



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:04 am BST

PDB ID : 1BPO  
Title : CLATHRIN HEAVY-CHAIN TERMINAL DOMAIN AND LINKER  
Authors : Harr, E.T.; Musacchio, A.; Harrison, S.C.; Kirchhausen, T.  
Deposited on : 1998-08-11  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

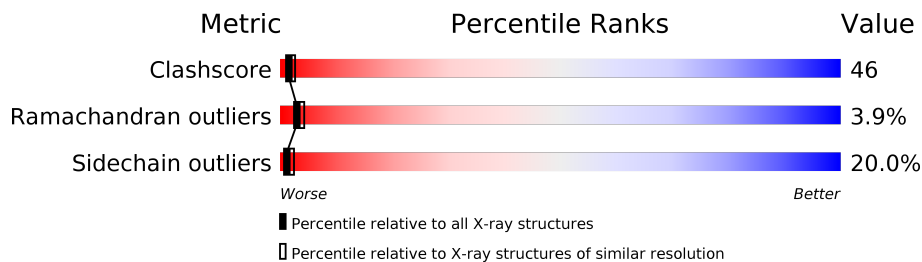
# 1 Overall quality at a glance

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	494	
1	B	494	
1	C	494	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11517 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 PROTEIN (CLATHRIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3812	2425	658	708	21	0	0	0
1	B	493	3858	2456	665	715	22	0	0	0
1	C	487	3812	2425	658	708	21	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total 16	O 16	0	0
2	B	9	Total 9	O 9	0	0
2	C	10	Total 10	O 10	0	0

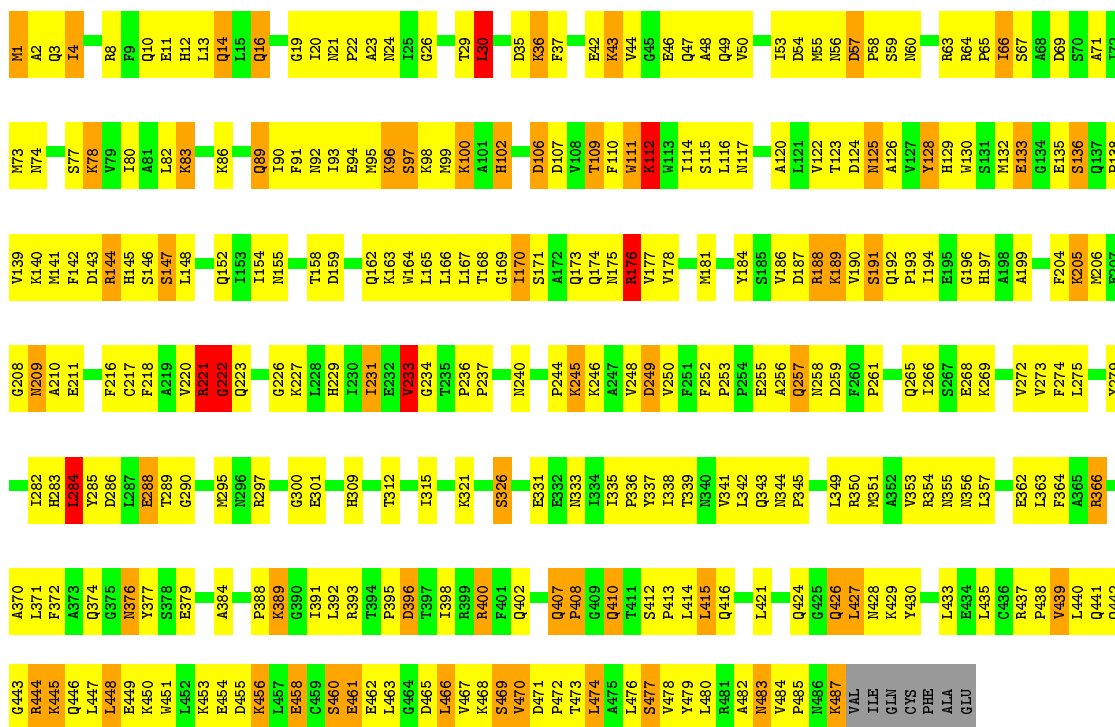
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

