



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YOV
Title : Insights into the Ubiquitin Transfer Cascade from the refined structure of the activating enzyme for NEDD8
Authors : Walden, H.; Podgorski, M.S.; Schulman, B.A.
Deposited on : 2005-01-28
Resolution : 2.60 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

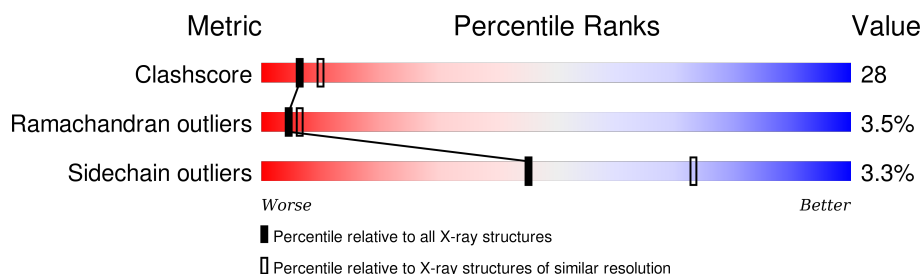
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	537	
1	C	537	
2	B	444	
2	D	444	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14604 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Amyloid protein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4208	2662	718	812	16			
1	C	526	Total	C	N	O	S	0	0	0
			4183	2644	714	809	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	CLONING ARTIFACT	UNP Q13564
A	-1	LYS	-	CLONING ARTIFACT	UNP Q13564
A	0	LEU	-	CLONING ARTIFACT	UNP Q13564
C	-2	MET	-	CLONING ARTIFACT	UNP Q13564
C	-1	LYS	-	CLONING ARTIFACT	UNP Q13564
C	0	LEU	-	CLONING ARTIFACT	UNP Q13564

- Molecule 2 is a protein called Ubiquitin-activating enzyme E1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	397	Total	C	N	O	S	0	0	0
			3089	1975	523	573	18			
2	D	382	Total	C	N	O	S	0	0	0
			2972	1901	502	551	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	CLONING ARTIFACT	UNP Q8TBC4
B	0	SER	-	CLONING ARTIFACT	UNP Q8TBC4
D	-1	GLY	-	CLONING ARTIFACT	UNP Q8TBC4
D	0	SER	-	CLONING ARTIFACT	UNP Q8TBC4

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

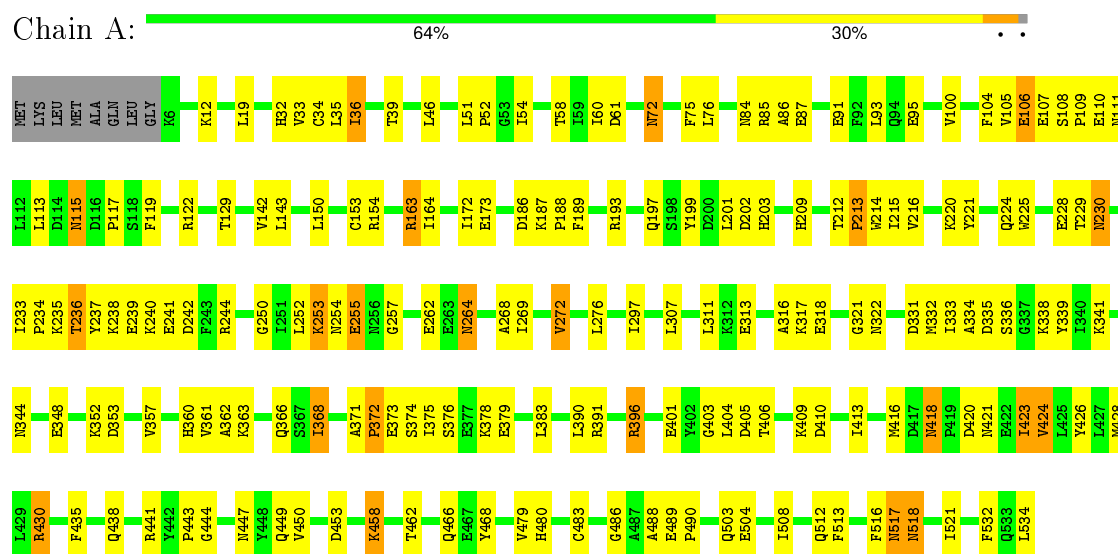
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total 53	O 53	0	0
4	B	62	Total 62	O 62	0	0
4	C	19	Total 19	O 19	0	0
4	D	16	Total 16	O 16	0	0

3 Residue-property plots

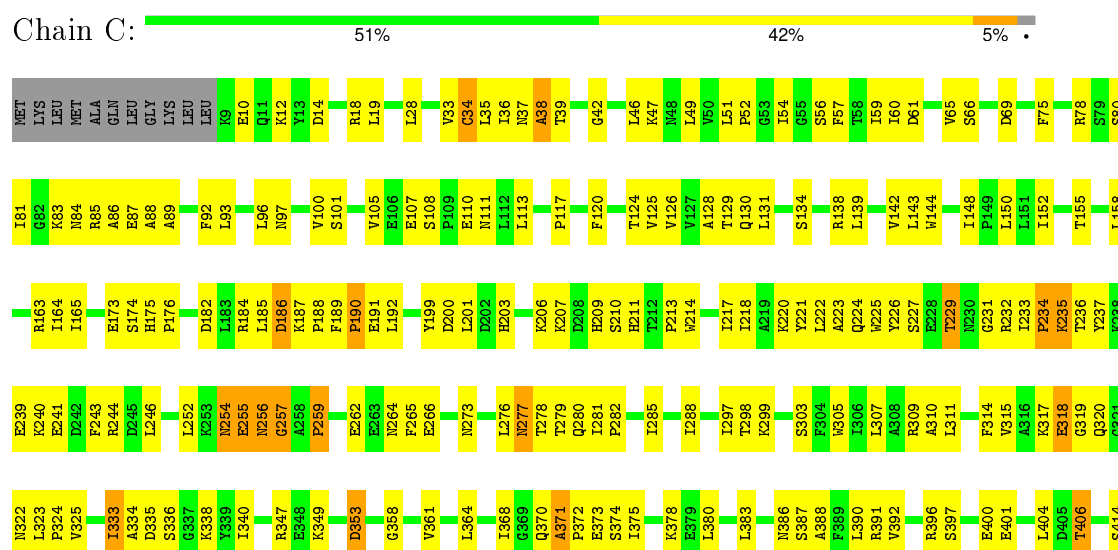
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

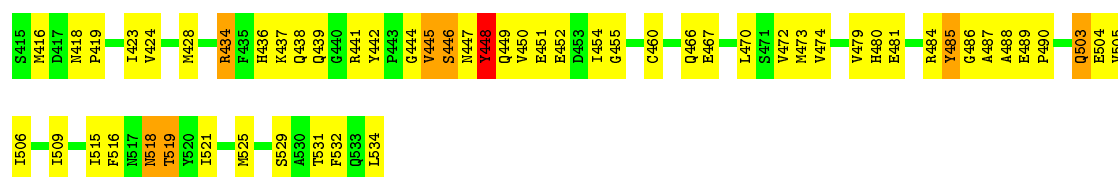
Note EDS was not executed.

• Molecule 1: Amyloid protein-binding protein 1



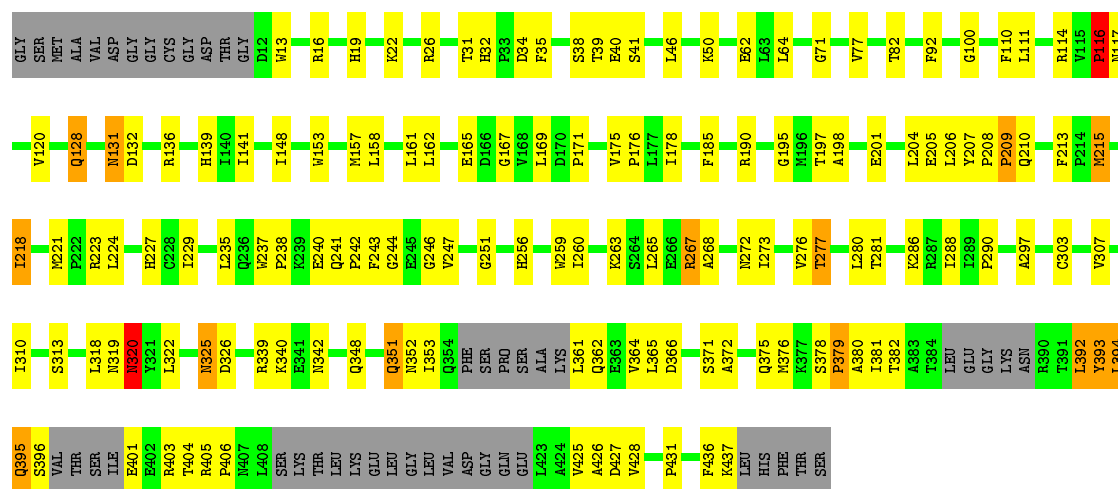
• Molecule 1: Amyloid protein-binding protein 1





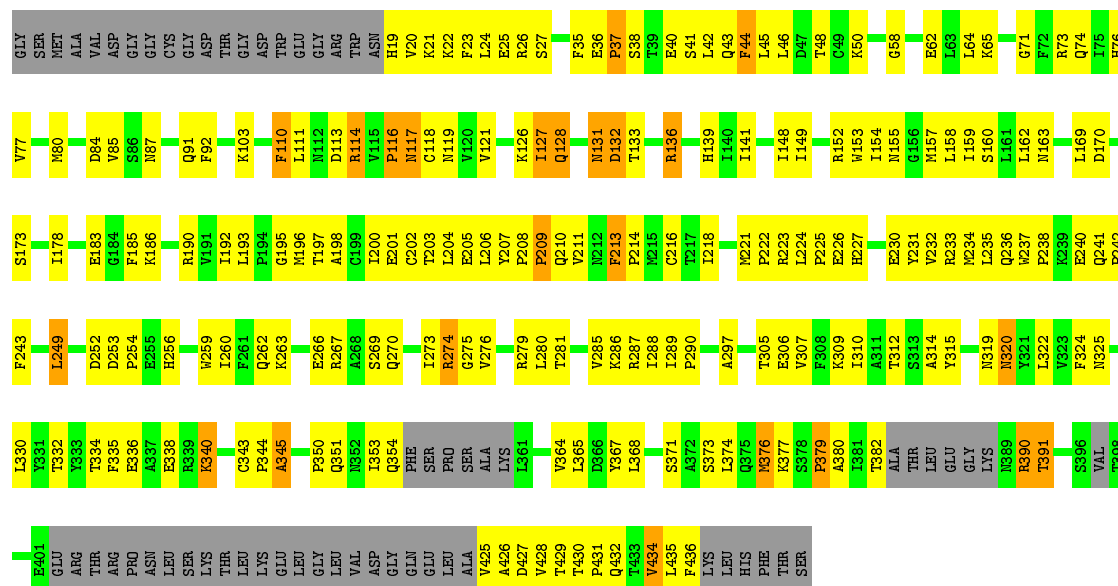
• Molecule 2: Ubiquitin-activating enzyme E1C

