.85	0.76
1:A:261:ASN:ND2	2:D:45:LYS:HZ2	1.83	0.76
1:B:225:ARG:HB2	1:B:225:ARG:NH2	2.02	0.75
1:A:194:MET:O	1:A:194:MET:HE2	1.87	0.75
1:C:285:LEU:HD13	1:C:293:PHE:HZ	1.50	0.75
1:B:225:ARG:CD	1:B:226:GLU:N	2.50	0.75
1:A:188:ILE:HG23	1:A:194:MET:HG2	1.68	0.75
1:B:614:ALA:HB2	3:B:701:HOH:O	1.86	0.75
1:B:218:LEU:HD13	1:B:231:ILE:HG12	1.68	0.74
1:C:478:ALA:O	1:C:482:GLN:HG3	1.87	0.74
1:A:225:ARG:NE	1:A:225:ARG:HA	2.03	0.74
1:C:280:GLN:HB3	3:C:851:HOH:O	1.86	0.74
1:B:228:LEU:CD1	1:B:265:HIS:HD2	1.99	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:169:ASN:HB2	3:A:828:HOH:O	1.88	0.74
1:B:533:ILE:HB	1:B:534:PRO:HD3	1.70	0.74
1:B:225:ARG:CZ	1:B:225:ARG:CB	2.58	0.74
1:B:202:MET:CE	1:B:218:LEU:HD23	2.17	0.74
1:B:223:HIS:HD2	1:B:223:HIS:H	1.34	0.74
1:A:171:ALA:O	1:A:175:VAL:HG23	1.88	0.74
1:C:186:HIS:HA	1:C:189:MET:HE3	1.70	0.73
1:B:541:VAL:HB	3:B:797:HOH:O	1.87	0.73
1:B:167:VAL:HG23	3:B:873:HOH:O	1.89	0.73
1:B:474:ARG:HH11	1:B:474:ARG:CB	2.01	0.72
1:B:260:HIS:O	1:B:264:LEU:HD23	1.89	0.72
1:C:207:ASP:HB3	1:C:210:THR:OG1	1.90	0.72
1:B:354:LYS:HB2	1:B:355:PRO:HD3	1.71	0.72
1:C:474:ARG:HB3	1:C:474:ARG:NH1	2.05	0.72
1:B:237:ILE:HG13	3:B:715:HOH:O	1.89	0.71
1:A:202:MET:CE	1:A:215:ALA:HA	2.20	0.71
1:A:219:HIS:CE1	2:D:49:VAL:HG11	2.25	0.71
1:B:478:ALA:O	1:B:482:GLN:HG3	1.90	0.71
1:B:225:ARG:HH11	1:B:225:ARG:CG	1.86	0.71
1:A:312:LYS:HE3	1:A:346:VAL:HG12	1.73	0.71
1:B:491:LEU:HD22	1:B:527:LEU:HD21	1.72	0.71
1:C:218:LEU:HD12	1:C:218:LEU:O	1.89	0.71
1:B:546:ASP:OD2	1:B:566:MET:HG3	1.91	0.71
1:C:618:LEU:HD23	3:C:799:HOH:O	1.91	0.71
1:B:207:ASP:HB3	1:B:210:THR:OG1	1.90	0.70
1:C:218:LEU:HD13	1:C:231:ILE:HG12	1.73	0.70
1:B:525:ALA:HB3	1:B:526:PRO:HD3	1.72	0.70
1:B:292:LYS:HE2	2:E:47:SER:OG	1.91	0.70
1:C:347:LEU:HD13	3:C:847:HOH:O	1.90	0.70
1:B:545:GLN:HG3	3:B:674:HOH:O	1.91	0.70
1:C:375:GLN:NE2	1:C:375:GLN:HA	2.07	0.70
1:B:373:PRO:HA	3:B:773:HOH:O	1.93	0.69
1:B:240:LEU:HB3	3:B:874:HOH:O	1.93	0.69
1:B:153:ILE:HB	1:B:154:PRO:HD3	1.75	0.69
1:B:498:LEU:HD11	1:B:514:ILE:CD1	2.22	0.69
1:A:202:MET:HE2	1:A:215:ALA:HA	1.72	0.69
1:C:259:LEU:HD13	3:C:817:HOH:O	1.91	0.69
1:A:414:ILE:HD13	1:A:414:ILE:H	1.57	0.69
1:C:192:PRO:O	1:C:196:SER:HB2	1.93	0.69
1:C:153:ILE:HB	1:C:154:PRO:HD3	1.75	0.69
1:C:280:GLN:HE21	1:C:314:ILE:CG2	2.03	0.69
1:A:647:ARG:HB3	1:A:647:ARG:HH11	1.58	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:565:ARG:HG3	1:C:568:GLU:HG3	1.75	0.69
3:B:688:HOH:O	1:C:329:ARG:HD3	1.92	0.69
1:C:540:LEU:HD13	3:C:760:HOH:O	1.93	0.69
1:B:280:GLN:H	1:B:280:GLN:HE21	0.74	0.68
1:C:634:GLU:HB2	3:C:855:HOH:O	1.93	0.68
1:A:358:VAL:CG1	1:A:395:GLN:HG3	2.23	0.68
1:A:599:PHE:HA	1:A:602:LEU:HD12	1.75	0.68
1:C:448:VAL:HG13	3:C:708:HOH:O	1.93	0.68
1:C:546:ASP:OD2	1:C:566:MET:HG3	1.93	0.68
1:C:292:LYS:HE2	2:F:47:SER:OG	1.93	0.68
1:B:620:GLU:O	1:B:623:GLN:HG3	1.93	0.68
1:B:222:SER:O	1:B:228:LEU:CD2	2.42	0.68
1:A:261:ASN:ND2	2:D:45:LYS:NZ	2.42	0.68
1:B:497:LEU:HD22	1:B:506:LEU:HD21	1.76	0.68
1:B:598:LEU:HB2	3:B:728:HOH:O	1.93	0.67
1:C:286:LEU:HD23	3:C:885:HOH:O	1.93	0.67
1:C:225:ARG:O	1:C:226:GLU:C	2.33	0.67
1:B:561:VAL:HA	3:B:835:HOH:O	1.93	0.67
1:B:565:ARG:HG3	1:B:568:GLU:HG3	1.77	0.67
1:C:627:ALA:O	1:C:631:ILE:HG13	1.95	0.67
1:C:525:ALA:HB3	1:C:526:PRO:HD3	1.77	0.67
1:B:232:PHE:O	1:B:234:SER:N	2.27	0.66
1:C:498:LEU:HD11	1:C:514:ILE:CD1	2.25	0.66
1:C:632:GLU:HG3	3:C:677:HOH:O	1.95	0.66
1:A:179:SER:N	3:A:767:HOH:O	2.28	0.66
1:A:174:MET:O	1:A:178:LEU:HD13	1.96	0.66
1:B:351:SER:O	1:B:352:SER:HB2	1.94	0.66
1:A:449:ARG:HD3	3:A:901:HOH:O	1.95	0.66
1:C:202:MET:HE3	1:C:218:LEU:HD23	1.77	0.66
1:C:265:HIS:N	1:C:265:HIS:ND1	2.44	0.65
1:A:647:ARG:HB3	1:A:647:ARG:NH1	2.10	0.65
1:C:202:MET:CE	1:C:218:LEU:HD23	2.27	0.65
1:C:155:GLU:HA	1:C:158:LYS:HD2	1.78	0.65
1:A:261:ASN:HD21	2:D:45:LYS:NZ	1.93	0.65
1:A:218:LEU:HD11	1:A:240:LEU:HD21	1.77	0.65
1:A:479:GLU:HG3	1:A:480:MET:N	2.11	0.65
1:B:429:CYS:SG	2:E:18:LEU:HD23	2.37	0.65
1:C:570:VAL:HA	3:C:760:HOH:O	1.96	0.65
1:C:621:LEU:HD12	3:C:799:HOH:O	1.96	0.64
1:A:151:ARG:N	3:A:939:HOH:O	2.28	0.64