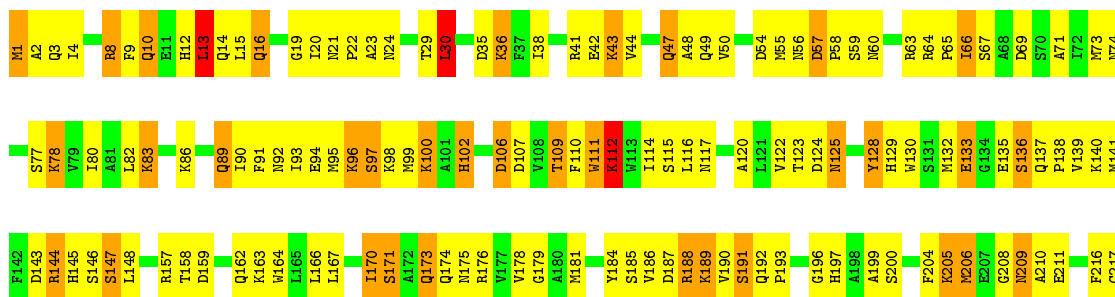
- Molecule 1: PROTEIN (CLATHRIN)

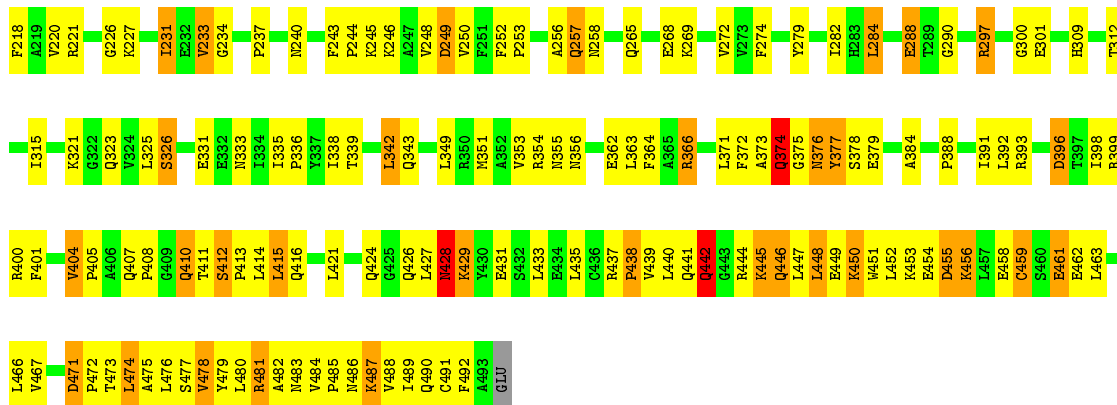
Chain A: 



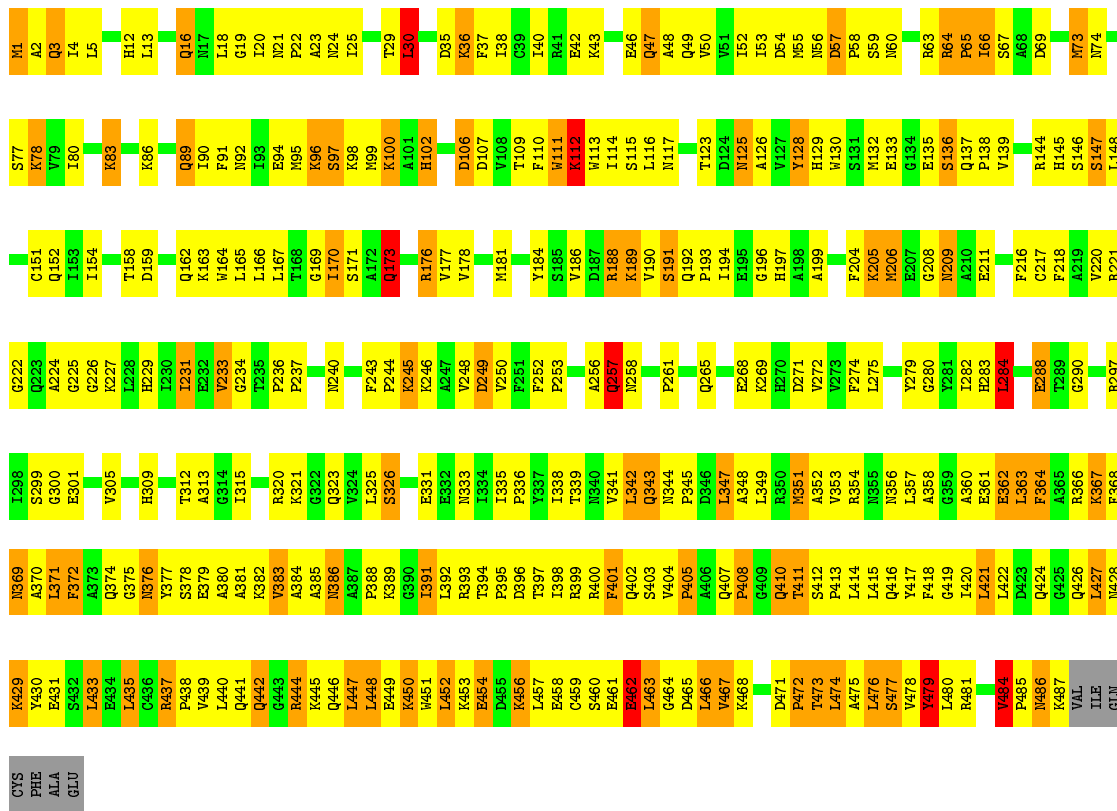
- Molecule 1: PROTEIN (CLATHRIN)