Chain B: 57% 29% 11%



• Molecule 2: Ubiquitin-activating enzyme E1C

Chain D: 42% 39% 5% 14%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.40 Å 123.60 Å 198.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14604	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/4290	0.63	0/5802
1	C	0.33	0/4265	0.59	1/5769 (0.0%)
2	B	0.45	0/3158	0.70	2/4300 (0.0%)
2	D	0.35	0/3036	0.61	1/4130 (0.0%)
All	All	0.39	0/14749	0.63	4/20001 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	320	ASN	N-CA-C	7.71	131.82	111.00
2	B	319	ASN	C-N-CA	6.24	137.29	121.70
2	D	37	PRO	N-CA-C	-5.93	96.68	112.10
1	C	519	THR	N-CA-C	5.16	124.92	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4208	0	4157	171	0
1	C	4183	0	4122	281	0
2	B	3089	0	3012	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2972	0	2914	240	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	53	0	0	7	0
4	B	62	0	0	9	0
4	C	19	0	0	6	0
4	D	16	0	0	1	0
All	All	14604	0	14205	789	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (789) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:ASN:ND2	1:C:519:THR:H	1.49	1.10
2:D:380:ALA:HB3	2:D:426:ALA:HB3	1.34	1.06
1:C:298:THR:HG22	1:C:299:LYS:H	1.20	1.04
2:D:27:SER:HB3	2:D:37:PRO:HG3	1.38	1.01
1:A:489:GLU:H	2:B:19:HIS:HD2	1.10	1.00
1:A:534:LEU:HD22	4:A:535:HOH:O	1.60	0.99
2:D:376:MET:HB3	2:D:427:ASP:OD2	1.65	0.96
2:B:50:LYS:H	2:B:139:HIS:HD2	1.13	0.95
2:B:32:HIS:HD2	2:B:34:ASP:H	1.12	0.95
2:D:74:GLN:HE22	2:D:119:ASN:HD22	1.00	0.94
2:D:204:LEU:HG	2:D:208:PRO:HG2	1.45	0.94
2:B:32:HIS:CD2	2:B:34:ASP:H	1.85	0.94
2:B:277:THR:HG22	2:B:280:LEU:H	1.33	0.94
1:A:244:ARG:HG2	1:A:272:VAL:HG11	1.50	0.93
1:C:347:ARG:HH12	2:D:274:ARG:HG3	1.31	0.92
2:B:128:GLN:HE21	2:B:128:GLN:H	1.16	0.92
2:D:153:TRP:CE2	2:D:431:PRO:HG3	2.05	0.92
2:B:207:TYR:C	2:B:209:PRO:HD2	1.92	0.90
2:D:50:LYS:H	2:D:139:HIS:HD2	1.19	0.90
2:D:434:VAL:HG12	2:D:435:LEU:H	1.35	0.90
1:C:518:ASN:ND2	1:C:519:THR:N	2.20	0.90
1:C:518:ASN:HD22	1:C:519:THR:N	1.69	0.90
2:B:204:LEU:O	2:B:208:PRO:HD2	1.72	0.89
2:D:35:PHE:CD1	2:D:314:ALA:HA	2.07	0.89
1:A:489:GLU:H	2:B:19:HIS:CD2	1.91	0.89
2:B:111:LEU:HD23	2:B:120:VAL:HG21	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:O	1:A:272:VAL:HG12	1.73	0.87
2:D:183:GLU:HG2	2:D:289:ILE:HD11	1.57	0.87
1:A:518:ASN:ND2	1:A:534:LEU:H	1.73	0.86
1:A:235:LYS:HB3	1:A:238:LYS:HE3	1.58	0.86
1:A:61:ASP:OD2	1:A:85:ARG:HD2	1.75	0.86
2:D:207:TYR:HB2	2:D:208:PRO:HD3	1.58	0.85
1:C:279:THR:HG22	1:C:322:ASN:HD22	1.38	0.85
1:C:84:ASN:HB3	1:C:87:GLU:HG2	1.59	0.84
1:A:396:ARG:HH12	1:A:534:LEU:C	1.81	0.83
1:C:130:GLN:HE22	1:C:155:THR:H	1.24	0.83
1:C:288:ILE:HG23	1:C:305:TRP:HZ3	1.42	0.83
1:C:234:PRO:HA	1:C:240:LYS:HZ3	1.42	0.82
1:C:59:ILE:HG22	1:C:60:ILE:H	1.45	0.82
1:A:201:LEU:HD12	1:A:220:LYS:HG2	1.61	0.82
2:B:50:LYS:H	2:B:139:HIS:CD2	1.98	0.82
2:B:31:THR:CG2	2:B:35:PHE:HB3	2.11	0.81
2:D:224:LEU:H	2:D:227:HIS:CD2	1.97	0.81
2:D:225:PRO:HB3	2:D:276:VAL:HG22	1.60	0.81
1:C:244:ARG:HH22	1:C:273:ASN:HD22	1.25	0.81
2:D:35:PHE:CE1	2:D:314:ALA:HA	2.16	0.81
2:B:141:ILE:HD12	2:B:158:LEU:HD21	1.63	0.80
2:D:377:LYS:N	2:D:427:ASP:OD2	2.13	0.80
1:C:438:GLN:HG2	1:C:439:GLN:HE22	1.45	0.80
2:D:430:THR:HG21	2:D:432:GLN:HG2	1.64	0.80
1:C:518:ASN:HD22	1:C:519:THR:H	1.27	0.80
1:C:186:ASP:O	1:C:188:PRO:HD3	1.83	0.79
2:D:427:ASP:OD1	2:D:428:VAL:N	2.16	0.79
2:D:27:SER:CB	2:D:37:PRO:HG3	2.13	0.78
1:A:396:ARG:HH11	1:A:396:ARG:HG3	1.48	0.78
1:A:518:ASN:HD22	1:A:534:LEU:H	1.30	0.77
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.65	0.77
1:C:298:THR:HG22	1:C:299:LYS:N	1.99	0.77
1:C:438:GLN:HG2	1:C:439:GLN:NE2	1.98	0.77
2:D:430:THR:CG2	2:D:432:GLN:HG2	2.15	0.76
2:D:224:LEU:H	2:D:227:HIS:HD2	1.32	0.76
2:D:190:ARG:HB2	2:D:320:ASN:O	1.86	0.76
2:B:403:ARG:O	2:B:406:PRO:HG2	1.84	0.76
1:A:517:ASN:O	1:A:517:ASN:ND2	2.18	0.76
1:A:238:LYS:HG3	1:A:239:GLU:H	1.50	0.76
1:C:234:PRO:HA	1:C:240:LYS:NZ	2.01	0.75
2:D:241:GLN:N	2:D:242:PRO:HD3	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:TRP:CE2	2:B:431:PRO:HG3	2.21	0.75
2:D:74:GLN:NE2	2:D:119:ASN:HD22	1.83	0.75
1:C:285:ILE:HD11	1:C:388:ALA:HA	1.68	0.75
2:B:64:LEU:HB3	2:B:111:LEU:HD22	1.67	0.74
1:A:143:LEU:HD12	1:A:150:LEU:HD22	1.69	0.74
1:A:46:LEU:HD23	1:A:93:LEU:HD13	1.69	0.74
1:C:225:TRP:NE1	1:C:233:ILE:HG12	2.02	0.74
1:C:518:ASN:OD1	1:C:534:LEU:N	2.21	0.74
2:B:32:HIS:HD2	2:B:34:ASP:N	1.86	0.74
2:D:236:GLN:HE22	2:D:263:LYS:HG2	1.53	0.74
1:C:113:LEU:O	1:C:117:PRO:HG3	1.87	0.74
2:D:186:LYS:NZ	2:D:325:ASN:HD21	1.86	0.74
1:C:232:ARG:C	1:C:234:PRO:HD2	2.07	0.73
1:A:357:VAL:O	1:A:361:VAL:HG23	1.88	0.73
1:C:59:ILE:HG22	1:C:60:ILE:N	2.03	0.73
2:B:403:ARG:C	2:B:406:PRO:HD2	2.09	0.73
1:C:233:ILE:N	1:C:234:PRO:HD2	2.04	0.73
1:C:36:ILE:HG23	1:C:37:ASN:ND2	2.04	0.73
1:A:534:LEU:HD13	4:A:535:HOH:O	1.88	0.72
2:D:202:CYS:HB3	2:D:343:CYS:SG	2.28	0.72
2:B:128:GLN:H	2:B:128:GLN:NE2	1.86	0.72
2:D:365:LEU:HG	2:D:379:PRO:HG2	1.72	0.71
2:B:427:ASP:OD1	2:B:428:VAL:N	2.23	0.71
2:D:44:PHE:O	2:D:48:THR:HB	1.90	0.71
1:A:215:ILE:H	1:A:332:MET:CE	2.04	0.71
1:C:347:ARG:NH1	2:D:274:ARG:HG3	2.04	0.71
1:A:409:LYS:O	1:A:413:ILE:HG12	1.91	0.71
1:A:173:GLU:O	1:A:512:GLN:O	2.09	0.71
1:A:236:THR:HA	1:A:240:LYS:HD2	1.73	0.70
2:D:43:GLN:NE2	2:D:46:LEU:HD12	2.06	0.70
2:D:131:ASN:HD22	2:D:133:THR:H	1.39	0.70
2:D:344:PRO:HG3	2:D:373:SER:O	1.91	0.70
2:B:376:MET:HB3	2:B:427:ASP:OD2	1.91	0.70
2:B:167:GLY:HA2	2:B:348:GLN:HE22	1.55	0.70
2:D:377:LYS:O	2:D:379:PRO:HD3	1.90	0.70
1:A:396:ARG:NH1	1:A:534:LEU:C	2.45	0.70
1:A:518:ASN:HB3	1:A:532:PHE:O	1.91	0.70
1:A:503:GLN:HE21	1:A:503:GLN:HA	1.55	0.70
1:A:517:ASN:O	1:A:518:ASN:HB2	1.91	0.69
2:D:204:LEU:O	2:D:208:PRO:HD2	1.91	0.69
2:D:223:ARG:H	2:D:227:HIS:HD2	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:ARG:HG2	2:D:117:ASN:O	1.92	0.69
1:A:84:ASN:ND2	1:A:87:GLU:H	1.90	0.69
2:B:237:TRP:O	2:B:240:GLU:O	2.09	0.69
1:C:282:PRO:HD2	1:C:285:ILE:HD12	1.73	0.69
1:C:10:GLU:HG2	1:C:10:GLU:O	1.92	0.69
1:C:36:ILE:CG2	1:C:128:ALA:HA	2.23	0.69
1:C:138:ARG:O	1:C:142:VAL:HG23	1.91	0.69
2:D:221:MET:N	2:D:222:PRO:HD3	2.06	0.69
2:D:237:TRP:HB3	2:D:238:PRO:HD3	1.75	0.69
2:B:405:ARG:N	2:B:406:PRO:HD2	2.08	0.69
2:D:368:LEU:HD13	2:D:376:MET:HE3	1.75	0.68
2:D:351:GLN:NE2	2:D:436:PHE:HE2	1.91	0.68
1:A:518:ASN:ND2	1:A:534:LEU:N	2.42	0.68
1:C:61:ASP:OD2	1:C:85:ARG:HD2	1.93	0.68
2:B:148:ILE:HD12	2:B:148:ILE:N	2.08	0.68
1:A:421:ASN:O	1:A:424:VAL:HG22	1.93	0.68
2:B:223:ARG:H	2:B:227:HIS:HD2	1.40	0.68
2:D:35:PHE:HD1	2:D:314:ALA:HA	1.58	0.68
1:A:503:GLN:HA	1:A:503:GLN:NE2	2.08	0.68
1:A:241:GLU:HA	1:A:244:ARG:HH11	1.56	0.68
1:C:218:ILE:O	1:C:222:LEU:HB2	1.93	0.68
2:B:50:LYS:N	2:B:139:HIS:HD2	1.91	0.68
2:B:31:THR:HG23	2:B:35:PHE:HB3	1.73	0.67
2:D:152:ARG:CZ	2:D:429:THR:HG21	2.24	0.67
2:D:74:GLN:HE22	2:D:119:ASN:ND2	1.84	0.67
2:D:41:SER:HA	2:D:44:PHE:CE2	2.29	0.67
1:C:311:LEU:HD21	1:C:387:SER:HB2	1.75	0.67
1:A:396:ARG:NH1	1:A:534:LEU:O	2.28	0.67
1:A:235:LYS:CB	1:A:238:LYS:HE3	2.24	0.67
1:C:134:SER:HB3	1:C:437:LYS:HE2	1.77	0.67
1:C:38:ALA:HB1	1:C:89:ALA:HB3	1.76	0.67