1:A:151:ARG:O	1:A:154:PRO:HD2	1.97	0.64
1:B:305:ALA:HA	3:B:941:HOH:O	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:225:ARG:C	1:B:227:GLY:N	2.46	0.64
1:B:156:LEU:HD13	1:B:175:VAL:HG22	1.80	0.64
1:C:228:LEU:HD22	1:C:228:LEU:N	1.99	0.64
1:A:188:ILE:HG23	1:A:194:MET:CG	2.28	0.64
1:C:491:LEU:HD22	1:C:527:LEU:HD21	1.80	0.64
1:A:280:GLN:CD	1:A:280:GLN:H	2.00	0.64
1:A:209:GLU:OE2	1:A:212:ARG:HD2	1.97	0.64
1:B:480:MET:HE2	3:B:846:HOH:O	1.96	0.64
1:B:627:ALA:O	1:B:631:ILE:HG13	1.97	0.64
1:C:223:HIS:CD2	1:C:223:HIS:H	2.15	0.64
1:C:281:LYS:HD2	3:C:768:HOH:O	1.97	0.64
1:A:326:ASN:HD22	1:A:329:ARG:NH2	1.93	0.63
1:C:439:CYS:HB2	3:C:761:HOH:O	1.97	0.63
1:B:483:ASN:ND2	1:B:486:ARG:HH12	1.96	0.63
1:A:537:VAL:O	1:A:541:VAL:HG23	1.98	0.63
1:C:643:LEU:HD11	3:C:902:HOH:O	1.98	0.63
1:B:226:GLU:O	1:B:230:ALA:N	2.28	0.63
1:B:265:HIS:N	1:B:265:HIS:ND1	2.46	0.63
1:A:614:ALA:O	1:A:617:VAL:HG12	1.97	0.63
1:B:285:LEU:HD13	1:B:293:PHE:HZ	1.62	0.63
1:C:185:ARG:HH11	1:C:185:ARG:HG2	1.64	0.63
1:B:182:GLU:HA	1:B:185:ARG:NH1	2.13	0.63
1:B:367:GLY:HA2	1:B:370:LEU:HG	1.79	0.62
1:B:182:GLU:HA	1:B:185:ARG:HH12	1.64	0.62
1:B:607:ILE:O	1:B:611:GLN:HG3	1.98	0.62
1:A:211:ALA:HB2	3:A:900:HOH:O	1.98	0.62
1:B:225:ARG:HD3	1:B:226:GLU:N	2.13	0.62
1:C:326:ASN:ND2	1:C:329:ARG:HH21	1.94	0.62
1:C:222:SER:O	1:C:228:LEU:HD13	1.99	0.62
1:C:614:ALA:HB1	3:C:721:HOH:O	2.00	0.62
1:C:367:GLY:HA2	1:C:370:LEU:HG	1.80	0.62
1:A:530:GLN:HG2	3:A:752:HOH:O	2.00	0.62
1:C:185:ARG:NE	1:C:220:ASN:HB3	2.15	0.62
1:C:228:LEU:CD1	1:C:265:HIS:HD2	2.12	0.61
1:A:207:ASP:HA	3:A:740:HOH:O	2.00	0.61
1:B:174:MET:HG2	3:B:859:HOH:O	1.99	0.61
1:A:285:LEU:HD13	1:A:293:PHE:HZ	1.66	0.61
1:C:598:LEU:HB2	3:C:769:HOH:O	1.99	0.61
1:B:240:LEU:HD13	1:B:258:THR:CG2	2.30	0.61
1:C:607:ILE:O	1:C:611:GLN:HG3	2.00	0.61
1:C:566:MET:O	1:C:570:VAL:HG23	2.00	0.61
1:B:289:THR:HB	3:B:820:HOH:O	1.99	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:ASN:HD21	2:D:45:LYS:HZ2	1.44	0.61
1:A:604:TYR:CZ	1:A:639:PRO:HB3	2.35	0.61
1:A:497:LEU:HD22	1:A:506:LEU:HD21	1.83	0.61
1:B:223:HIS:CD2	1:B:223:HIS:N	2.68	0.60
1:B:155:GLU:O	1:B:158:LYS:HG2	2.00	0.60
1:B:470:HIS:HD2	3:E:56:HOH:O	1.85	0.60
1:C:641:THR:HG21	3:C:803:HOH:O	2.02	0.60
1:B:163:GLU:HA	3:B:730:HOH:O	1.99	0.60
1:A:302:GLN:HB2	1:A:343:VAL:HG22	1.82	0.60
1:C:311:SER:O	1:C:315:ILE:HG13	2.00	0.60
1:A:180:LYS:HE3	3:A:747:HOH:O	2.00	0.60
1:C:228:LEU:CD2	1:C:228:LEU:N	2.59	0.60
1:C:483:ASN:ND2	1:C:486:ARG:HH12	2.00	0.60
1:B:281:LYS:HE2	3:B:821:HOH:O	2.01	0.60
2:D:13:GLY:O	2:D:14:ALA:HB3	2.02	0.60
1:A:476:GLN:HG3	3:A:702:HOH:O	2.00	0.59
1:B:591:ARG:HD3	3:B:759:HOH:O	2.00	0.59
1:C:631:ILE:HG22	1:C:636:ALA:HB3	1.83	0.59
1:A:604:TYR:OH	1:A:639:PRO:HD3	2.02	0.59
1:A:401:LEU:O	1:A:405:LEU:HG	2.02	0.59
1:A:433:LYS:HD3	3:A:918:HOH:O	2.02	0.59
1:C:621:LEU:HB2	3:C:799:HOH:O	2.03	0.59
1:C:156:LEU:HD13	1:C:175:VAL:HG22	1.84	0.59
1:A:643:LEU:HD22	1:A:651:VAL:HG11	1.84	0.59
1:B:218:LEU:CD1	1:B:231:ILE:HG12	2.31	0.59
1:B:284:ALA:O	1:B:287:ASN:ND2	2.36	0.59
1:C:447:LEU:O	1:C:451:VAL:HG23	2.03	0.59
1:A:607:ILE:O	1:A:611:GLN:HG3	2.03	0.59
1:C:339:THR:O	1:C:343:VAL:HG23	2.02	0.58
1:A:560:PHE:HB2	3:A:904:HOH:O	2.02	0.58
1:C:225:ARG:O	1:C:228:LEU:HD23	2.03	0.58
1:A:154:PRO:C	1:A:158:LYS:HZ2	2.07	0.58
1:B:449:ARG:HH11	1:B:449:ARG:HG2	1.67	0.58
1:B:375:GLN:NE2	1:B:375:GLN:HA	2.17	0.58
1:A:326:ASN:ND2	1:A:329:ARG:HH21	1.99	0.58
1:A:638:ALA:HB3	1:A:639:PRO:CD	2.34	0.58
1:A:219:HIS:HE1	2:D:49:VAL:HG11	1.66	0.58
1:C:202:MET:HE2	1:C:215:ALA:HA	1.84	0.58
1:B:566:MET:O	1:B:570:VAL:HG23	2.04	0.58
1:B:596:ILE:O	1:B:600:VAL:HG23	2.04	0.58
1:C:458:GLU:HG2	1:C:506:LEU:HD22	1.85	0.58
1:C:497:LEU:HD22	1:C:506:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:185:ARG:HH11	1:C:185:ARG:CG	2.17	0.58
1:B:240:LEU:HB3	1:B:259:LEU:CD1	2.33	0.58
1:A:202:MET:HB2	1:A:214:THR:HB	1.85	0.58
1:A:180:LYS:HB3	3:A:835:HOH:O	2.02	0.58
1:C:469:ARG:CZ	1:C:512:GLY:HA3	2.34	0.58
1:C:284:ALA:O	1:C:287:ASN:ND2	2.37	0.58
1:B:631:ILE:HG22	1:B:636:ALA:HB3	1.86	0.57