Chain B: 





• Molecule 1: PROTEIN (CLATHRIN)



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	205.82Å 205.82Å 87.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	95.0 (6.00-2.60)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.226 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11517	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	0.92	4/3889 (0.1%)	1.04	12/5270 (0.2%)
1	B	0.87	1/3936 (0.0%)	1.01	7/5334 (0.1%)
1	C	0.89	6/3889 (0.2%)	1.00	9/5270 (0.2%)
All	All	0.90	11/11714 (0.1%)	1.02	28/15874 (0.2%)

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	A	0	2
1	C	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	484	VAL	CB-CG2	15.09	1.84	1.52
1	A	174	GLN	CA-CB	-12.07	1.27	1.53
1	A	174	GLN	C-N	-7.87	1.16	1.34
1	A	222	GLY	C-N	-7.84	1.16	1.34
1	C	151	CYS	CB-SG	-6.16	1.71	1.82
1	C	484	VAL	C-N	5.90	1.45	1.34
1	C	305	VAL	CB-CG1	-5.41	1.41	1.52
1	B	491	CYS	CB-SG	5.11	1.91	1.82
1	A	233	VAL	CB-CG2	-5.10	1.42	1.52
1	C	471	ASP	C-N	-5.07	1.24	1.34
1	C	305	VAL	CB-CG2	-5.02	1.42	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLY	C-N-CA	14.03	156.78	121.70
1	A	222	GLY	O-C-N	-12.62	102.51	122.70
1	C	484	VAL	CA-CB-CG2	-12.56	92.06	110.90
1	B	174	GLN	CB-CA-C	11.42	133.23	110.40
1	A	222	GLY	CA-C-N	8.27	135.39	117.20
1	A	400	ARG	NE-CZ-NH1	-7.39	116.61	120.30
1	C	484	VAL	CG1-CB-CG2	-7.19	99.40	110.90
1	A	284	LEU	CA-CB-CG	7.10	131.63	115.30
1	C	284	LEU	CA-CB-CG	7.05	131.53	115.30
1	B	284	LEU	CA-CB-CG	7.03	131.47	115.30
1	C	457	LEU	CA-CB-CG	6.91	131.19	115.30
1	B	30	LEU	CA-CB-CG	6.69	130.69	115.30
1	B	13	LEU	CA-CB-CG	6.68	130.67	115.30
1	B	297	ARG	NE-CZ-NH1	-6.65	116.98	120.30
1	C	73	MET	CG-SD-CE	-6.65	89.57	100.20
1	A	30	LEU	CA-CB-CG	6.45	130.12	115.30
1	C	30	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	393	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	B	8	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	A	221	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	174	GLN	O-C-N	-5.53	113.86	122.70
1	B	41	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	64	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	357	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	38	ILE	N-CA-C	-5.30	96.69	111.00
1	C	65	PRO	N-CA-C	-5.17	98.65	112.10
1	A	427	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	176	ARG	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	GLY	Mainchain,Peptide
1	C	479	TYR	Sidechain

## 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	3812	0	3848	326	0
1	B	3858	0	3897	309	1
1	C	3812	0	3850	440	0
2	A	16	0	0	1	0
2	B	9	0	0	0	0
2	C	10	0	0	1	0
All	All	11517	0	11595	1055	1

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 46.