2:B:425:VAL:HG12	2:B:426:ALA:N	2.10	0.67
1:C:336:SER:O	1:C:340:ILE:HG12	1.95	0.66
2:D:434:VAL:HG12	2:D:435:LEU:N	2.10	0.66
1:C:226:TYR:CE1	1:C:231:GLY:O	2.49	0.66
1:A:109:PRO:O	1:A:113:LEU:HD23	1.96	0.66
1:C:438:GLN:HE21	1:C:439:GLN:HE22	1.41	0.66
2:B:40:GLU:HB2	4:B:483:HOH:O	1.94	0.66
2:D:376:MET:CB	2:D:427:ASP:OD2	2.44	0.66
1:A:458:LYS:HD3	1:A:458:LYS:O	1.95	0.66
4:B:485:HOH:O	2:D:126:LYS:HD2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:HG22	1:A:237:TYR:CD1	2.31	0.65
1:A:84:ASN:HD22	1:A:87:GLU:H	1.45	0.64
1:A:317:LYS:HD2	1:A:360:HIS:HE1	1.61	0.64
2:D:425:VAL:HG12	2:D:426:ALA:N	2.12	0.64
1:C:368:ILE:HG22	1:C:370:GLN:HB2	1.78	0.64
1:C:516:PHE:CD1	1:C:518:ASN:O	2.51	0.64
2:D:153:TRP:CZ2	2:D:431:PRO:HG3	2.32	0.64
1:C:244:ARG:NH2	1:C:273:ASN:HD22	1.95	0.64
1:A:119:PHE:O	1:A:122:ARG:HG2	1.98	0.64
2:D:202:CYS:HB2	2:D:340:LYS:HB3	1.81	0.63
1:C:442:TYR:HB2	1:C:445:VAL:CG2	2.28	0.63
2:D:320:ASN:HB2	4:D:451:HOH:O	1.97	0.63
1:C:280:GLN:O	1:C:282:PRO:HD3	1.99	0.63
1:C:143:LEU:HD22	1:C:148:ILE:HG21	1.80	0.63
2:D:210:GLN:HG2	2:D:211:VAL:N	2.14	0.63
2:B:213:PHE:HB3	2:B:218:ILE:HD13	1.81	0.63
2:B:31:THR:HG23	2:B:35:PHE:CB	2.29	0.63
1:C:349:LYS:HB2	4:C:541:HOH:O	1.99	0.63
2:B:405:ARG:H	2:B:406:PRO:HD2	1.62	0.63
2:B:197:THR:HG22	2:B:198:ALA:N	2.13	0.63
2:D:374:LEU:HD21	2:D:436:PHE:CZ	2.34	0.62
2:D:240:GLU:HB2	2:D:242:PRO:HD3	1.79	0.62
1:C:516:PHE:CE1	1:C:518:ASN:O	2.53	0.62
2:D:186:LYS:HZ2	2:D:325:ASN:HD21	1.45	0.62
1:C:37:ASN:HB2	1:C:129:THR:OG1	1.99	0.62
1:A:435:PHE:CD2	1:A:443:PRO:HD3	2.35	0.62
1:A:12:LYS:HE2	4:B:491:HOH:O	1.98	0.62
2:D:43:GLN:C	2:D:45:LEU:H	2.03	0.62
2:B:148:ILE:H	2:B:148:ILE:HD12	1.63	0.62
1:C:262:GLU:HB3	1:C:264:ASN:OD1	2.00	0.62
1:A:254:ASN:HB2	1:A:255:GLU:OE2	2.00	0.62
2:D:236:GLN:NE2	2:D:263:LYS:HE2	2.14	0.62
1:C:364:LEU:O	1:C:368:ILE:HD13	2.00	0.62
1:A:33:VAL:HG12	1:A:54:ILE:HD13	1.80	0.62
1:C:416:MET:HG3	1:C:472:VAL:HG11	1.82	0.62
1:A:111:ASN:ND2	1:A:115:ASN:HD21	1.96	0.61
1:C:449:GLN:HG2	4:C:548:HOH:O	2.00	0.61
1:C:201:LEU:HD22	1:C:209:HIS:ND1	2.15	0.61
1:C:371:ALA:HB1	1:C:372:PRO:HD2	1.81	0.61
2:D:24:LEU:O	2:D:37:PRO:HA	2.00	0.61
1:C:87:GLU:HG3	1:C:88:ALA:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ILE:HG23	1:C:37:ASN:HD22	1.64	0.61
1:C:298:THR:CG2	1:C:299:LYS:H	2.03	0.61
2:B:62:GLU:HG2	2:B:297:ALA:HA	1.82	0.61
1:A:362:ALA:O	1:A:366:GLN:HG3	2.00	0.61
1:A:534:LEU:CD2	4:A:535:HOH:O	2.32	0.61
1:A:421:ASN:HD22	1:A:423:ILE:HB	1.64	0.61
1:A:272:VAL:HG23	1:A:276:LEU:HD11	1.81	0.61
1:A:115:ASN:O	1:A:117:PRO:HD3	2.01	0.61
1:A:371:ALA:HB1	1:A:372:PRO:HD2	1.81	0.61
1:C:233:ILE:HD13	1:C:243:PHE:CG	2.36	0.61
1:C:442:TYR:HB2	1:C:445:VAL:HG21	1.82	0.61
2:B:162:LEU:HD22	2:B:169:LEU:HD11	1.83	0.61
2:D:243:PHE:HD1	2:D:256:HIS:HD1	1.47	0.60
1:A:317:LYS:HB2	1:A:318:GLU:OE2	2.01	0.60
1:A:449:GLN:HB3	1:A:453:ASP:OD2	2.00	0.60
2:D:203:THR:HG22	2:D:203:THR:O	2.00	0.60
1:A:331:ASP:HB2	2:B:224:LEU:HD11	1.84	0.60
1:A:111:ASN:HD21	1:A:115:ASN:HD21	1.49	0.60
2:B:128:GLN:N	2:B:128:GLN:HE21	1.95	0.60
1:C:184:ARG:NE	1:C:325:VAL:HG12	2.17	0.60
2:B:365:LEU:O	2:B:365:LEU:HD23	2.01	0.60
1:C:225:TRP:CD1	1:C:233:ILE:HG12	2.37	0.60
2:D:365:LEU:O	2:D:365:LEU:HD23	2.01	0.60
1:A:235:LYS:HD2	1:A:239:GLU:OE2	2.02	0.60
1:C:38:ALA:HB1	1:C:89:ALA:CB	2.31	0.60
2:D:236:GLN:HE22	2:D:263:LYS:CG	2.14	0.60
2:D:380:ALA:CB	2:D:426:ALA:HB3	2.21	0.60
1:C:236:THR:HB	1:C:239:GLU:CD	2.22	0.60
2:D:243:PHE:HD1	2:D:256:HIS:ND1	2.00	0.60
2:B:224:LEU:H	2:B:227:HIS:CD2	2.20	0.60
2:B:39:THR:HG23	4:B:483:HOH:O	2.00	0.60
1:C:189:PHE:CE1	1:C:192:LEU:HB2	2.37	0.60
1:C:299:LYS:HA	1:C:368:ILE:HG23	1.82	0.59
2:B:229:ILE:HD13	2:B:281:THR:HA	1.84	0.59
1:A:240:LYS:O	1:A:244:ARG:HG3	2.02	0.59
2:D:197:THR:HG22	2:D:198:ALA:N	2.17	0.59
1:C:36:ILE:HG22	1:C:128:ALA:HA	1.83	0.59
1:A:423:ILE:HD13	1:A:423:ILE:O	2.02	0.59
1:C:319:GLY:O	1:C:320:GLN:HB2	2.03	0.59
2:B:38:SER:HB3	2:B:41:SER:OG	2.02	0.59
1:A:430:ARG:NH2	4:A:577:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ILE:HD11	1:C:315:VAL:HG11	1.83	0.59
1:C:12:LYS:HA	2:D:85:VAL:HG12	1.84	0.59
1:C:78:ARG:HH11	1:C:78:ARG:HG3	1.68	0.59
2:D:152:ARG:NE	2:D:429:THR:HG21	2.17	0.58
1:C:224:GLN:OE1	1:C:246:LEU:HD11	2.03	0.58
1:C:255:GLU:O	1:C:256:ASN:C	2.40	0.58
2:B:195:GLY:O	2:B:339:ARG:NH1	2.36	0.58
1:A:110:GLU:OE1	1:A:110:GLU:HA	2.02	0.58
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.86	0.58
1:A:458:LYS:HD3	1:A:458:LYS:C	2.23	0.58
2:D:353:ILE:HG21	2:D:367:TYR:CE2	2.38	0.58
2:D:430:THR:HG22	2:D:432:GLN:H	1.69	0.58
1:A:46:LEU:HD23	1:A:93:LEU:CD1	2.32	0.58
1:C:240:LYS:O	1:C:244:ARG:HG3	2.04	0.58
1:C:59:ILE:O	1:C:60:ILE:HG13	2.04	0.58
2:D:249:LEU:HD11	2:D:253:ASP:HB3	1.84	0.58
1:A:163:ARG:NH1	1:A:401:GLU:OE2	2.36	0.58
1:A:235:LYS:HB3	1:A:238:LYS:CE	2.32	0.58
2:D:224:LEU:HD12	2:D:227:HIS:CE1	2.38	0.58
2:D:131:ASN:HD22	2:D:131:ASN:C	2.07	0.58
1:C:128:ALA:HB1	1:C:131:LEU:HD11	1.86	0.57
1:C:39:THR:HG23	1:C:42:GLY:H	1.69	0.57
1:A:376:SER:OG	1:A:378:LYS:HG2	2.03	0.57
1:A:193:ARG:O	1:A:197:GLN:HG3	2.04	0.57
2:B:251:GLY:O	2:B:286:LYS:HE2	2.04	0.57
2:D:178:ILE:HD12	2:D:307:VAL:HG22	1.87	0.57
2:B:208:PRO:N	2:B:209:PRO:HD2	2.19	0.57
1:C:404:LEU:HD21	1:C:467:GLU:HG2	1.84	0.57
1:C:434:ARG:HH11	1:C:434:ARG:HG2	1.69	0.57
1:C:428:MET:HE1	1:C:479:VAL:HA	1.87	0.57
1:A:341:LYS:NZ	4:A:582:HOH:O	2.37	0.57
1:C:59:ILE:CG2	1:C:60:ILE:H	2.16	0.57
1:C:505:VAL:O	1:C:509:ILE:HG12	2.03	0.57
1:C:445:VAL:HG22	1:C:486:GLY:O	2.04	0.57
2:D:27:SER:HB3	2:D:37:PRO:CG	2.24	0.57
2:D:131:ASN:HD21	2:D:133:THR:HB	1.69	0.57
1:C:378:LYS:NZ	1:C:378:LYS:HB3	2.20	0.56
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.86	0.56
2:D:64:LEU:HD21	2:D:77:VAL:HG22	1.86	0.56
2:B:64:LEU:HD21	2:B:77:VAL:HG22	1.86	0.56
2:D:42:LEU:O	2:D:46:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HD2	1:A:360:HIS:CE1	2.41	0.56
1:A:172:ILE:HA	1:A:390:LEU:HD22	1.86	0.56
1:C:279:THR:CG2	1:C:322:ASN:HD22	2.13	0.56
1:A:72:ASN:ND2	1:A:72:ASN:C	2.59	0.56
2:D:50:LYS:H	2:D:139:HIS:CD2	2.11	0.56
2:D:236:GLN:HE22	2:D:263:LYS:HE2	1.71	0.56
1:A:297:ILE:HG21	1:A:368:ILE:HD11	1.86	0.56
2:D:232:VAL:HA	2:D:236:GLN:HB3	1.88	0.56
2:B:16:ARG:HH12	2:B:117:ASN:HD22	1.54	0.55
2:D:429:THR:O	2:D:429:THR:HG22	2.05	0.55
1:C:33:VAL:CG2	1:C:34:CYS:N	2.70	0.55
1:C:518:ASN:HB3	1:C:532:PHE:O	2.06	0.55
2:B:204:LEU:C	2:B:206:LEU:H	2.10	0.55
2:B:425:VAL:HG12	2:B:426:ALA:H	1.70	0.55
2:B:208:PRO:O	2:B:210:GLN:N	2.39	0.55
2:B:169:LEU:O	2:B:171:PRO:HD3	2.05	0.55
1:A:396:ARG:HG3	1:A:396:ARG:NH1	2.18	0.55
2:D:434:VAL:O	2:D:435:LEU:HG	2.06	0.55
1:A:215:ILE:H	1:A:332:MET:HE3	1.70	0.55
1:A:418:ASN:ND2	1:A:420:ASP:H	2.05	0.55
1:A:214:TRP:HB2	1:A:268:ALA:HA	1.89	0.55
1:A:480:HIS:HE1	4:B:471:HOH:O	1.90	0.55
1:C:262:GLU:O	1:C:266:GLU:HG2	2.07	0.54
1:C:314:PHE:HZ	1:C:353:ASP:OD2	1.90	0.54
2:D:324:PHE:HD1	2:D:332:THR:HG22	1.73	0.54
1:A:224:GLN:O	1:A:228:GLU:HG3	2.08	0.54
1:A:396:ARG:NH1	1:A:534:LEU:OXT	2.40	0.54
2:B:403:ARG:O	2:B:406:PRO:CG	2.54	0.54
1:C:254:ASN:O	1:C:255:GLU:C	2.45	0.54