1:C:461:THR:O	1:C:465:ILE:HG13	2.04	0.57
1:B:447:LEU:O	1:B:451:VAL:HG23	2.04	0.57
1:B:242:LYS:HD3	1:B:243:MET:HE2	1.86	0.57
1:C:660:PHE:C	1:C:662:MET:H	2.06	0.57
1:A:533:ILE:HB	1:A:534:PRO:HD3	1.86	0.57
1:C:225:ARG:C	1:C:225:ARG:CD	2.60	0.57
1:C:493:VAL:HG11	3:C:708:HOH:O	2.03	0.57
1:B:458:GLU:HA	1:B:461:THR:OG1	2.05	0.57
1:C:596:ILE:O	1:C:600:VAL:HG23	2.05	0.57
1:A:620:GLU:O	1:A:623:GLN:HG2	2.04	0.57
1:A:345:LYS:NZ	2:D:25:GLY:HA3	2.20	0.57
1:B:218:LEU:HD12	1:B:218:LEU:O	2.04	0.57
1:C:242:LYS:HD3	1:C:243:MET:HE2	1.86	0.57
1:B:192:PRO:O	1:B:196:SER:HB2	2.04	0.56
1:B:490:GLY:O	1:B:494:VAL:HG23	2.05	0.56
1:C:232:PHE:O	1:C:234:SER:N	2.38	0.56
2:E:13:GLY:O	2:E:14:ALA:HB3	2.06	0.56
1:B:155:GLU:O	1:B:158:LYS:CG	2.53	0.56
1:A:476:GLN:HB3	3:A:821:HOH:O	2.04	0.56
1:A:566:MET:O	1:A:570:VAL:HG23	2.06	0.56
1:A:608:GLU:CD	1:A:648:ASN:HD22	2.09	0.56
1:B:458:GLU:HG2	1:B:506:LEU:HD22	1.86	0.56
1:C:257:THR:HG23	2:F:45:LYS:HD2	1.88	0.56
1:A:591:ARG:HD3	1:A:627:ALA:CB	2.28	0.56
1:C:240:LEU:HD13	1:C:258:THR:HG22	1.87	0.56
1:B:311:SER:O	1:B:315:ILE:HG13	2.06	0.56
1:B:638:ALA:HB3	1:B:639:PRO:CD	2.36	0.56
1:A:280:GLN:HB2	3:A:866:HOH:O	2.06	0.55
1:B:292:LYS:HG3	3:B:805:HOH:O	2.06	0.55
1:C:265:HIS:O	1:C:266:GLN:C	2.44	0.55
1:A:462:GLU:HB3	1:A:463:PRO:CD	2.37	0.55
1:B:631:ILE:HB	1:B:662:MET:HE2	1.88	0.55
1:A:225:ARG:O	1:A:229:LEU:HG	2.06	0.55
1:B:218:LEU:HD21	1:B:240:LEU:HD21	1.87	0.55
1:C:537:VAL:O	1:C:540:LEU:HB3	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:MET:O	1:B:198:ILE:HG13	2.05	0.55
1:B:660:PHE:C	1:B:662:MET:H	2.08	0.55
1:A:202:MET:O	1:A:205:THR:HG22	2.07	0.55
1:C:483:ASN:HD21	1:C:486:ARG:HH22	1.54	0.55
2:F:15:ASN:HB2	3:F:422:HOH:O	2.07	0.55
1:B:326:ASN:ND2	1:B:329:ARG:HH21	1.97	0.55
1:A:477:GLU:HG2	3:A:821:HOH:O	2.05	0.55
1:B:333:TYR:CE2	1:B:335:LYS:HB2	2.42	0.55
1:A:398:MET:O	1:A:402:LEU:HG	2.06	0.55
1:B:225:ARG:HD3	1:B:225:ARG:C	2.28	0.55
1:C:465:ILE:HD11	1:C:497:LEU:HD13	1.89	0.55
1:B:255:ALA:HA	3:B:874:HOH:O	2.07	0.54
1:A:567:GLU:H	1:A:567:GLU:CD	2.11	0.54
1:A:405:LEU:HB2	1:A:424:LEU:HD21	1.90	0.54
1:C:206:ASN:ND2	3:C:771:HOH:O	2.39	0.54
1:C:185:ARG:HD3	1:C:221:LEU:HD23	1.89	0.54
1:C:230:ALA:O	1:C:234:SER:OG	2.25	0.54
1:A:309:GLN:O	1:A:312:LYS:HB2	2.07	0.54
1:B:502:SER:HB3	1:B:506:LEU:HD23	1.88	0.54
1:B:634:GLU:HB2	3:B:760:HOH:O	2.07	0.54
1:A:491:LEU:HB2	1:A:492:PRO:HD3	1.89	0.54
1:A:354:LYS:HB2	1:A:355:PRO:CD	2.37	0.54
2:F:13:GLY:O	2:F:14:ALA:HB3	2.07	0.54
1:A:195:VAL:HG21	1:A:230:ALA:HB1	1.89	0.54
1:B:266:GLN:O	1:B:267:GLU:O	2.26	0.54
1:C:465:ILE:HD11	1:C:497:LEU:CD1	2.37	0.54
1:B:339:THR:O	1:B:343:VAL:HG23	2.08	0.54
1:C:535:ARG:NH2	1:C:539:LEU:HD21	2.22	0.54
1:C:449:ARG:HG2	1:C:449:ARG:HH11	1.72	0.54
1:A:641:THR:O	1:A:644:LEU:HB2	2.07	0.54
1:C:636:ALA:O	1:C:640:LEU:HG	2.08	0.53
1:B:259:LEU:HD12	3:B:874:HOH:O	2.09	0.53
1:C:596:ILE:N	1:C:597:PRO:HD2	2.22	0.53
1:C:611:GLN:HA	3:C:806:HOH:O	2.08	0.53
1:B:483:ASN:HD21	1:B:486:ARG:HH22	1.56	0.53
1:C:602:LEU:HB2	3:C:721:HOH:O	2.08	0.53
1:B:312:LYS:N	3:B:941:HOH:O	2.41	0.53
1:C:223:HIS:CD2	1:C:223:HIS:N	2.76	0.53
1:B:602:LEU:HD13	3:B:701:HOH:O	2.08	0.53
1:B:170:LYS:O	1:B:174:MET:HG3	2.09	0.53
1:C:225:ARG:O	1:C:227:GLY:N	2.41	0.53
1:B:225:ARG:HD3	1:B:226:GLU:CA	2.39	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:308:ASN:O	1:A:312:LYS:HG3	2.09	0.53
1:B:162:ASP:OD1	1:B:163:GLU:N	2.36	0.53
1:B:292:LYS:NZ	3:B:822:HOH:O	2.41	0.53
1:B:643:LEU:HD22	1:B:651:VAL:HG11	1.91	0.53
1:A:316:LEU:HD22	1:A:353:ASN:CG	2.29	0.53
1:C:490:GLY:O	1:C:494:VAL:HG23	2.09	0.53
1:B:240:LEU:HD12	3:B:715:HOH:O	2.08	0.53
1:A:364:GLN:HG2	3:A:790:HOH:O	2.09	0.53
1:C:228:LEU:HD11	1:C:265:HIS:CD2	2.42	0.52
1:C:255:ALA:HB1	3:C:817:HOH:O	2.08	0.52
1:B:483:ASN:HD22	1:B:486:ARG:HH12	1.57	0.52
1:B:469:ARG:CZ	1:B:512:GLY:HA3	2.39	0.52
1:B:219:HIS:CE1	2:E:49:VAL:HG11	2.44	0.52
1:B:265:HIS:O	1:B:266:GLN:C	2.48	0.52
1:C:333:TYR:CE2	1:C:335:LYS:HB2	2.44	0.52
1:C:195:VAL:O	1:C:199:VAL:HG23	2.09	0.52
1:C:266:GLN:NE2	1:C:267:GLU:HG2	2.24	0.52