All (1055) 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:484:VAL:CB	1:C:484:VAL:CG2	1.84	1.55
1:B:21:ASN:HD21	1:B:23:ALA:HB3	1.12	1.12
1:C:173:GLN:OE1	1:C:173:GLN:HA	1.47	1.12
1:B:73:MET:HE1	1:B:80:ILE:HB	1.33	1.10
1:A:444:ARG:HH11	1:A:444:ARG:HB2	1.05	1.10
1:A:73:MET:HE1	1:A:80:ILE:HB	1.30	1.07
1:C:438:PRO:HA	1:C:441:GLN:HB2	1.37	1.06
1:A:21:ASN:HD21	1:A:23:ALA:HB3	1.20	1.04
1:C:73:MET:HE1	1:C:80:ILE:HB	1.35	1.02
1:B:21:ASN:ND2	1:B:23:ALA:HB3	1.75	1.02
1:C:442:GLN:HB3	1:C:444:ARG:CD	1.89	1.02
1:C:401:PHE:O	1:C:404:VAL:HB	1.61	1.01
1:B:1:MET:SD	1:C:1:MET:HA	2.03	0.99
1:C:374:GLN:HE21	1:C:376:ASN:HB2	1.28	0.97
1:C:484:VAL:CA	1:C:484:VAL:CG2	2.45	0.94
1:C:64:ARG:HH11	1:C:96:LYS:HE3	1.32	0.94
1:C:164:TRP:CE2	1:C:233:VAL:HG13	2.02	0.94
1:C:361:GLU:H	1:C:361:GLU:CD	1.70	0.94
1:B:123:THR:HG22	1:B:125:ASN:H	1.32	0.94
1:A:64:ARG:HH11	1:A:96:LYS:HE3	1.31	0.93
1:B:64:ARG:HH11	1:B:96:LYS:HE3	1.33	0.93
1:B:24:ASN:ND2	1:B:42:GLU:HG2	1.82	0.93
1:B:371:LEU:HD13	1:B:379:GLU:HB3	1.48	0.93
1:A:24:ASN:ND2	1:A:42:GLU:HG2	1.82	0.93
1:C:21:ASN:HD21	1:C:23:ALA:HB3	1.30	0.93
1:A:21:ASN:ND2	1:A:23:ALA:HB3	1.83	0.93
1:A:444:ARG:HH11	1:A:444:ARG:CB	1.81	0.92
1:A:73:MET:CE	1:A:80:ILE:HB	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:HG22	1:A:125:ASN:H	1.34	0.90
1:C:407:GLN:HE22	1:C:410:GLN:HE21	1.15	0.90
1:C:24:ASN:ND2	1:C:42:GLU:HG2	1.86	0.90
1:C:374:GLN:HG2	1:C:375:GLY:H	1.36	0.90
1:A:100:LYS:HE2	1:A:130:TRP:NE1	1.86	0.90
1:C:484:VAL:CG2	1:C:484:VAL:CG1	2.51	0.89
1:A:64:ARG:NH1	1:A:96:LYS:HE3	1.87	0.89
1:A:164:TRP:CE2	1:A:233:VAL:HG13	2.07	0.88
1:C:439:VAL:HG21	1:C:451:TRP:HH2	1.37	0.88
1:B:374:GLN:NE2	1:B:374:GLN:H	1.71	0.87
1:A:444:ARG:HB2	1:A:444:ARG:NH1	1.88	0.87
1:B:374:GLN:HE21	1:B:374:GLN:H	1.18	0.87
1:C:64:ARG:NH1	1:C:96:LYS:HE3	1.90	0.87
1:A:398:ILE:HD12	1:A:430:TYR:CD2	2.09	0.86
1:C:407:GLN:HE22	1:C:410:GLN:NE2	1.73	0.86
1:C:13:LEU:HD11	1:C:58:PRO:HB2	1.57	0.86
1:B:64:ARG:NH1	1:B:96:LYS:HE3	1.89	0.85
1:C:21:ASN:ND2	1:C:23:ALA:HB3	1.92	0.85
1:A:377:TYR:HB3	1:A:413:PRO:HB3	1.56	0.85
1:C:442:GLN:HB3	1:C:444:ARG:HD3	1.57	0.85
1:C:2:ALA:HB1	1:C:4:ILE:O	1.75	0.85
1:B:374:GLN:N	1:B:374:GLN:HE21	1.73	0.85
1:B:1:MET:SD	1:C:1:MET:HG2	2.16	0.84
1:C:50:VAL:HG23	1:C:66:ILE:HB	1.59	0.84
1:A:24:ASN:HD22	1:A:42:GLU:HG2	1.40	0.84
1:C:353:VAL:HG23	1:C:364:PHE:CZ	2.12	0.84
1:C:396:ASP:HA	1:C:399:ARG:NH1	1.93	0.84
1:C:173:GLN:HG2	1:C:178:VAL:HG21	1.56	0.84