1:A:221:TYR:OH	1:A:250:GLY:HA3	2.07	0.54
1:C:225:TRP:CE2	1:C:233:ILE:HG12	2.42	0.54
1:C:396:ARG:HB2	4:C:539:HOH:O	2.06	0.54
1:A:235:LYS:HB2	1:A:239:GLU:HG3	1.90	0.54
1:C:110:GLU:CD	1:C:110:GLU:H	2.11	0.54
2:B:32:HIS:HB3	2:B:313:SER:O	2.07	0.54
1:A:241:GLU:HA	1:A:244:ARG:NH1	2.22	0.54
1:C:223:ALA:O	1:C:226:TYR:HB2	2.08	0.54
1:C:525:MET:HG3	2:D:315:TYR:CE2	2.43	0.54
2:D:218:ILE:N	2:D:218:ILE:HD12	2.22	0.54
1:C:126:VAL:O	1:C:150:LEU:HD12	2.08	0.54
1:C:38:ALA:HB3	1:C:85:ARG:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.89	0.54
2:D:425:VAL:HG12	2:D:426:ALA:H	1.71	0.54
1:A:215:ILE:HG13	1:A:332:MET:CE	2.38	0.54
2:D:286:LYS:HB2	2:D:288:ILE:HG13	1.89	0.54
1:A:35:LEU:HD22	1:A:46:LEU:HD22	1.90	0.53
1:A:373:GLU:C	1:A:375:ILE:H	2.10	0.53
2:D:390:ARG:O	2:D:391:THR:CB	2.55	0.53
1:C:438:GLN:HE21	1:C:439:GLN:NE2	2.06	0.53
2:B:215:MET:CE	2:B:235:LEU:HD11	2.38	0.53
2:D:351:GLN:NE2	2:D:436:PHE:CE2	2.76	0.53
1:C:297:ILE:CD1	1:C:368:ILE:HD11	2.39	0.53
2:D:287:ARG:HH11	2:D:287:ARG:HG2	1.72	0.53
2:D:430:THR:HG22	2:D:432:GLN:N	2.23	0.53
1:A:353:ASP:O	1:A:357:VAL:HG23	2.09	0.53
1:C:174:SER:HB3	1:C:176:PRO:HD3	1.90	0.53
1:C:244:ARG:NH2	1:C:273:ASN:ND2	2.55	0.53
1:A:108:SER:HB2	1:A:109:PRO:HD2	1.90	0.53
1:C:105:VAL:HG12	1:C:107:GLU:H	1.73	0.53
1:C:235:LYS:HG2	4:C:543:HOH:O	2.08	0.53
2:D:170:ASP:O	2:D:173:SER:HB3	2.09	0.53
1:C:108:SER:HB3	1:C:111:ASN:HD22	1.74	0.53
2:B:318:LEU:C	2:B:320:ASN:H	2.12	0.53
2:B:64:LEU:HB3	2:B:111:LEU:CD2	2.38	0.53
2:B:352:ASN:HA	2:B:437:LYS:O	2.09	0.53
1:C:233:ILE:HB	1:C:276:LEU:HD13	1.91	0.53
1:C:217:ILE:HD11	1:C:264:ASN:ND2	2.24	0.52
2:B:361:LEU:O	2:B:364:VAL:HG22	2.09	0.52
1:C:84:ASN:ND2	1:C:86:ALA:HB3	2.24	0.52
2:D:58:GLY:HA2	2:D:91:GLN:HG3	1.90	0.52
1:C:484:ARG:HH11	1:C:484:ARG:HG2	1.75	0.52
1:A:253:LYS:HB2	1:A:257:GLY:O	2.10	0.52
2:D:204:LEU:CG	2:D:208:PRO:HG2	2.31	0.52
2:B:244:GLY:O	2:B:247:VAL:HG23	2.09	0.52
1:C:10:GLU:OE2	2:D:279:ARG:NH2	2.43	0.52
1:A:229:THR:O	1:A:230:ASN:CB	2.57	0.52
1:C:255:GLU:O	1:C:256:ASN:O	2.27	0.52
2:B:353:ILE:HG13	2:B:353:ILE:O	2.09	0.52
1:C:10:GLU:OE2	2:D:279:ARG:NH1	2.42	0.52
2:B:46:LEU:HD23	2:B:71:GLY:O	2.09	0.52
1:C:236:THR:HB	1:C:239:GLU:OE1	2.10	0.51
2:D:429:THR:O	2:D:429:THR:CG2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LYS:HA	1:A:366:GLN:OE1	2.09	0.51
2:D:131:ASN:ND2	2:D:133:THR:H	2.07	0.51
1:A:462:THR:O	1:A:466:GLN:HG3	2.11	0.51
1:C:144:TRP:CZ3	1:C:397:SER:HA	2.45	0.51
2:D:214:PRO:O	2:D:218:ILE:HD13	2.11	0.51
1:A:235:LYS:HD3	1:A:238:LYS:HE3	1.92	0.51
1:C:33:VAL:HG22	1:C:34:CYS:N	2.25	0.51
2:B:197:THR:HG22	2:B:198:ALA:H	1.75	0.51
1:C:158:LEU:HG	2:D:23:PHE:HE2	1.75	0.51
1:C:454:ILE:HG23	1:C:455:GLY:N	2.25	0.51
1:C:489:GLU:H	2:D:19:HIS:CE1	2.28	0.51
1:A:60:ILE:HD11	1:A:119:PHE:HE2	1.76	0.51
1:C:310:ALA:CB	1:C:361:VAL:HG22	2.41	0.51
2:B:401:GLU:O	2:B:404:THR:CB	2.59	0.51
1:A:344:ASN:O	1:A:348:GLU:HG2	2.10	0.51
2:B:365:LEU:HD23	2:B:365:LEU:C	2.31	0.51
1:C:434:ARG:NH1	1:C:434:ARG:HG2	2.26	0.51
2:D:157:MET:O	2:D:160:SER:HB3	2.10	0.51
1:C:374:SER:C	1:C:375:ILE:HD12	2.31	0.51
2:D:48:THR:HG22	2:D:48:THR:O	2.11	0.51
1:C:244:ARG:NH2	1:C:273:ASN:HB2	2.25	0.51
2:B:178:ILE:HD11	2:B:310:ILE:HD12	1.93	0.50
2:B:325:ASN:HD22	2:B:326:ASP:N	2.09	0.50
1:C:54:ILE:O	1:C:100:VAL:HG22	2.12	0.50
2:D:226:GLU:OE2	2:D:280:LEU:HD21	2.10	0.50
1:C:164:ILE:HD13	1:C:515:ILE:HD12	1.93	0.50
1:C:277:ASN:C	1:C:277:ASN:HD22	2.14	0.50
1:A:19:LEU:HG	2:B:290:PRO:HB3	1.92	0.50
2:D:281:THR:O	2:D:285:VAL:HG23	2.10	0.50
2:D:207:TYR:HB2	2:D:208:PRO:CD	2.36	0.50
1:A:371:ALA:HB3	1:A:374:SER:HB3	1.91	0.50
1:C:317:LYS:HB2	1:C:318:GLU:OE1	2.11	0.50
1:C:419:PRO:O	1:C:424:VAL:HG21	2.12	0.50
2:D:373:SER:O	2:D:374:LEU:HD12	2.12	0.50
1:C:10:GLU:OE2	2:D:279:ARG:CZ	2.60	0.50
1:A:376:SER:OG	1:A:379:GLU:HG3	2.11	0.50
1:A:489:GLU:N	2:B:19:HIS:HD2	1.93	0.50
2:B:148:ILE:CD1	2:B:148:ILE:H	2.23	0.50
1:C:46:LEU:HD21	1:C:57:PHE:CD1	2.47	0.50
2:D:46:LEU:HD23	2:D:71:GLY:O	2.12	0.50
1:A:352:LYS:HG2	4:A:568:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:GLN:HB3	2:B:436:PHE:CD2	2.46	0.50
2:D:241:GLN:N	2:D:242:PRO:CD	2.72	0.50
1:C:18:ARG:HB3	2:D:290:PRO:HG3	1.93	0.50
1:C:128:ALA:HB1	1:C:131:LEU:CD1	2.42	0.50
1:C:51:LEU:HD11	2:D:92:PHE:HB3	1.93	0.50
2:D:58:GLY:HA2	2:D:91:GLN:CG	2.42	0.50
1:A:212:THR:HG22	1:A:216:VAL:HB	1.93	0.50
2:D:266:GLU:O	2:D:269:SER:HB3	2.11	0.50
1:C:370:GLN:O	1:C:371:ALA:HB2	2.11	0.50
1:A:36:ILE:O	1:A:60:ILE:O	2.29	0.50
2:D:197:THR:CG2	2:D:198:ALA:N	2.75	0.50
1:C:400:GLU:O	1:C:406:THR:HB	2.11	0.50
2:D:287:ARG:NH1	2:D:287:ARG:HG2	2.27	0.49
2:D:434:VAL:CG1	2:D:435:LEU:H	2.18	0.49
2:D:240:GLU:CB	2:D:242:PRO:HD3	2.42	0.49
1:C:174:SER:O	1:C:175:HIS:HB2	2.13	0.49
1:C:518:ASN:CG	1:C:519:THR:H	2.09	0.49
1:C:234:PRO:HD3	1:C:276:LEU:HB3	1.93	0.49
1:C:244:ARG:HH21	1:C:273:ASN:HB2	1.78	0.49
1:A:202:ASP:OD1	1:A:203:HIS:N	2.45	0.49
1:C:87:GLU:HG3	1:C:88:ALA:H	1.77	0.49
1:A:84:ASN:HD21	1:A:86:ALA:HB3	1.77	0.49
1:C:150:LEU:HD23	1:C:165:ILE:HD12	1.94	0.49
2:D:230:GLU:HG3	2:D:234:MET:CE	2.42	0.49
1:A:534:LEU:CD1	4:A:535:HOH:O	2.51	0.49
1:C:424:VAL:HG13	1:C:474:VAL:HG13	1.95	0.49
2:D:186:LYS:HZ2	2:D:325:ASN:ND2	2.10	0.49
1:C:481:GLU:OE1	1:C:484:ARG:HD2	2.12	0.49
1:C:221:TYR:HD2	1:C:246:LEU:HG	1.76	0.49
1:A:426:TYR:HB2	1:A:521:ILE:HD11	1.95	0.49
1:A:187:LYS:N	1:A:188:PRO:HD3	2.27	0.49
1:C:92:PHE:HD2	2:D:114:ARG:NH2	2.11	0.49
1:A:229:THR:O	1:A:230:ASN:HB2	2.11	0.49
1:C:315:VAL:HG13	1:C:322:ASN:N	2.27	0.49
2:D:236:GLN:HE21	2:D:259:TRP:HH2	1.60	0.49
1:A:215:ILE:HG13	1:A:332:MET:HE3	1.95	0.49
1:C:189:PHE:HB3	1:C:349:LYS:NZ	2.28	0.49
1:A:72:ASN:HD22	1:A:72:ASN:C	2.16	0.49
1:C:59:ILE:CG2	1:C:60:ILE:N	2.73	0.48
2:D:236:GLN:NE2	2:D:263:LYS:HG2	2.24	0.48
1:C:65:VAL:HG12	1:C:66:SER:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:ASP:HB3	2:B:136:ARG:NH1	2.28	0.48
2:B:148:ILE:CD1	2:B:148:ILE:N	2.76	0.48
1:C:444:GLY:O	1:C:446:SER:N	2.45	0.48
1:C:143:LEU:HD12	1:C:150:LEU:HD22	1.95	0.48
1:A:264:ASN:HD22	1:A:264:ASN:H	1.59	0.48
2:D:373:SER:C	2:D:374:LEU:HD12	2.34	0.48
2:D:126:LYS:HG3	2:D:128:GLN:HG2	1.94	0.48
1:C:150:LEU:HD21	1:C:152:ILE:HD11	1.95	0.48
1:A:264:ASN:HD22	1:A:264:ASN:N	2.11	0.48
1:C:186:ASP:CG	1:C:187:LYS:H	2.16	0.48
1:C:18:ARG:HH21	2:D:288:ILE:HD12	1.78	0.48
1:C:61:ASP:CB	1:C:86:ALA:HB2	2.44	0.48
1:C:254:ASN:O	1:C:255:GLU:O	2.31	0.48
1:A:447:ASN:ND2	2:B:26:ARG:HH21	2.12	0.48
1:A:32:HIS:HE1	1:A:58:THR:OG1	1.97	0.48
2:B:394:LEU:O	2:B:396:SER:N	2.46	0.48
1:A:504:GLU:HG3	1:A:516:PHE:CE2	2.48	0.48
2:B:242:PRO:HG3	2:B:259:TRP:CZ2	2.49	0.48
2:D:322:LEU:C	2:D:322:LEU:HD23	2.34	0.48
1:C:371:ALA:HB3	1:C:374:SER:OG	2.13	0.48
2:D:36:GLU:O	2:D:38:SER:N	2.47	0.48
1:C:175:HIS:N	1:C:176:PRO:CD	2.77	0.48
2:B:361:LEU:HD23	2:B:361:LEU:C	2.34	0.48
2:B:208:PRO:N	2:B:209:PRO:CD	2.77	0.48
1:C:454:ILE:HG23	1:C:455:GLY:H	1.79	0.48
1:C:503:GLN:OE1	1:C:503:GLN:HA	2.13	0.48
1:C:368:ILE:N	1:C:368:ILE:HD12	2.29	0.48
1:C:236:THR:HB	1:C:239:GLU:CG	2.44	0.48
1:A:117:PRO:C	1:A:119:PHE:H	2.16	0.48
1:C:484:ARG:O	1:C:486:GLY:N	2.47	0.48
1:C:470:LEU:C	1:C:472:VAL:H	2.17	0.48