1:C:219:HIS:HA	1:C:258:THR:OG1	2.09	0.52
1:C:643:LEU:HD22	1:C:651:VAL:HG11	1.92	0.52
1:A:565:ARG:HD3	3:A:895:HOH:O	2.09	0.52
1:A:316:LEU:HD22	1:A:353:ASN:OD1	2.10	0.52
1:C:347:LEU:HA	3:C:870:HOH:O	2.10	0.52
1:C:240:LEU:HB3	1:C:259:LEU:HD11	1.90	0.52
1:C:483:ASN:HD22	1:C:486:ARG:HH12	1.58	0.52
1:A:474:ARG:HD2	2:D:15:ASN:OD1	2.09	0.52
1:C:202:MET:SD	1:C:243:MET:HG3	2.50	0.52
1:C:565:ARG:HB2	3:C:901:HOH:O	2.09	0.52
1:C:157:THR:O	1:C:161:ASN:ND2	2.43	0.52
1:A:510:THR:O	1:A:514:ILE:HG13	2.09	0.52
1:C:185:ARG:CD	1:C:221:LEU:HD23	2.40	0.52
1:B:279:LEU:HB2	1:B:280:GLN:NE2	2.25	0.52
1:C:355:PRO:O	1:C:359:GLU:HB2	2.10	0.52
1:B:544:HIS:HB3	3:B:674:HOH:O	2.10	0.52
1:B:284:ALA:HB1	3:B:704:HOH:O	2.10	0.52
1:A:474:ARG:NH1	2:D:15:ASN:HB3	2.24	0.52
1:C:261:ASN:O	1:C:265:HIS:CE1	2.62	0.51
1:C:602:LEU:HD12	3:C:721:HOH:O	2.09	0.51
1:A:181:LYS:HA	3:A:705:HOH:O	2.10	0.51
1:B:641:THR:O	1:B:644:LEU:HB2	2.10	0.51
1:C:285:LEU:HD13	1:C:293:PHE:CZ	2.38	0.51
1:A:225:ARG:HE	1:A:225:ARG:HA	1.76	0.51
1:B:230:ALA:O	1:B:234:SER:OG	2.27	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:232:PHE:HA	3:B:944:HOH:O	2.09	0.51
1:A:194:MET:O	1:A:198:ILE:HG13	2.10	0.51
1:B:465:ILE:HD11	1:B:497:LEU:CD1	2.40	0.51
1:C:209:GLU:OE1	1:C:209:GLU:HA	2.10	0.51
1:B:596:ILE:N	1:B:597:PRO:CD	2.73	0.51
1:B:229:LEU:O	1:B:233:LYS:HG3	2.10	0.51
1:A:598:LEU:HD11	3:A:731:HOH:O	2.09	0.51
1:B:636:ALA:O	1:B:640:LEU:HG	2.11	0.51
1:A:599:PHE:O	1:A:602:LEU:HB2	2.11	0.51
1:B:393:THR:HG21	2:E:18:LEU:HD21	1.93	0.51
1:A:345:LYS:HZ3	2:D:25:GLY:HA3	1.75	0.51
1:C:541:VAL:HB	3:C:704:HOH:O	2.10	0.51
1:B:225:ARG:CD	1:B:225:ARG:C	2.78	0.51
1:C:658:VAL:O	1:C:662:MET:HB2	2.11	0.51
1:B:283:VAL:HA	1:B:286:LEU:HG	1.93	0.51
1:C:225:ARG:C	1:C:227:GLY:H	2.13	0.51
1:A:316:LEU:HD13	1:A:353:ASN:OD1	2.11	0.51
1:C:240:LEU:HD13	1:C:258:THR:CG2	2.40	0.51
1:C:229:LEU:O	1:C:233:LYS:HG3	2.12	0.50
1:B:242:LYS:HD3	1:B:243:MET:CE	2.42	0.50
1:A:169:ASN:CG	1:A:210:THR:HG1	2.14	0.50
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.76	0.50
1:C:631:ILE:HB	1:C:662:MET:HE2	1.93	0.50
1:C:266:GLN:O	1:C:267:GLU:O	2.29	0.50
1:A:188:ILE:CD1	3:A:767:HOH:O	2.58	0.50
1:C:520:CYS:O	1:C:523:ASN:HB2	2.11	0.50
2:F:49:VAL:HG23	2:F:50:ASN:N	2.27	0.50
1:B:491:LEU:HD22	1:B:527:LEU:CD2	2.42	0.50
1:C:641:THR:O	1:C:644:LEU:HB2	2.12	0.50
1:C:318:SER:HA	3:C:746:HOH:O	2.12	0.50
2:D:49:VAL:HG23	2:D:50:ASN:N	2.27	0.50
1:B:535:ARG:NH2	1:B:539:LEU:HD21	2.27	0.50
1:C:638:ALA:HB3	1:C:639:PRO:CD	2.41	0.50
1:C:225:ARG:HG3	1:C:225:ARG:NH2	2.25	0.50
1:C:225:ARG:O	1:C:228:LEU:CD2	2.60	0.50
1:B:537:VAL:O	1:B:540:LEU:HB3	2.12	0.50
1:C:240:LEU:HB3	1:C:259:LEU:CD1	2.42	0.50
1:A:643:LEU:HD22	1:A:651:VAL:CG1	2.42	0.50
1:C:256:ILE:HG22	1:C:257:THR:N	2.26	0.50
1:B:253:PHE:N	1:B:253:PHE:CD2	2.79	0.50
1:A:477:GLU:OE1	1:A:480:MET:HB2	2.12	0.49
1:A:625:LYS:O	1:A:628:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:647:ARG:HB3	1:B:647:ARG:NH1	2.27	0.49
1:A:600:VAL:HG23	3:A:947:HOH:O	2.10	0.49
1:C:660:PHE:O	1:C:662:MET:N	2.46	0.49
1:A:565:ARG:HB3	1:A:567:GLU:OE1	2.12	0.49
1:C:535:ARG:CZ	1:C:539:LEU:HD21	2.42	0.49
1:C:194:MET:O	1:C:198:ILE:HG13	2.12	0.49
1:B:256:ILE:CG2	1:B:257:THR:N	2.75	0.49
1:B:212:ARG:HD3	3:B:931:HOH:O	2.13	0.49
1:B:312:LYS:HG3	3:B:941:HOH:O	2.12	0.49
1:C:498:LEU:HD11	1:C:514:ILE:HD11	1.94	0.49
1:A:631:ILE:CG2	1:A:662:MET:HE1	2.42	0.49
1:C:265:HIS:O	1:C:266:GLN:O	2.29	0.49
1:B:548:GLN:NE2	3:B:929:HOH:O	2.46	0.49
1:C:533:ILE:HB	1:C:534:PRO:CD	2.42	0.49
1:A:393:THR:HG21	2:D:18:LEU:HD21	1.94	0.49
1:C:226:GLU:O	1:C:230:ALA:N	2.32	0.49
1:C:375:GLN:NE2	1:C:375:GLN:CA	2.75	0.49
1:B:624:ASP:HA	3:B:868:HOH:O	2.11	0.49
1:C:294:LEU:O	1:C:298:THR:HG23	2.13	0.49
1:B:222:SER:O	1:B:228:LEU:HD21	2.11	0.49
1:B:351:SER:O	1:B:352:SER:CB	2.61	0.49
2:E:49:VAL:HG23	2:E:50:ASN:N	2.27	0.49
1:B:488:HIS:HE1	3:B:782:HOH:O	1.94	0.49
1:A:240:LEU:HB2	1:A:259:LEU:HD21	1.95	0.49
1:C:507:ILE:O	1:C:511:VAL:HG23	2.13	0.49
1:C:640:LEU:HD11	1:C:658:VAL:CG1	2.43	0.49
1:C:346:VAL:O	1:C:349:VAL:HG22	2.12	0.48
1:C:458:GLU:HA	1:C:461:THR:OG1	2.13	0.48