1:A:309:HIS:HD2	1:A:312:THR:OG1	1.59	0.83
1:A:100:LYS:HE2	1:A:130:TRP:HE1	1.42	0.83
1:A:398:ILE:HD12	1:A:430:TYR:CE2	2.13	0.83
1:B:24:ASN:HD22	1:B:42:GLU:HG2	1.38	0.83
1:C:452:LEU:HD21	1:C:478:VAL:HG22	1.59	0.83
1:C:89:GLN:NE2	1:C:98:LYS:HD2	1.94	0.83
1:B:471:ASP:HB3	1:B:474:LEU:HB2	1.60	0.82
1:C:477:SER:O	1:C:481:ARG:HG2	1.80	0.82
1:C:89:GLN:HE21	1:C:98:LYS:HD2	1.45	0.82
1:B:73:MET:HE1	1:B:80:ILE:CB	2.09	0.82
1:C:398:ILE:HG23	1:C:414:LEU:HD11	1.60	0.82
1:C:438:PRO:CA	1:C:441:GLN:HB2	2.10	0.82
1:C:123:THR:HG22	1:C:125:ASN:H	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:PRO:HA	1:C:441:GLN:NE2	1.96	0.81
1:B:407:GLN:HG2	1:B:408:PRO:HD2	1.62	0.81
1:C:345:PRO:HA	1:C:348:ALA:HB3	1.63	0.81
1:A:216:PHE:HD2	1:A:231:ILE:HD11	1.47	0.80
1:B:9:PHE:CD2	1:C:5:LEU:HD23	2.16	0.80
1:C:176:ARG:HD3	1:C:177:VAL:H	1.45	0.80
1:C:394:THR:O	1:C:397:THR:HB	1.81	0.80
1:C:450:LYS:O	1:C:454:GLU:HG3	1.82	0.80
1:C:374:GLN:NE2	1:C:376:ASN:HB2	1.95	0.80
1:C:271:ASP:HB2	1:C:354:ARG:NH2	1.96	0.79
1:B:477:SER:O	1:B:481:ARG:HG2	1.81	0.79
1:C:386:ASN:N	1:C:386:ASN:HD22	1.79	0.79
1:A:92:ASN:OD1	1:A:94:GLU:HB3	1.83	0.78
1:C:412:SER:O	1:C:416:GLN:HG3	1.83	0.78
1:B:50:VAL:HG23	1:B:66:ILE:HB	1.65	0.78
1:C:448:LEU:HD21	1:C:474:LEU:HG	1.65	0.78
1:B:439:VAL:HG13	1:B:444:ARG:HB2	1.63	0.78
1:C:413:PRO:HA	1:C:416:GLN:HB2	1.65	0.78
1:C:74:ASN:HD22	1:C:77:SER:H	1.31	0.78
1:B:175:ASN:O	1:B:176:ARG:HD3	1.84	0.77
1:C:24:ASN:HD22	1:C:42:GLU:HG2	1.47	0.77
1:C:271:ASP:HB2	1:C:354:ARG:HH21	1.49	0.77
1:B:450:LYS:O	1:B:454:GLU:HG3	1.85	0.77
1:C:363:LEU:HD12	1:C:363:LEU:H	1.49	0.77
1:A:449:GLU:HG3	1:A:474:LEU:HD11	1.65	0.77
1:C:176:ARG:HD3	1:C:177:VAL:N	1.99	0.77
1:C:382:LYS:HA	1:C:420:ILE:HD13	1.66	0.77
1:A:89:GLN:NE2	1:A:98:LYS:HD2	1.99	0.76
1:A:221:ARG:HG3	1:A:252:PHE:CE1	2.20	0.76
1:C:428:ASN:OD1	1:C:431:GLU:HB2	1.86	0.76
1:A:50:VAL:HG23	1:A:66:ILE:HB	1.68	0.76
1:A:181:MET:CE	1:A:196:GLY:HA3	2.16	0.75
1:C:371:LEU:HD13	1:C:380:ALA:HA	1.67	0.75
1:B:100:LYS:HE2	1:B:130:TRP:NE1	2.02	0.75
1:C:438:PRO:HA	1:C:441:GLN:CB	2.15	0.75
1:C:353:VAL:HG23	1:C:364:PHE:HZ	1.49	0.75
1:B:12:HIS:NE2	1:B:326:SER:HB3	2.02	0.75
1:A:74:ASN:HD22	1:A:77:SER:H	1.32	0.75
1:B:216:PHE:HD2	1:B:231:ILE:HD11	1.48	0.74
1:C:361:GLU:HA	1:C:391:ILE:HD12	1.68	0.74
1:A:89:GLN:HE21	1:A:98:LYS:HD2	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:SER:OG	1:B:173:GLN:NE2	2.20	0.74