2:B:136:ARG:HG2	2:B:161:LEU:HD22	1.96	0.48
1:C:297:ILE:HD11	1:C:368:ILE:HD11	1.94	0.47
1:C:236:THR:HB	1:C:239:GLU:HG3	1.96	0.47
2:D:225:PRO:HG3	2:D:273:ILE:HG22	1.96	0.47
1:A:318:GLU:N	1:A:318:GLU:OE2	2.38	0.47
1:C:485:TYR:C	1:C:487:ALA:H	2.17	0.47
1:A:54:ILE:O	1:A:100:VAL:HG22	2.14	0.47
1:C:277:ASN:HD22	1:C:278:THR:N	2.12	0.47
2:D:132:ASP:HA	2:D:157:MET:HE1	1.96	0.47
1:A:199:TYR:OH	1:A:338:LYS:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:TYR:CD2	2:B:223:ARG:HB3	2.49	0.47
1:A:172:ILE:HA	1:A:390:LEU:CD2	2.43	0.47
1:A:164:ILE:HD11	1:A:508:ILE:HD11	1.96	0.47
2:D:221:MET:N	2:D:222:PRO:CD	2.77	0.47
1:A:366:GLN:C	1:A:368:ILE:H	2.16	0.47
2:D:368:LEU:HD22	2:D:374:LEU:HD23	1.96	0.47
1:A:331:ASP:OD1	2:B:223:ARG:HD2	2.15	0.47
2:B:425:VAL:CG1	2:B:426:ALA:N	2.76	0.47
1:C:78:ARG:HD3	1:C:81:ILE:HD12	1.96	0.47
2:D:233:ARG:HD2	2:D:285:VAL:HA	1.96	0.47
2:B:393:TYR:O	2:B:395:GLN:N	2.43	0.47
2:D:20:VAL:C	2:D:22:LYS:H	2.18	0.47
2:D:208:PRO:O	2:D:210:GLN:N	2.48	0.47
1:C:525:MET:HG3	2:D:315:TYR:CD2	2.50	0.47
2:D:64:LEU:HB3	2:D:111:LEU:CD1	2.44	0.47
1:C:163:ARG:NH1	1:C:401:GLU:OE2	2.48	0.47
2:D:27:SER:CB	2:D:37:PRO:CG	2.89	0.47
2:D:193:LEU:H	2:D:197:THR:HB	1.78	0.47
2:D:319:ASN:HD22	2:D:336:GLU:HB2	1.79	0.47
1:C:47:LYS:HE3	2:D:65:LYS:NZ	2.30	0.47
2:D:148:ILE:HD13	2:D:208:PRO:HA	1.97	0.47
2:B:213:PHE:HB3	2:B:218:ILE:CD1	2.45	0.47
1:C:428:MET:CE	1:C:479:VAL:HA	2.45	0.47
1:C:49:LEU:O	1:C:52:PRO:HG2	2.15	0.47
1:A:229:THR:O	1:A:230:ASN:ND2	2.47	0.47
1:C:164:ILE:CD1	1:C:515:ILE:HD12	2.44	0.47
1:C:130:GLN:HE22	1:C:155:THR:N	2.04	0.47
2:D:131:ASN:ND2	2:D:133:THR:HB	2.29	0.47
2:D:163:ASN:N	2:D:173:SER:OG	2.48	0.47
1:C:436:HIS:ND1	1:C:441:ARG:O	2.45	0.47
2:D:224:LEU:HD12	2:D:227:HIS:NE2	2.30	0.46
1:C:37:ASN:C	1:C:39:THR:H	2.18	0.46
2:D:40:GLU:O	2:D:43:GLN:HB3	2.15	0.46
1:C:213:PRO:O	1:C:217:ILE:HG13	2.14	0.46
2:B:157:MET:O	2:B:157:MET:HE3	2.15	0.46
2:D:353:ILE:O	2:D:354:GLN:HB3	2.15	0.46
1:C:75:PHE:CE2	1:C:93:LEU:HD23	2.50	0.46
1:A:91:GLU:O	1:A:95:GLU:HG2	2.15	0.46
2:B:153:TRP:CZ2	2:B:431:PRO:HG3	2.50	0.46
1:C:472:VAL:HG12	1:C:473:MET:N	2.31	0.46
1:C:224:GLN:OE1	1:C:246:LEU:HD21	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:GLY:HA2	1:C:380:LEU:HD21	1.97	0.46
2:D:21:LYS:HA	2:D:25:GLU:HG2	1.97	0.46
1:C:285:ILE:HD13	1:C:323:LEU:HD11	1.98	0.46
2:D:232:VAL:HG11	2:D:260:ILE:HG23	1.97	0.46
1:C:442:TYR:HB2	1:C:445:VAL:HG23	1.97	0.46
1:C:33:VAL:CG1	1:C:54:ILE:HD12	2.46	0.46
2:D:213:PHE:HB3	2:D:218:ILE:HD11	1.96	0.46
1:A:307:LEU:HB3	1:A:383:LEU:CD2	2.42	0.46
1:C:35:LEU:HG	1:C:37:ASN:H	1.81	0.46
1:C:201:LEU:HD13	1:C:209:HIS:HE1	1.80	0.46
2:B:392:LEU:O	2:B:393:TYR:CB	2.63	0.46
1:C:214:TRP:O	1:C:218:ILE:HG12	2.15	0.46
1:C:368:ILE:CG2	1:C:370:GLN:HB2	2.45	0.46
2:D:46:LEU:O	2:D:73:ARG:HB2	2.15	0.46
1:C:317:LYS:C	1:C:319:GLY:H	2.19	0.46
1:A:189:PHE:O	1:A:193:ARG:HG3	2.16	0.46
1:C:404:LEU:HD22	1:C:467:GLU:O	2.16	0.46
2:D:425:VAL:CG1	2:D:426:ALA:N	2.78	0.46
1:C:189:PHE:HB2	1:C:190:PRO:HD2	1.97	0.46
1:C:217:ILE:HD13	1:C:265:PHE:CD1	2.50	0.46
1:C:416:MET:SD	1:C:423:ILE:HG23	2.56	0.46
1:C:158:LEU:HG	2:D:23:PHE:CE2	2.50	0.46
2:D:216:CYS:SG	2:D:221:MET:HE1	2.56	0.46
2:B:224:LEU:H	2:B:227:HIS:HD2	1.63	0.46
1:C:199:TYR:O	1:C:220:LYS:HE2	2.15	0.46
2:B:82:THR:HG23	2:B:100:GLY:O	2.16	0.46
2:D:152:ARG:HB3	2:D:429:THR:HG23	1.98	0.46
1:A:321:GLY:O	1:A:322:ASN:ND2	2.49	0.46
2:D:152:ARG:CB	2:D:429:THR:HG23	2.46	0.45
2:D:152:ARG:NH2	2:D:201:GLU:OE1	2.42	0.45
1:A:113:LEU:CD1	1:A:142:VAL:HG21	2.46	0.45
1:A:447:ASN:HD22	2:B:26:ARG:NH2	2.13	0.45
1:A:209:HIS:HD2	1:A:262:GLU:OE2	1.99	0.45
2:D:38:SER:C	2:D:40:GLU:N	2.68	0.45
2:D:43:GLN:HE21	2:D:43:GLN:HA	1.81	0.45
2:D:76:HIS:CD2	2:D:121:VAL:HB	2.51	0.45
2:B:110:PHE:C	2:B:110:PHE:CD2	2.89	0.45
2:D:149:ILE:HD11	2:D:377:LYS:NZ	2.31	0.45
1:A:416:MET:CE	1:A:424:VAL:HG13	2.46	0.45
1:A:235:LYS:CD	1:A:238:LYS:HE3	2.47	0.45
1:C:191:GLU:CD	1:C:191:GLU:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:PHE:CZ	2:D:330:LEU:HD11	2.52	0.45
1:A:163:ARG:NH2	1:A:396:ARG:O	2.49	0.45
1:C:189:PHE:CZ	1:C:192:LEU:HB2	2.52	0.45
2:B:243:PHE:O	2:B:247:VAL:HG21	2.17	0.45
2:B:256:HIS:O	2:B:260:ILE:HG12	2.16	0.45
1:A:513:PHE:CD1	1:A:513:PHE:N	2.84	0.45
1:C:486:GLY:O	1:C:487:ALA:HB3	2.17	0.45
2:B:378:SER:N	2:B:379:PRO:HD3	2.31	0.45
1:C:347:ARG:HH12	2:D:274:ARG:CG	2.16	0.45
1:C:18:ARG:CB	2:D:290:PRO:HG3	2.47	0.45
1:C:108:SER:HB3	1:C:111:ASN:ND2	2.31	0.45
1:C:445:VAL:O	1:C:446:SER:HB3	2.16	0.45
1:C:201:LEU:C	1:C:203:HIS:H	2.20	0.45
1:C:386:ASN:O	1:C:390:LEU:HD23	2.16	0.45
1:A:75:PHE:O	1:A:76:LEU:HD23	2.17	0.45
1:C:211:HIS:HD2	2:D:221:MET:SD	2.40	0.45
1:C:14:ASP:O	1:C:18:ARG:HG2	2.17	0.45
1:A:213:PRO:HG3	1:A:334:ALA:CB	2.47	0.45
2:D:374:LEU:HD21	2:D:436:PHE:HZ	1.79	0.45
1:C:309:ARG:HB3	1:C:364:LEU:HD21	1.99	0.44
1:C:200:ASP:OD1	1:C:203:HIS:HB2	2.17	0.44
2:D:87:ASN:OD1	2:D:103:LYS:HE2	2.17	0.44
2:B:64:LEU:HD21	2:B:77:VAL:CG2	2.47	0.44
1:C:36:ILE:HG21	1:C:128:ALA:HA	1.98	0.44
1:A:421:ASN:ND2	1:A:423:ILE:HB	2.29	0.44
2:B:197:THR:CG2	2:B:198:ALA:N	2.80	0.44
2:D:23:PHE:CD1	2:D:23:PHE:N	2.85	0.44
1:C:19:LEU:HD13	2:D:185:PHE:CE1	2.52	0.44
1:A:105:VAL:C	1:A:107:GLU:H	2.20	0.44
1:C:303:SER:O	1:C:307:LEU:HG	2.17	0.44
2:B:405:ARG:N	2:B:406:PRO:CD	2.73	0.44
1:C:484:ARG:HG2	1:C:484:ARG:NH1	2.32	0.44
2:D:353:ILE:HD13	2:D:367:TYR:HE2	1.82	0.44
2:D:43:GLN:NE2	2:D:43:GLN:HA	2.32	0.44
2:D:128:GLN:H	2:D:128:GLN:CD	2.19	0.44
2:D:141:ILE:CD1	2:D:158:LEU:HD21	2.46	0.44
1:A:334:ALA:O	2:B:221:MET:HE2	2.17	0.44
1:A:209:HIS:CD2	1:A:252:LEU:HG	2.51	0.44
1:C:521:ILE:O	1:C:529:SER:HA	2.18	0.44
1:C:143:LEU:HD22	1:C:148:ILE:CG2	2.47	0.44
1:C:314:PHE:CE2	1:C:324:PRO:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:PHE:HB3	2:D:218:ILE:CD1	2.48	0.44
2:B:185:PHE:HB3	2:B:326:ASP:HB3	1.99	0.44
2:B:131:ASN:OD1	2:B:132:ASP:OD1	2.35	0.44
2:B:272:ASN:ND2	4:B:475:HOH:O	2.48	0.44
2:B:139:HIS:O	2:B:176:PRO:HD2	2.17	0.44
2:D:243:PHE:N	2:D:243:PHE:CD2	2.85	0.44
2:D:353:ILE:HD13	2:D:367:TYR:CE2	2.52	0.44
2:D:364:VAL:O	2:D:367:TYR:HB3	2.17	0.44
2:B:318:LEU:C	2:B:320:ASN:N	2.71	0.44
1:C:454:ILE:HD12	1:C:480:HIS:CG	2.53	0.44
2:B:340:LYS:HD2	4:B:502:HOH:O	2.17	0.44
2:D:368:LEU:HB3	2:D:376:MET:HE3	1.98	0.44
1:C:201:LEU:HD22	1:C:209:HIS:CE1	2.53	0.44
1:A:428:MET:CE	1:A:479:VAL:HA	2.48	0.44
2:D:338:GLU:O	2:D:340:LYS:N	2.47	0.44
2:D:38:SER:C	2:D:40:GLU:H	2.19	0.44
2:D:237:TRP:CZ2	2:D:249:LEU:HB2	2.52	0.44
2:D:430:THR:HG22	2:D:432:GLN:HG2	1.95	0.44
1:C:96:LEU:HD22	2:D:92:PHE:HB2	1.99	0.44
2:D:26:ARG:HH11	2:D:26:ARG:HG2	1.82	0.44
1:C:233:ILE:O	1:C:234:PRO:O	2.36	0.43
2:D:202:CYS:HB3	2:D:343:CYS:HB2	1.99	0.43
1:C:190:PRO:HB2	1:C:191:GLU:OE2	2.17	0.43
2:D:305:THR:HG22	2:D:309:LYS:HE3	2.00	0.43
2:B:13:TRP:CZ3	2:B:116:PRO:HG2	2.53	0.43
1:C:335:ASP:HB3	1:C:338:LYS:CG	2.48	0.43
1:C:125:VAL:HG12	1:C:126:VAL:N	2.33	0.43
2:B:82:THR:HG23	2:B:100:GLY:C	2.38	0.43
2:D:136:ARG:HH11	2:D:136:ARG:HG3	1.83	0.43
2:D:204:LEU:C	2:D:206:LEU:H	2.22	0.43
1:C:66:SER:H	1:C:69:ASP:HB2	1.84	0.43