1:B:414:ILE:CD1	1:B:414:ILE:N	2.56	0.48
1:A:354:LYS:CB	1:A:355:PRO:CD	2.91	0.48
1:A:415:ASN:HA	3:A:917:HOH:O	2.13	0.48
1:B:240:LEU:HB3	1:B:259:LEU:HD11	1.95	0.48
1:C:351:SER:O	1:C:352:SER:CB	2.57	0.48
1:A:474:ARG:NH2	3:A:940:HOH:O	2.45	0.48
1:A:544:HIS:CD2	1:A:598:LEU:HD11	2.49	0.48
1:A:218:LEU:HD13	1:A:258:THR:HG21	1.95	0.48
1:C:320:GLY:N	1:C:321:PRO:CD	2.77	0.48
1:A:324:LEU:HD22	1:A:340:THR:HG23	1.96	0.48
1:C:189:MET:HE1	1:C:224:HIS:CD2	2.49	0.48
1:B:545:GLN:HG2	3:B:913:HOH:O	2.13	0.48
1:C:438:VAL:HG12	1:C:443:GLY:HA3	1.96	0.48
1:C:489:TYR:HA	3:C:678:HOH:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:225:ARG:HD2	1:C:226:GLU:CA	2.43	0.48
1:A:498:LEU:HD11	1:A:514:ILE:CD1	2.43	0.48
1:A:617:VAL:HG13	1:A:618:LEU:N	2.28	0.48
1:C:350:CYS:HB3	3:C:870:HOH:O	2.14	0.48
1:B:595:THR:HA	3:B:693:HOH:O	2.13	0.48
1:A:428:THR:O	1:A:435:LYS:HE2	2.13	0.48
1:B:256:ILE:HG22	1:B:257:THR:N	2.29	0.48
3:B:863:HOH:O	1:C:289:THR:HG21	2.14	0.48
1:A:339:THR:HA	3:A:958:HOH:O	2.13	0.48
1:C:521:PRO:HA	1:C:524:HIS:CE1	2.49	0.48
1:A:609:ASN:O	1:A:613:VAL:HG22	2.14	0.48
1:A:438:VAL:HG11	1:A:471:LEU:HD11	1.96	0.48
1:A:634:GLU:O	1:A:634:GLU:HG3	2.13	0.48
1:C:226:GLU:HA	1:C:226:GLU:OE1	2.14	0.47
1:C:622:ALA:O	1:C:628:ALA:HB2	2.14	0.47
1:C:189:MET:CE	1:C:224:HIS:CD2	2.97	0.47
1:C:640:LEU:HD22	1:C:655:ALA:HA	1.95	0.47
1:B:461:THR:O	1:B:465:ILE:HG13	2.14	0.47
1:B:658:VAL:O	1:B:662:MET:HB2	2.14	0.47
1:B:467:ALA:O	1:B:471:LEU:HG	2.14	0.47
1:C:414:ILE:CD1	1:C:414:ILE:N	2.60	0.47
1:A:367:GLY:HA2	1:A:370:LEU:HG	1.95	0.47
1:A:311:SER:O	1:A:315:ILE:HG13	2.14	0.47
1:C:228:LEU:HD11	1:C:265:HIS:HD2	1.78	0.47
1:B:449:ARG:NH1	1:B:449:ARG:HG2	2.29	0.47
1:A:225:ARG:HE	1:A:228:LEU:HD12	1.79	0.47
1:C:502:SER:HB3	1:C:506:LEU:HD23	1.96	0.47
1:B:535:ARG:CZ	1:B:539:LEU:HD21	2.45	0.47
1:A:186:HIS:HA	1:A:189:MET:HE2	1.96	0.47
1:B:240:LEU:HD13	1:B:258:THR:HG22	1.96	0.47
1:A:429:CYS:SG	2:D:18:LEU:HD23	2.55	0.47
1:B:209:GLU:OE1	1:B:209:GLU:HA	2.13	0.47
1:C:224:HIS:O	1:C:228:LEU:HD22	2.15	0.47
1:B:618:LEU:HD22	1:B:631:ILE:HD13	1.95	0.47
1:B:622:ALA:O	1:B:628:ALA:HB2	2.15	0.47
1:B:520:CYS:O	1:B:523:ASN:HB2	2.15	0.47
1:B:265:HIS:O	1:B:266:GLN:O	2.33	0.47
1:B:257:THR:HG23	2:E:45:LYS:HD2	1.97	0.47
1:C:658:VAL:HG12	1:C:662:MET:HE3	1.97	0.47
1:A:202:MET:CE	1:A:218:LEU:HD21	2.37	0.47
1:C:525:ALA:HB3	3:C:744:HOH:O	2.15	0.47
1:C:533:ILE:HB	1:C:534:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:261:ASN:O	1:B:265:HIS:CE1	2.68	0.47
1:C:165:GLN:HB3	3:C:835:HOH:O	2.15	0.47
1:B:303:ILE:HG23	3:B:903:HOH:O	2.14	0.47
1:B:465:ILE:HD11	1:B:497:LEU:HD13	1.97	0.46
1:B:640:LEU:HD22	1:B:655:ALA:HA	1.96	0.46
1:B:444:ILE:O	1:B:448:VAL:HG23	2.14	0.46
1:B:660:PHE:O	1:B:662:MET:N	2.48	0.46
1:B:355:PRO:O	1:B:359:GLU:HB2	2.15	0.46
1:B:218:LEU:HD11	1:B:231:ILE:CG2	2.45	0.46
1:A:178:LEU:O	1:A:184:SER:HB2	2.16	0.46
1:A:350:CYS:SG	1:A:353:ASN:ND2	2.89	0.46
1:C:335:LYS:HE2	2:F:40:ASP:CG	2.36	0.46
1:B:229:LEU:O	1:B:232:PHE:HB3	2.15	0.46
1:C:283:VAL:HA	1:C:286:LEU:HG	1.97	0.46
1:B:640:LEU:HD11	1:B:658:VAL:CG1	2.46	0.46
1:B:517:LEU:HB3	1:B:523:ASN:HD22	1.80	0.46
1:A:485:VAL:HG12	1:A:485:VAL:O	2.15	0.46
1:A:436:MET:HE3	3:A:843:HOH:O	2.16	0.46
1:B:240:LEU:CB	1:B:259:LEU:HD11	2.46	0.46
1:C:281:LYS:HD3	3:C:719:HOH:O	2.15	0.46
1:B:422:GLY:O	1:B:425:SER:HB3	2.16	0.46
1:B:225:ARG:CD	1:B:226:GLU:CA	2.93	0.46
1:C:660:PHE:C	1:C:662:MET:N	2.69	0.46
1:C:256:ILE:CG2	1:C:257:THR:N	2.77	0.46
1:B:181:LYS:HA	3:B:684:HOH:O	2.15	0.46
1:B:507:ILE:O	1:B:511:VAL:HG23	2.15	0.46
1:C:618:LEU:HD22	1:C:631:ILE:HD13	1.96	0.46
1:C:263:LEU:HD21	1:C:273:VAL:HG21	1.98	0.46
1:B:474:ARG:HB2	3:B:720:HOH:O	2.16	0.46
1:B:311:SER:HB2	3:B:941:HOH:O	2.15	0.46
1:B:273:VAL:HG11	1:B:304:LEU:HD11	1.96	0.46
1:B:202:MET:HE2	1:B:215:ALA:HA	1.97	0.46
1:B:599:PHE:O	1:B:602:LEU:HB2	2.16	0.46
1:C:161:ASN:H	1:C:161:ASN:ND2	2.13	0.46
1:C:419:CYS:O	1:C:423:ILE:HG13	2.16	0.46
1:C:162:ASP:OD1	1:C:163:GLU:N	2.39	0.46
1:B:255:ALA:CA	3:B:874:HOH:O	2.63	0.45
1:C:448:VAL:CG1	3:C:708:HOH:O	2.59	0.45