1:C:216:PHE:HD2	1:C:231:ILE:HD11	1.51	0.74
1:C:92:ASN:OD1	1:C:94:GLU:HB3	1.87	0.74
1:A:301:GLU:HG3	1:A:321:LYS:HD3	1.67	0.74
1:C:391:ILE:HG23	1:C:392:LEU:HG	1.70	0.74
1:A:176:ARG:CG	1:A:177:VAL:H	1.99	0.74
1:C:413:PRO:HG3	1:C:416:GLN:NE2	2.03	0.73
1:A:412:SER:OG	1:A:415:LEU:HD23	1.88	0.73
1:A:170:ILE:HB	1:A:177:VAL:HG12	1.69	0.73
1:C:73:MET:HE1	1:C:80:ILE:CB	2.17	0.73
1:A:220:VAL:O	1:A:226:GLY:HA2	1.88	0.73
1:A:12:HIS:NE2	1:A:326:SER:HB3	2.04	0.73
1:B:90:ILE:O	1:B:99:MET:HB2	1.88	0.73
1:A:171:SER:O	1:A:178:VAL:HG22	1.88	0.73
1:B:164:TRP:CE2	1:B:233:VAL:HG13	2.23	0.72
1:B:73:MET:CE	1:B:80:ILE:HB	2.15	0.72
1:B:373:ALA:O	1:B:375:GLY:N	2.22	0.72
1:A:473:THR:HG23	1:C:171:SER:HA	1.71	0.72
1:C:433:LEU:O	1:C:437:ARG:HB2	1.89	0.72
1:C:442:GLN:HB3	1:C:444:ARG:HD2	1.71	0.72
1:A:442:GLN:CB	1:A:444:ARG:HH12	2.02	0.72
1:B:453:LYS:C	1:B:455:ASP:H	1.92	0.72
1:C:484:VAL:CG2	1:C:484:VAL:C	2.58	0.72
1:C:407:GLN:NE2	1:C:410:GLN:HE21	1.87	0.72
1:B:309:HIS:HD2	1:B:312:THR:OG1	1.71	0.72
1:C:222:GLY:O	1:C:225:GLY:N	2.23	0.72
1:C:412:SER:C	1:C:416:GLN:HG3	2.11	0.71
1:A:148:LEU:HD22	1:A:167:LEU:HD23	1.73	0.71
1:C:338:ILE:HA	1:C:342:LEU:HB2	1.71	0.71
1:B:92:ASN:OD1	1:B:94:GLU:HB3	1.90	0.71
1:C:435:LEU:O	1:C:438:PRO:HD2	1.90	0.71
1:A:166:LEU:HD22	1:A:216:PHE:HE1	1.55	0.71
1:C:374:GLN:HE21	1:C:376:ASN:CB	2.01	0.71
1:C:407:GLN:O	1:C:410:GLN:HG2	1.90	0.71
1:B:453:LYS:O	1:B:455:ASP:OD2	2.08	0.70
1:C:181:MET:CE	1:C:196:GLY:HA3	2.21	0.70
1:A:301:GLU:HG3	1:A:321:LYS:CD	2.20	0.70
1:C:253:PRO:HD2	1:C:256:ALA:CB	2.21	0.70
1:B:407:GLN:HG2	1:B:408:PRO:CD	2.21	0.70
1:C:439:VAL:HG21	1:C:451:TRP:CH2	2.24	0.70
1:A:181:MET:HE1	1:A:196:GLY:HA3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:PHE:C	1:C:366:ARG:H	1.93	0.70
1:A:456:LYS:HZ2	1:A:456:LYS:HB3	1.56	0.70
1:B:116:LEU:HD22	1:B:116:LEU:H	1.56	0.70
1:B:440:LEU:HD21	1:B:448:LEU:HD22	1.72	0.69
1:A:412:SER:O	1:A:416:GLN:HG3	1.92	0.69
1:B:158:THR:HG22	1:B:159:ASP:O	1.92	0.69
1:B:272:VAL:HG11	1:B:284:LEU:HD13	1.75	0.69
1:C:486:ASN:O	1:C:487:LYS:HG3	1.92	0.69
1:C:445:LYS:O	1:C:449:GLU:HG3	1.91	0.69
1:C:484:VAL:HG23	1:C:484:VAL:C	2.13	0.69
1:A:158:THR:HG21	1:A:162:GLN:HG2	1.74	0.69
1:B:428:ASN:N	1:B:428:ASN:OD1	2.23	0.69
1:C:486:ASN:O	1:C:487:LYS:CG	2.41	0.69
1:B:297:ARG:HH21	1:B:300:GLY:HA2	1.58	0.68
1:B:439:VAL:HA	1:B:442:GLN:HE21	1.59	0.68
1:C:145:HIS:NE2	1:C:193:PRO:HG3	2.09	0.68
1:B:301:GLU:HG3	1:B:321:LYS:HD3	1.75	0.68