2:D:178:ILE:HD12	2:D:307:VAL:CG2	2.47	0.43
1:C:503:GLN:OE1	1:C:506:ILE:HB	2.18	0.43
2:D:306:GLU:O	2:D:310:ILE:HG13	2.19	0.43
1:A:313:GLU:O	1:A:316:ALA:HB3	2.18	0.43
2:D:267:ARG:O	2:D:270:GLN:HB3	2.17	0.43
2:B:128:GLN:N	2:B:128:GLN:NE2	2.60	0.43
2:D:43:GLN:HE22	2:D:46:LEU:HD12	1.82	0.43
2:D:44:PHE:C	2:D:48:THR:HB	2.38	0.43
1:A:105:VAL:HG12	1:A:107:GLU:HB2	2.00	0.43
1:C:173:GLU:HG2	4:C:540:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:434:VAL:O	2:D:435:LEU:CG	2.67	0.43
1:C:236:THR:CG2	1:C:237:TYR:N	2.82	0.43
2:B:425:VAL:CG1	2:B:426:ALA:H	2.30	0.43
2:D:154:ILE:HG23	2:D:155:ASN:N	2.33	0.43
2:D:35:PHE:CE1	2:D:314:ALA:CA	2.97	0.43
1:C:233:ILE:HG13	1:C:233:ILE:H	1.52	0.43
1:C:503:GLN:NE2	2:D:185:PHE:CE2	2.86	0.43
2:B:340:LYS:HE2	2:B:342:ASN:OD1	2.18	0.43
1:C:450:VAL:O	1:C:452:GLU:N	2.52	0.43
1:A:517:ASN:HD22	1:A:517:ASN:C	2.18	0.43
1:A:117:PRO:C	1:A:119:PHE:N	2.72	0.43
1:C:467:GLU:HG2	1:C:467:GLU:O	2.18	0.43
2:B:267:ARG:NH1	4:B:457:HOH:O	2.52	0.43
1:C:531:THR:HG22	1:C:532:PHE:N	2.34	0.43
2:D:236:GLN:HE22	2:D:263:LYS:CE	2.30	0.43
2:D:231:TYR:HD1	2:D:235:LEU:HD12	1.84	0.43
2:D:252:ASP:O	2:D:254:PRO:HD3	2.19	0.43
1:C:333:ILE:N	1:C:333:ILE:HD12	2.32	0.43
2:D:192:ILE:CD1	2:D:200:ILE:HG13	2.49	0.43
1:C:438:GLN:NE2	1:C:439:GLN:HE22	2.11	0.43
1:C:143:LEU:CD1	1:C:150:LEU:HD13	2.48	0.43
1:C:189:PHE:HB3	1:C:349:LYS:HZ2	1.84	0.43
1:C:416:MET:C	1:C:418:ASN:N	2.70	0.43
1:C:397:SER:OG	1:C:400:GLU:HG3	2.19	0.43
2:B:268:ALA:HB1	2:B:273:ILE:O	2.18	0.43
1:C:225:TRP:CD1	1:C:233:ILE:CG1	3.02	0.43
1:C:139:LEU:O	1:C:143:LEU:HG	2.19	0.43
2:D:85:VAL:C	2:D:87:ASN:H	2.23	0.43
2:B:190:ARG:HB2	2:B:320:ASN:O	2.19	0.43
1:C:226:TYR:CD1	1:C:231:GLY:O	2.72	0.42
1:C:213:PRO:HG3	1:C:334:ALA:HB1	2.01	0.42
1:C:33:VAL:O	1:C:57:PHE:HA	2.19	0.42
1:A:213:PRO:HB2	1:A:216:VAL:HG23	2.00	0.42
1:C:163:ARG:NH2	1:C:396:ARG:O	2.52	0.42
2:B:428:VAL:O	2:B:428:VAL:HG12	2.19	0.42
2:B:235:LEU:C	2:B:238:PRO:HD2	2.40	0.42
1:A:423:ILE:HD13	1:A:426:TYR:HB3	2.01	0.42
1:A:33:VAL:CG1	1:A:54:ILE:HD13	2.48	0.42
1:C:448:TYR:HD1	2:D:26:ARG:NH1	2.17	0.42
2:D:376:MET:CE	2:D:425:VAL:HG11	2.49	0.42
2:D:343:CYS:C	2:D:345:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:GLU:CG	2:D:279:ARG:HH12	2.32	0.42
2:B:303:CYS:O	2:B:307:VAL:HG23	2.18	0.42
2:D:207:TYR:C	2:D:209:PRO:HD2	2.39	0.42
1:C:234:PRO:O	1:C:235:LYS:C	2.58	0.42
1:A:33:VAL:HG22	1:A:34:CYS:N	2.34	0.42
1:C:75:PHE:CZ	1:C:96:LEU:HD11	2.55	0.42
1:C:227:SER:O	1:C:229:THR:N	2.52	0.42
1:C:383:LEU:HD12	1:C:383:LEU:O	2.18	0.42
1:A:403:GLY:HA3	1:A:406:THR:OG1	2.20	0.42
1:A:335:ASP:OD1	1:A:336:SER:N	2.53	0.42
2:D:35:PHE:HE1	2:D:314:ALA:HA	1.77	0.42
1:C:80:SER:O	1:C:81:ILE:C	2.58	0.42
2:D:210:GLN:HG2	2:D:211:VAL:H	1.81	0.42
2:D:224:LEU:HB2	2:D:227:HIS:CD2	2.55	0.42
2:D:279:ARG:HH11	2:D:279:ARG:HG3	1.83	0.42
1:C:217:ILE:HD11	1:C:264:ASN:HD22	1.84	0.42
2:D:169:LEU:HD22	2:D:195:GLY:O	2.20	0.42
1:A:488:ALA:C	1:A:490:PRO:HD3	2.39	0.42
2:D:368:LEU:HB3	2:D:376:MET:CE	2.50	0.42
2:D:64:LEU:HB3	2:D:111:LEU:HD13	2.02	0.42
2:D:159:ILE:HG23	2:D:162:LEU:HD12	2.00	0.42
1:A:225:TRP:HH2	1:A:242:ASP:HB3	1.85	0.42
1:A:212:THR:CG2	1:A:216:VAL:HB	2.49	0.42
1:A:186:ASP:C	1:A:188:PRO:HD3	2.40	0.42
1:C:182:ASP:OD1	1:C:182:ASP:O	2.38	0.42
1:C:488:ALA:C	1:C:490:PRO:HD3	2.40	0.42
2:B:158:LEU:HD22	2:B:175:VAL:HB	2.01	0.42
2:D:262:GLN:O	2:D:266:GLU:HG3	2.20	0.42
1:A:404:LEU:HD23	1:A:468:TYR:CE2	2.55	0.42
1:A:238:LYS:HG3	1:A:239:GLU:N	2.28	0.42
1:C:288:ILE:HD11	1:C:392:VAL:HG23	2.02	0.42
1:C:185:LEU:HD13	1:C:218:ILE:HG21	2.01	0.42
1:C:481:GLU:OE2	1:C:525:MET:HE2	2.19	0.42
2:D:35:PHE:HE1	2:D:314:ALA:CB	2.33	0.41
2:D:127:ILE:HA	2:D:127:ILE:HD13	1.79	0.41
1:C:233:ILE:O	1:C:234:PRO:C	2.59	0.41
2:B:381:ILE:HG22	2:B:382:THR:N	2.35	0.41
1:C:206:LYS:HG3	1:C:207:LYS:N	2.35	0.41
1:C:460:CYS:HB3	4:C:536:HOH:O	2.19	0.41
2:B:204:LEU:O	2:B:206:LEU:N	2.53	0.41
1:C:113:LEU:HD21	1:C:120:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:HG3	1:A:104:PHE:CZ	2.55	0.41
2:B:13:TRP:CH2	2:B:116:PRO:HG2	2.55	0.41
1:C:504:GLU:OE1	1:C:516:PHE:HD2	2.03	0.41
1:C:436:HIS:C	1:C:438:GLN:H	2.23	0.41
1:A:225:TRP:NE1	1:A:233:ILE:HG12	2.35	0.41
2:D:334:THR:HG22	2:D:335:PHE:N	2.34	0.41
1:A:486:GLY:O	2:B:22:LYS:NZ	2.53	0.41
2:D:80:MET:HG3	2:D:80:MET:O	2.20	0.41
2:D:233:ARG:CD	2:D:285:VAL:HA	2.51	0.41
1:C:163:ARG:CD	1:C:518:ASN:ND2	2.83	0.41
1:C:241:GLU:OE2	1:C:244:ARG:HD2	2.20	0.41
1:A:84:ASN:ND2	1:A:106:GLU:HG2	2.36	0.41
1:C:189:PHE:CB	1:C:349:LYS:NZ	2.83	0.41
1:C:78:ARG:HD3	1:C:81:ILE:CD1	2.51	0.41
2:D:226:GLU:CD	2:D:226:GLU:H	2.24	0.41
1:A:428:MET:HE2	1:A:479:VAL:HA	2.01	0.41
1:A:51:LEU:N	1:A:52:PRO:HD2	2.35	0.41
1:A:39:THR:HB	1:A:489:GLU:OE1	2.21	0.41
1:C:210:SER:HA	1:C:262:GLU:OE1	2.20	0.41
1:C:36:ILE:HG23	1:C:36:ILE:O	2.20	0.41
2:D:41:SER:C	2:D:43:GLN:N	2.73	0.41
1:A:444:GLY:HA3	1:A:483:CYS:O	2.21	0.41
1:C:373:GLU:O	1:C:373:GLU:HG2	2.21	0.41
2:D:425:VAL:CG2	2:D:436:PHE:HD1	2.33	0.41
1:C:84:ASN:O	1:C:87:GLU:HG2	2.21	0.41
1:C:236:THR:O	1:C:240:LYS:HG3	2.20	0.41
1:A:311:LEU:HD11	1:A:383:LEU:HD11	2.03	0.41
1:C:184:ARG:NH2	1:C:323:LEU:O	2.41	0.41
1:C:218:ILE:O	1:C:222:LEU:CB	2.67	0.41
2:B:62:GLU:HG3	4:B:446:HOH:O	2.19	0.41
1:C:49:LEU:HB3	1:C:54:ILE:HD13	2.02	0.41
2:D:162:LEU:HA	2:D:173:SER:OG	2.21	0.41
2:B:362:GLN:O	2:B:366:ASP:OD1	2.39	0.41
2:B:322:LEU:HD23	2:B:322:LEU:C	2.41	0.41
1:C:56:SER:HB3	1:C:101:SER:HB2	2.02	0.41
2:D:110:PHE:O	2:D:110:PHE:HD2	2.04	0.41
1:C:234:PRO:O	1:C:236:THR:N	2.53	0.41
2:D:43:GLN:O	2:D:45:LEU:N	2.54	0.41
2:D:44:PHE:CD1	2:D:44:PHE:O	2.73	0.41
2:D:249:LEU:CD1	2:D:256:HIS:HB2	2.51	0.41
2:D:249:LEU:HD13	2:D:256:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:HD22	2:B:26:ARG:HH21	1.69	0.41
2:B:31:THR:HG21	2:B:35:PHE:HB3	2.00	0.40
1:C:124:THR:HG22	1:C:125:VAL:HG23	2.03	0.40
1:C:78:ARG:C	1:C:80:SER:H	2.24	0.40
1:A:215:ILE:N	1:A:332:MET:HE3	2.36	0.40
2:D:84:ASP:CG	2:D:85:VAL:N	2.75	0.40
1:C:65:VAL:HB	1:C:81:ILE:HA	2.03	0.40
2:B:286:LYS:HB2	2:B:288:ILE:HG13	2.02	0.40
1:A:390:LEU:O	1:A:391:ARG:HG2	2.22	0.40
2:D:382:THR:HG23	2:D:390:ARG:C	2.42	0.40
2:D:430:THR:HA	2:D:431:PRO:HD3	1.87	0.40
2:D:36:GLU:HB3	2:D:38:SER:OG	2.21	0.40
1:A:373:GLU:C	1:A:375:ILE:N	2.75	0.40
2:B:241:GLN:NE2	2:B:246:GLY:H	2.19	0.40
2:B:263:LYS:HA	2:B:263:LYS:HD3	1.92	0.40
2:B:364:VAL:HG23	2:B:381:ILE:CD1	2.51	0.40
2:D:116:PRO:O	2:D:118:CYS:N	2.52	0.40
1:C:257:GLY:O	1:C:259:PRO:HD3	2.22	0.40
1:A:129:THR:HA	1:A:153:CYS:O	2.21	0.40
2:D:425:VAL:CG1	2:D:426:ALA:H	2.33	0.40
2:D:24:LEU:HD21	2:D:312:THR:HG21	2.04	0.40
1:C:28:LEU:HA	1:C:509:ILE:HG21	2.03	0.40
1:C:46:LEU:HD23	1:C:93:LEU:HD13	2.03	0.40
2:B:265:LEU:HD23	2:B:276:VAL:HB	2.03	0.40
2:B:372:ALA:O	2:B:375:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	527/537 (98%)	477 (90%)	39 (7%)	11 (2%)	9 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	524/537 (98%)	438 (84%)	65 (12%)	21 (4%)	4	4
2	B	387/444 (87%)	351 (91%)	24 (6%)	12 (3%)	5	8
2	D	372/444 (84%)	298 (80%)	54 (14%)	20 (5%)	2	2
All	All	1810/1962 (92%)	1564 (86%)	182 (10%)	64 (4%)	4	6