1:C:402:LEU:O	1:C:406:VAL:HG23	2.15	0.45
1:B:498:LEU:HD11	1:B:514:ILE:HD11	1.95	0.45
1:A:620:GLU:OE1	1:A:620:GLU:HA	2.15	0.45
2:E:13:GLY:N	3:E:66:HOH:O	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:638:ALA:HB3	1:B:639:PRO:HD3	1.99	0.45
1:C:239:ALA:HB2	3:C:682:HOH:O	2.15	0.45
1:C:170:LYS:O	1:C:174:MET:HG3	2.17	0.45
1:B:206:ASN:HB2	3:B:783:HOH:O	2.15	0.45
1:C:345:LYS:HD3	1:C:380:ASN:HD22	1.80	0.45
1:C:185:ARG:HD2	1:C:220:ASN:O	2.16	0.45
1:A:617:VAL:CG1	1:A:618:LEU:N	2.78	0.45
1:A:345:LYS:HD3	1:A:380:ASN:HD22	1.81	0.45
1:C:413:ASP:HB3	1:C:416:VAL:HG23	1.99	0.45
1:B:431:ASN:OD1	1:B:433:LYS:HB2	2.16	0.45
1:B:294:LEU:O	1:B:298:THR:HG23	2.17	0.45
1:C:335:LYS:HE2	2:F:40:ASP:OD1	2.16	0.45
1:A:316:LEU:CD1	1:A:321:PRO:HG2	2.46	0.45
1:C:269:ALA:O	1:C:273:VAL:HG23	2.17	0.45
1:C:467:ALA:O	1:C:471:LEU:HG	2.17	0.45
1:C:240:LEU:CB	1:C:259:LEU:HD11	2.47	0.45
1:C:517:LEU:HB3	1:C:523:ASN:HD22	1.80	0.45
1:B:283:VAL:HG12	3:B:768:HOH:O	2.16	0.45
1:C:638:ALA:N	1:C:639:PRO:HD2	2.31	0.45
1:B:600:VAL:HG13	1:B:636:ALA:HB2	1.98	0.45
1:B:157:THR:O	1:B:161:ASN:ND2	2.50	0.45
1:B:195:VAL:O	1:B:199:VAL:HG23	2.17	0.45
1:C:444:ILE:O	1:C:448:VAL:HG23	2.16	0.45
1:C:253:PHE:N	1:C:253:PHE:CD2	2.83	0.45
1:C:228:LEU:HD12	1:C:265:HIS:NE2	2.32	0.45
1:B:266:GLN:HA	3:B:697:HOH:O	2.17	0.45
1:B:266:GLN:NE2	1:B:267:GLU:HG2	2.32	0.45
1:B:660:PHE:C	1:B:662:MET:N	2.70	0.45
1:C:178:LEU:O	1:C:184:SER:HB3	2.17	0.45
1:B:221:LEU:O	1:B:227:GLY:HA3	2.17	0.45
1:B:224:HIS:O	1:B:227:GLY:HA3	2.17	0.45
1:B:161:ASN:ND2	1:B:161:ASN:H	2.15	0.45
1:C:229:LEU:O	1:C:232:PHE:HB3	2.17	0.44
1:A:479:GLU:HA	1:A:482:GLN:OE1	2.17	0.44
1:C:219:HIS:CE1	2:F:49:VAL:HG11	2.52	0.44
1:A:156:LEU:HD13	1:A:175:VAL:HG22	1.98	0.44
1:A:363:MET:HB2	3:A:683:HOH:O	2.17	0.44
2:D:41:LEU:O	2:D:45:LYS:HG3	2.16	0.44
1:C:449:ARG:HG2	1:C:449:ARG:NH1	2.32	0.44
1:B:320:GLY:N	1:B:321:PRO:CD	2.80	0.44
1:B:280:GLN:N	1:B:280:GLN:NE2	2.21	0.44
1:A:201:THR:O	1:A:205:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:242:LYS:HD3	1:C:243:MET:CE	2.47	0.44
2:D:13:GLY:O	2:D:14:ALA:CB	2.65	0.44
1:C:431:ASN:HB3	1:C:434:ASN:HB2	2.00	0.44
1:A:242:LYS:HE2	3:A:801:HOH:O	2.16	0.44
1:B:240:LEU:HB3	1:B:259:LEU:HD12	1.99	0.44
1:B:160:LEU:O	1:B:168:VAL:HG13	2.18	0.44
1:A:583:ASP:O	1:A:587:ARG:HG3	2.17	0.44
1:C:607:ILE:HD12	1:C:610:ILE:HD12	1.99	0.44
1:B:185:ARG:HD3	1:B:220:ASN:O	2.18	0.44
1:A:474:ARG:CD	2:D:15:ASN:OD1	2.65	0.44
1:C:600:VAL:HG13	1:C:636:ALA:HB2	1.98	0.44
1:B:263:LEU:HD21	1:B:273:VAL:HG21	2.00	0.44
1:B:521:PRO:HA	1:B:524:HIS:CE1	2.53	0.44
1:A:414:ILE:H	1:A:414:ILE:CD1	2.21	0.44
1:C:252:LEU:HD12	3:C:709:HOH:O	2.18	0.44
1:B:271:MET:HB2	3:B:808:HOH:O	2.18	0.44
1:C:429:CYS:SG	2:F:18:LEU:HD23	2.58	0.44
1:B:346:VAL:O	1:B:349:VAL:HG22	2.18	0.43
1:A:188:ILE:HD11	3:A:767:HOH:O	2.18	0.43
1:C:431:ASN:OD1	1:C:433:LYS:HB2	2.18	0.43
1:A:174:MET:CE	3:A:781:HOH:O	2.65	0.43
1:A:449:ARG:HG2	1:A:449:ARG:HH11	1.83	0.43
1:B:638:ALA:N	1:B:639:PRO:HD2	2.33	0.43
1:B:206:ASN:ND2	3:B:783:HOH:O	2.50	0.43
1:A:507:ILE:O	1:A:511:VAL:HG23	2.18	0.43
1:A:153:ILE:HB	1:A:154:PRO:CD	2.41	0.43
1:C:611:GLN:O	1:C:614:ALA:HB3	2.18	0.43
1:B:607:ILE:HD12	1:B:610:ILE:HD12	1.99	0.43
1:C:469:ARG:NE	1:C:512:GLY:HA3	2.34	0.43
1:A:521:PRO:HA	1:A:524:HIS:CE1	2.53	0.43
1:C:312:LYS:HD3	3:C:870:HOH:O	2.17	0.43
1:C:386:ARG:HD2	2:F:21:PHE:CD2	2.53	0.43
1:B:228:LEU:CD1	1:B:265:HIS:CD2	2.83	0.43
1:A:405:LEU:CB	1:A:424:LEU:HD21	2.48	0.43
1:A:458:GLU:HA	1:A:461:THR:OG1	2.18	0.43
1:B:345:LYS:HD3	1:B:380:ASN:HD22	1.84	0.43
1:A:210:THR:O	1:A:214:THR:HG23	2.19	0.43
1:A:202:MET:HE3	1:A:215:ALA:HA	2.00	0.43
1:B:156:LEU:HD13	1:B:175:VAL:CG2	2.47	0.43
1:B:235:GLY:HA3	3:B:726:HOH:O	2.18	0.43
1:C:495:VAL:O	1:C:498:LEU:HB2	2.19	0.43
1:C:401:LEU:O	1:C:405:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:THR:O	1:B:205:THR:HG22	2.17	0.43
1:B:271:MET:HG3	3:B:788:HOH:O	2.19	0.43
1:A:581:ALA:O	1:A:587:ARG:NH1	2.49	0.43
1:B:481:ALA:O	1:B:485:VAL:HG23	2.19	0.43
1:C:282:MET:SD	1:C:300:CYS:HB3	2.59	0.43
1:A:202:MET:HB2	1:A:214:THR:CB	2.48	0.42