1:A:471:ASP:HB3	1:A:474:LEU:HB2	1.75	0.68
1:A:476:LEU:HD21	1:C:170:ILE:HD12	1.75	0.68
1:B:91:PHE:CE2	1:B:96:LYS:HE2	2.29	0.68
1:C:468:LYS:HD3	1:C:475:ALA:HB3	1.76	0.68
1:A:86:LYS:HE3	1:A:107:ASP:CG	2.13	0.68
1:A:73:MET:HE1	1:A:80:ILE:CB	2.18	0.68
1:B:220:VAL:O	1:B:226:GLY:HA2	1.94	0.68
1:A:117:ASN:HB2	1:A:132:MET:HG2	1.76	0.68
1:B:396:ASP:HA	1:B:399:ARG:HD2	1.74	0.68
1:B:297:ARG:NH2	1:B:300:GLY:HA2	2.09	0.68
1:A:100:LYS:HG2	1:A:130:TRP:CZ2	2.30	0.67
1:A:476:LEU:HD11	1:C:177:VAL:HG22	1.76	0.67
1:C:382:LYS:HA	1:C:420:ILE:CD1	2.24	0.67
1:B:166:LEU:HD22	1:B:216:PHE:HE1	1.59	0.67
1:C:139:VAL:HG12	1:C:139:VAL:O	1.94	0.67
1:B:376:ASN:O	1:B:378:SER:N	2.27	0.67
1:C:100:LYS:HE2	1:C:130:TRP:NE1	2.10	0.67
1:C:363:LEU:CD1	1:C:363:LEU:H	2.04	0.67
1:B:373:ALA:C	1:B:375:GLY:N	2.46	0.67
1:C:269:LYS:HE2	1:C:331:GLU:OE2	1.95	0.67
1:C:417:TYR:C	1:C:419:GLY:H	1.94	0.67
1:C:467:VAL:HG11	1:C:474:LEU:HD12	1.77	0.67
1:A:91:PHE:CE2	1:A:96:LYS:HE2	2.29	0.67
1:B:158:THR:HG21	1:B:162:GLN:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:HIS:HD2	1:B:221:ARG:H	1.42	0.67
1:A:176:ARG:HG2	1:A:177:VAL:H	1.60	0.66
1:B:371:LEU:HD13	1:B:379:GLU:CB	2.21	0.66
1:C:16:GLN:OE1	1:C:22:PRO:HB3	1.94	0.66
1:A:269:LYS:HE2	1:A:331:GLU:OE2	1.96	0.66
1:B:428:ASN:OD1	1:B:431:GLU:OE1	2.13	0.66
1:B:477:SER:O	1:B:481:ARG:CG	2.43	0.66
1:B:1:MET:CG	1:C:1:MET:HA	2.26	0.66
1:B:301:GLU:HG3	1:B:321:LYS:CD	2.26	0.66
1:C:421:LEU:HD13	1:C:431:GLU:OE1	1.96	0.66
1:C:426:GLN:CD	1:C:458:GLU:HB2	2.16	0.66
1:C:220:VAL:O	1:C:226:GLY:HA2	1.96	0.66
1:C:117:ASN:HB2	1:C:132:MET:HG2	1.78	0.66
1:B:128:TYR:O	1:B:129:HIS:HD2	1.78	0.66
1:C:421:LEU:HA	1:C:424:GLN:HB2	1.78	0.66
1:B:148:LEU:HD22	1:B:167:LEU:HD23	1.76	0.65
1:A:227:LYS:HD3	1:A:249:ASP:HA	1.76	0.65
1:B:117:ASN:HB2	1:B:132:MET:HG2	1.77	0.65
1:B:439:VAL:HA	1:B:442:GLN:NE2	2.11	0.65
1:C:166:LEU:HD22	1:C:216:PHE:HE1	1.61	0.65
1:C:447:LEU:HD23	1:C:451:TRP:CZ2	2.31	0.65
1:A:154:ILE:HD13	1:A:170:ILE:HG12	1.79	0.65
1:A:90:ILE:O	1:A:99:MET:HB2	1.95	0.65
1:C:438:PRO:O	1:C:441:GLN:HB2	1.95	0.65
1:C:211:GLU:HB2	1:C:240:ASN:OD1	1.97	0.65
1:C:402:GLN:C	1:C:404:VAL:H	1.99	0.65
1:C:158:THR:HG22	1:C:159:ASP:O	1.95	0.65
1:B:463:LEU:O	1:B:467:VAL:HG23	1.97	0.65
1:B:190:VAL:HG12	1:B:191:SER:N	2.12	0.65
1:A:91:PHE:HE2	1:A:96:LYS:HE2	1.62	0.64
1:B:211:GLU:HB2	1:B:240:ASN:OD1	1.97	0.64
1:A:158:THR:HG22	1:A:159:ASP:O	1.97	0.64
1:A:190:VAL:HG12	1:A:191:SER:N	2.11	0.64