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
2	B	320	ASN
2	B	395	GLN
1	C	229	THR
1	C	234	PRO
1	C	235	LYS
1	C	255	GLU
1	C	256	ASN
1	C	446	SER
2	D	116	PRO
2	D	340	LYS
2	D	391	THR
1	A	230	ASN
1	A	438	GLN
1	A	450	VAL
2	B	205	GLU
2	B	379	PRO
2	B	392	LEU
2	B	393	TYR
1	C	83	LYS
1	C	333	ILE
1	C	448	TYR
1	C	451	GLU
2	D	117	ASN
2	D	274	ARG
2	D	275	GLY
1	A	236	THR
1	A	333	ILE
2	B	371	SER
2	B	394	LEU
1	C	186	ASP
1	C	318	GLU
1	C	445	VAL

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Mol	Chain	Res	Type
1	C	447	ASN
1	C	485	TYR
2	D	132	ASP
2	D	196	MET
2	D	209	PRO
2	D	320	ASN
2	D	371	SER
2	D	376	MET
1	A	36	ILE
2	B	92	PHE
2	B	380	ALA
1	C	254	ASN
1	C	257	GLY
2	D	44	PHE
1	A	106	GLU
1	A	368	ILE
1	A	372	PRO
1	C	38	ALA
1	C	252	LEU
2	D	205	GLU
2	D	345	ALA
2	D	390	ARG
2	B	209	PRO
1	C	190	PRO
2	D	249	LEU
2	D	434	VAL
2	B	116	PRO
2	D	350	PRO
1	A	234	PRO
2	D	379	PRO
1	C	371	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	461/467 (99%)	442 (96%)	19 (4%)	37	66
1	C	458/467 (98%)	445 (97%)	13 (3%)	51	78
2	B	335/387 (87%)	323 (96%)	12 (4%)	42	71
2	D	325/387 (84%)	317 (98%)	8 (2%)	55	81
All	All	1579/1708 (92%)	1527 (97%)	52 (3%)	45	73