2:E:41:LEU:O	2:E:45:LYS:HG3	2.19	0.42
1:C:499:HIS:ND1	1:C:499:HIS:N	2.67	0.42
1:C:221:LEU:O	1:C:227:GLY:HA3	2.19	0.42
1:C:165:GLN:NE2	3:C:903:HOH:O	2.51	0.42
1:B:178:LEU:O	1:B:184:SER:HB3	2.19	0.42
1:C:201:THR:O	1:C:205:THR:HG22	2.18	0.42
1:B:225:ARG:HG3	1:B:226:GLU:CA	2.46	0.42
1:B:262:LEU:CD1	3:B:715:HOH:O	2.68	0.42
1:C:342:ARG:O	1:C:346:VAL:HG23	2.19	0.42
2:F:41:LEU:O	2:F:45:LYS:HG3	2.18	0.42
1:B:629:GLU:CD	3:B:710:HOH:O	2.57	0.42
1:A:155:GLU:O	1:A:158:LYS:HB2	2.20	0.42
1:A:179:SER:O	1:A:185:ARG:NH2	2.52	0.42
1:B:151:ARG:O	1:B:154:PRO:HD2	2.19	0.42
1:A:649:GLU:CB	3:A:688:HOH:O	2.67	0.42
1:A:176:HIS:CG	1:A:176:HIS:O	2.72	0.42
1:A:358:VAL:HG13	1:A:395:GLN:HG3	1.99	0.42
1:C:521:PRO:C	1:C:523:ASN:H	2.22	0.42
1:B:155:GLU:HA	1:B:158:LYS:HD2	2.01	0.42
1:A:631:ILE:HG22	1:A:636:ALA:CB	2.49	0.42
1:A:600:VAL:HG21	1:A:634:GLU:HG2	2.00	0.42
1:A:350:CYS:HA	3:A:718:HOH:O	2.20	0.42
1:C:160:LEU:O	1:C:168:VAL:HG13	2.19	0.42
1:A:231:ILE:O	1:A:231:ILE:HG22	2.19	0.42
1:C:490:GLY:O	1:C:493:VAL:HG12	2.20	0.42
1:A:643:LEU:HA	1:A:643:LEU:HD23	1.76	0.42
1:A:538:GLN:OE1	1:A:538:GLN:HA	2.18	0.42
1:B:401:LEU:O	1:B:405:LEU:HG	2.18	0.42
1:C:447:LEU:HA	1:C:450:THR:OG1	2.20	0.42
1:B:489:TYR:N	1:B:489:TYR:CD1	2.88	0.42
1:A:375:GLN:HA	1:A:375:GLN:NE2	2.35	0.42
1:B:202:MET:SD	1:B:243:MET:HG3	2.60	0.42
1:A:523:ASN:C	1:A:526:PRO:HD2	2.40	0.42
1:C:525:ALA:N	1:C:526:PRO:CD	2.83	0.42
1:A:546:ASP:C	1:A:548:GLN:H	2.23	0.42
1:B:632:GLU:HG3	3:B:708:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:615:ALA:HB1	1:A:654:TYR:HB3	2.02	0.42
1:A:162:ASP:OD1	1:A:163:GLU:N	2.53	0.42
1:C:523:ASN:C	1:C:526:PRO:HD2	2.40	0.41
1:C:162:ASP:CG	1:C:163:GLU:H	2.22	0.41
1:B:443:GLY:O	1:B:444:ILE:C	2.58	0.41
1:A:444:ILE:HG23	1:A:485:VAL:HG22	2.01	0.41
1:A:193:GLN:O	1:A:197:ALA:HB2	2.19	0.41
1:B:413:ASP:HB3	1:B:416:VAL:HG23	2.01	0.41
1:C:273:VAL:HG11	1:C:304:LEU:HD11	2.02	0.41
1:C:542:ARG:NH2	1:C:546:ASP:OD1	2.53	0.41
1:C:156:LEU:HD13	1:C:175:VAL:CG2	2.48	0.41
1:A:474:ARG:CZ	2:D:15:ASN:CB	2.99	0.41
1:A:477:GLU:OE1	1:A:480:MET:SD	2.78	0.41
1:A:162:ASP:OD1	1:A:164:ASP:N	2.51	0.41
1:C:442:GLY:HA2	3:C:733:HOH:O	2.20	0.41
1:C:268:GLY:O	1:C:272:ALA:HB2	2.21	0.41
1:A:479:GLU:HG3	1:A:480:MET:H	1.83	0.41
1:B:162:ASP:CG	1:B:163:GLU:H	2.23	0.41
1:A:342:ARG:HB2	3:A:958:HOH:O	2.19	0.41
1:A:520:CYS:HA	1:A:521:PRO:HD2	1.92	0.41
1:C:647:ARG:NH1	1:C:647:ARG:HB3	2.36	0.41
1:B:232:PHE:C	1:B:234:SER:H	2.22	0.41
1:A:229:LEU:HD23	1:A:266:GLN:OE1	2.19	0.41
1:B:462:GLU:HB3	1:B:463:PRO:CD	2.50	0.41
1:B:282:MET:SD	1:B:300:CYS:HB3	2.60	0.41
1:B:202:MET:CE	1:B:215:ALA:HA	2.51	0.41
1:A:155:GLU:HA	1:A:158:LYS:HZ2	1.85	0.41
1:C:347:LEU:O	1:C:353:ASN:HB3	2.21	0.41
1:C:491:LEU:HB2	1:C:492:PRO:HD3	2.02	0.41
1:B:163:GLU:HB2	3:B:758:HOH:O	2.20	0.41
1:C:246:SER:HA	1:C:247:PRO:HD3	1.96	0.41
1:C:595:THR:HG1	1:C:599:PHE:HE2	1.65	0.41
1:C:599:PHE:O	1:C:602:LEU:HB2	2.20	0.41
1:C:202:MET:HE1	1:C:218:LEU:HD23	2.00	0.41
2:D:25:GLY:HA2	3:D:64:HOH:O	2.21	0.41
1:C:427:LEU:O	1:C:434:ASN:ND2	2.54	0.41
1:B:453:ARG:HD3	3:B:709:HOH:O	2.21	0.41
1:C:462:GLU:HB3	1:C:463:PRO:CD	2.51	0.41
1:B:592:GLY:HA3	3:B:845:HOH:O	2.20	0.41
1:A:335:LYS:NZ	3:A:864:HOH:O	2.52	0.41
1:B:595:THR:HG1	1:B:599:PHE:HE2	1.66	0.41
1:C:491:LEU:HD22	1:C:527:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:ALA:N	3:A:900:HOH:O	2.53	0.41
1:B:163:GLU:HB2	3:B:790:HOH:O	2.21	0.41
1:B:413:ASP:HB3	1:B:416:VAL:CG2	2.51	0.41
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.89	0.41
1:C:261:ASN:O	1:C:265:HIS:ND1	2.54	0.40
1:A:638:ALA:HB3	1:A:639:PRO:HD3	2.03	0.40
1:B:427:LEU:O	1:B:434:ASN:ND2	2.55	0.40
1:B:499:HIS:N	1:B:499:HIS:ND1	2.68	0.40
1:B:594:ASN:ND2	3:B:784:HOH:O	2.54	0.40
1:C:614:ALA:CB	3:C:721:HOH:O	2.61	0.40
1:C:658:VAL:HG12	1:C:662:MET:CE	2.51	0.40
1:A:493:VAL:O	1:A:497:LEU:HG	2.20	0.40
2:E:13:GLY:O	2:E:14:ALA:CB	2.70	0.40
1:C:317:ALA:HB1	3:C:754:HOH:O	2.21	0.40
1:C:596:ILE:N	1:C:597:PRO:CD	2.82	0.40
1:B:270:LYS:HB2	3:B:696:HOH:O	2.22	0.40
1:C:225:ARG:HA	1:C:228:LEU:CD2	2.52	0.40
1:C:281:LYS:HE3	3:C:699:HOH:O	2.21	0.40
1:B:647:ARG:HB3	1:B:647:ARG:HH11	1.85	0.40
1:B:431:ASN:HB3	1:B:434:ASN:HB2	2.03	0.40
1:B:262:LEU:HD11	3:B:715:HOH:O	2.21	0.40
1:A:599:PHE:CG	1:A:617:VAL:HG11	2.57	0.40
1:C:599:PHE:O	1:C:600:VAL:C	2.60	0.40
1:C:316:LEU:HD13	1:C:353:ASN:OD1	2.22	0.40
1:B:285:LEU:C	1:B:287:ASN:H	2.24	0.40
1:C:413:ASP:HB3	1:C:416:VAL:CG2	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:C:223:HIS:O	1:C:225:ARG:NH2[2_655]	2.02	0.18

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	498/540 (92%)	469 (94%)	22 (4%)	7 (1%)	16	27
1	B	498/540 (92%)	449 (90%)	39 (8%)	10 (2%)	11	17
1	C	498/540 (92%)	449 (90%)	39 (8%)	10 (2%)	11	17
2	D	20/49 (41%)	17 (85%)	1 (5%)	2 (10%)	1	1
2	E	20/49 (41%)	17 (85%)	2 (10%)	1 (5%)	3	3
2	F	20/49 (41%)	17 (85%)	2 (10%)	1 (5%)	3	3
All	All	1554/1767 (88%)	1418 (91%)	105 (7%)	31 (2%)	11	17

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	15	ASN
1	B	225	ARG
1	B	232	PHE
1	B	233	LYS
1	B	266	GLN
1	B	267	GLU
1	B	268	GLY
1	C	232	PHE
1	C	233	LYS
1	C	266	GLN
1	C	267	GLU
1	C	268	GLY
1	A	164	ASP
1	A	352	SER
1	B	205	THR
1	B	352	SER
1	B	476	GLN
1	B	661	ARG
2	E	15	ASN
1	C	205	THR
1	C	352	SER
1	C	476	GLN
1	C	661	ARG
2	F	15	ASN
1	A	430	ASN
2	D	14	ALA
1	A	208	VAL
1	A	209	GLU
1	A	457	ARG
1	C	603	LEU

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Mol	Chain	Res	Type
1	A	638	ALA

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	409/448 (91%)	393 (96%)	16 (4%)	43	70
1	B	409/448 (91%)	361 (88%)	48 (12%)	8	14
1	C	409/448 (91%)	361 (88%)	48 (12%)	8	14
2	D	18/41 (44%)	18 (100%)	0	100	100
2	E	18/41 (44%)	18 (100%)	0	100	100
2	F	18/41 (44%)	18 (100%)	0	100	100
All	All	1281/1467 (87%)	1169 (91%)	112 (9%)	15	27

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	ARG
1	A	275	LEU
1	A	280	GLN
1	A	302	GLN
1	A	322	GLN
1	A	352	SER
1	A	359	GLU
1	A	414	ILE
1	A	440	GLN
1	A	456	ASP
1	A	459	ASP
1	A	505	PRO
1	A	560	PHE
1	A	593	LEU
1	A	632	GLU
1	A	661	ARG
1	B	160	LEU
1	B	161	ASN

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Mol	Chain	Res	Type
1	B	164	ASP
1	B	169	ASN
1	B	170	LYS
1	B	182	GLU
1	B	184	SER
1	B	188	ILE
1	B	194	MET
1	B	196	SER
1	B	210	THR
1	B	218	LEU
1	B	223	HIS
1	B	224	HIS
1	B	225	ARG
1	B	228	LEU
1	B	229	LEU
1	B	233	LYS
1	B	234	SER
1	B	250	SER
1	B	256	ILE
1	B	258	THR
1	B	259	LEU
1	B	264	LEU
1	B	265	HIS
1	B	280	GLN
1	B	302	GLN
1	B	322	GLN
1	B	352	SER
1	B	353	ASN
1	B	359	GLU
1	B	368	LEU
1	B	375	GLN
1	B	395	GLN
1	B	414	ILE
1	B	436	MET
1	B	450	THR
1	B	453	ARG
1	B	465	ILE
1	B	474	ARG
1	B	479	GLU
1	B	499	HIS
1	B	546	ASP
1	B	560	PHE

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Mol	Chain	Res	Type
1	B	567	GLU
1	B	605	SER
1	B	624	ASP
1	B	632	GLU
1	C	160	LEU
1	C	161	ASN
1	C	164	ASP
1	C	169	ASN
1	C	170	LYS
1	C	184	SER
1	C	185	ARG
1	C	188	ILE
1	C	190	ARG
1	C	194	MET
1	C	196	SER
1	C	218	LEU
1	C	223	HIS
1	C	224	HIS
1	C	225	ARG
1	C	226	GLU
1	C	228	LEU
1	C	233	LYS
1	C	234	SER
1	C	250	SER
1	C	256	ILE
1	C	258	THR
1	C	259	LEU
1	C	264	LEU
1	C	265	HIS
1	C	271	MET
1	C	302	GLN
1	C	322	GLN
1	C	352	SER
1	C	353	ASN
1	C	359	GLU
1	C	368	LEU
1	C	375	GLN
1	C	395	GLN
1	C	413	ASP
1	C	414	ILE
1	C	436	MET
1	C	450	THR

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Mol	Chain	Res	Type
1	C	453	ARG
1	C	465	ILE
1	C	474	ARG
1	C	479	GLU
1	C	499	HIS
1	C	546	ASP
1	C	560	PHE
1	C	605	SER
1	C	624	ASP
1	C	632	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	HIS
1	A	261	ASN
1	A	280	GLN
1	A	302	GLN
1	A	322	GLN
1	A	326	ASN
1	A	375	GLN
1	A	380	ASN
1	A	476	GLN
1	A	544	HIS
1	A	548	GLN
1	A	594	ASN
1	A	648	ASN
1	B	161	ASN
1	B	219	HIS
1	B	223	HIS
1	B	224	HIS
1	B	280	GLN
1	B	302	GLN
1	B	322	GLN
1	B	326	ASN
1	B	375	GLN
1	B	380	ASN
1	B	470	HIS
1	B	483	ASN
1	B	488	HIS
1	B	544	HIS
1	B	594	ASN

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Mol	Chain	Res	Type
1	C	161	ASN
1	C	219	HIS
1	C	223	HIS
1	C	224	HIS
1	C	302	GLN
1	C	322	GLN
1	C	326	ASN
1	C	375	GLN
1	C	380	ASN
1	C	434	ASN
1	C	470	HIS
1	C	483	ASN
1	C	578	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.