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	115	ASN
1	A	154	ARG
1	A	163	ARG
1	A	213	PRO
1	A	253	LYS
1	A	255	GLU
1	A	264	ASN
1	A	272	VAL
1	A	396	ARG
1	A	405	ASP
1	A	410	ASP
1	A	418	ASN
1	A	423	ILE
1	A	424	VAL
1	A	430	ARG
1	A	441	ARG
1	A	458	LYS
1	A	517	ASN
2	B	114	ARG
2	B	116	PRO
2	B	128	GLN
2	B	131	ASN
2	B	165	GLU
2	B	201	GLU
2	B	215	MET
2	B	218	ILE
2	B	267	ARG
2	B	277	THR
2	B	325	ASN

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Mol	Chain	Res	Type
2	B	351	GLN
1	C	34	CYS
1	C	97	ASN
1	C	259	PRO
1	C	277	ASN
1	C	353	ASP
1	C	391	ARG
1	C	406	THR
1	C	414	SER
1	C	434	ARG
1	C	448	TYR
1	C	466	GLN
1	C	503	GLN
1	C	518	ASN
2	D	110	PHE
2	D	113	ASP
2	D	114	ARG
2	D	127	ILE
2	D	128	GLN
2	D	131	ASN
2	D	136	ARG
2	D	213	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	32	HIS
1	A	48	ASN
1	A	72	ASN
1	A	84	ASN
1	A	111	ASN
1	A	209	HIS
1	A	211	HIS
1	A	224	GLN
1	A	264	ASN
1	A	296	ASN
1	A	320	GLN
1	A	344	ASN
1	A	359	ASN
1	A	360	HIS
1	A	370	GLN

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Mol	Chain	Res	Type
1	A	418	ASN
1	A	421	ASN
1	A	438	GLN
1	A	439	GLN
1	A	447	ASN
1	A	480	HIS
1	A	503	GLN
1	A	517	ASN
1	A	518	ASN
2	B	19	HIS
2	B	32	HIS
2	B	87	ASN
2	B	117	ASN
2	B	125	ASN
2	B	128	GLN
2	B	131	ASN
2	B	139	HIS
2	B	227	HIS
2	B	236	GLN
2	B	262	GLN
2	B	325	ASN
2	B	348	GLN
2	B	351	GLN
1	C	37	ASN
1	C	72	ASN
1	C	84	ASN
1	C	97	ASN
1	C	111	ASN
1	C	130	GLN
1	C	145	ASN
1	C	147	GLN
1	C	273	ASN
1	C	277	ASN
1	C	322	ASN
1	C	359	ASN
1	C	370	GLN
1	C	439	GLN
1	C	512	GLN
1	C	518	ASN
1	C	527	GLN
2	D	43	GLN
2	D	74	GLN

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Mol	Chain	Res	Type
2	D	76	HIS
2	D	87	ASN
2	D	131	ASN
2	D	139	HIS
2	D	227	HIS
2	D	236	GLN
2	D	282	GLN
2	D	319	ASN
2	D	325	ASN
2	D	351	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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