1:A:461:GLU:HG3	1:A:484:VAL:HG11	1.80	0.64
1:A:350:ARG:NH2	2:A:505:HOH:O	2.30	0.64
1:A:211:GLU:HB2	1:A:240:ASN:OD1	1.96	0.64
1:A:1:MET:O	1:A:3:GLN:OE1	2.14	0.64
1:A:116:LEU:HD22	1:A:116:LEU:H	1.62	0.64
1:A:173:GLN:CD	1:A:178:VAL:HG21	2.18	0.64
1:A:343:GLN:O	1:A:345:PRO:HD3	1.98	0.64
1:A:86:LYS:HE3	1:A:107:ASP:OD1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLN:OE1	1:B:22:PRO:HB3	1.97	0.64
1:C:158:THR:HG21	1:C:162:GLN:HG2	1.79	0.64
1:C:476:LEU:HD23	1:C:476:LEU:C	2.18	0.64
1:C:309:HIS:HD2	1:C:312:THR:OG1	1.81	0.64
1:C:362:GLU:HG2	1:C:363:LEU:N	2.12	0.64
1:C:413:PRO:CG	1:C:416:GLN:HE21	2.11	0.64
1:C:440:LEU:HD11	1:C:467:VAL:HG22	1.80	0.64
1:A:439:VAL:HG11	1:A:447:LEU:HD23	1.80	0.64
1:B:158:THR:HG23	1:B:162:GLN:HA	1.80	0.64
1:B:384:ALA:HA	1:B:392:LEU:HD12	1.80	0.64
1:C:301:GLU:HG3	1:C:321:LYS:HD3	1.80	0.64
1:C:116:LEU:H	1:C:116:LEU:HD22	1.63	0.63
1:C:158:THR:HG23	1:C:162:GLN:HA	1.79	0.63
1:C:347:LEU:HD12	1:C:347:LEU:O	1.98	0.63
1:B:373:ALA:C	1:B:375:GLY:H	2.01	0.63
1:A:272:VAL:HG11	1:A:284:LEU:HD13	1.80	0.63
1:A:339:THR:O	1:A:343:GLN:HA	1.98	0.63
1:C:417:TYR:C	1:C:419:GLY:N	2.52	0.63
1:B:231:ILE:O	1:B:231:ILE:HG12	1.97	0.63
1:C:301:GLU:HG3	1:C:321:LYS:CD	2.29	0.63
1:C:353:VAL:HG22	1:C:386:ASN:O	1.99	0.63
1:C:413:PRO:HG3	1:C:416:GLN:HE21	1.61	0.63
1:C:91:PHE:CE2	1:C:96:LYS:HE2	2.34	0.63
1:C:369:ASN:N	1:C:369:ASN:OD1	2.30	0.63
1:A:158:THR:HG23	1:A:162:GLN:HA	1.80	0.63
1:B:393:ARG:NH2	1:B:431:GLU:OE1	2.29	0.63
1:A:188:ARG:O	1:A:190:VAL:N	2.31	0.63
1:B:95:MET:HG3	1:B:97:SER:OG	1.99	0.63
1:C:197:HIS:HD2	1:C:221:ARG:H	1.45	0.63
1:B:145:HIS:NE2	1:B:193:PRO:HG3	2.14	0.62
1:B:269:LYS:HE2	1:B:331:GLU:OE2	1.99	0.62
1:A:442:GLN:HB3	1:A:444:ARG:HH12	1.64	0.62
1:B:24:ASN:HD22	1:B:42:GLU:CG	2.11	0.62
1:A:237:PRO:HD2	1:A:240:ASN:OD1	1.99	0.62
1:C:372:PHE:CE2	1:C:400:ARG:HD2	2.34	0.62
1:A:145:HIS:NE2	1:A:193:PRO:HG3	2.14	0.62
1:A:371:LEU:HD13	1:A:379:GLU:HB3	1.80	0.62
1:B:221:ARG:HA	1:B:226:GLY:HA2	1.81	0.62
1:A:274:PHE:CD2	1:A:284:LEU:HD22	2.35	0.62
1:B:65:PRO:O	1:B:66:ILE:HG13	1.98	0.62
1:B:237:PRO:HD2	1:B:240:ASN:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:TYR:O	1:C:419:GLY:N	2.33	0.62
1:B:450:LYS:HG2	1:B:454:GLU:CD	2.20	0.62
1:B:91:PHE:HE2	1:B:96:LYS:HE2	1.63	0.62
1:C:363:LEU:N	1:C:363:LEU:HD12	2.14	0.62
1:C:368:PHE:HD2	1:C:400:ARG:CZ	2.13	0.62
1:C:368:PHE:HD2	1:C:400:ARG:NH2	1.97	0.62
1:C:440:LEU:HD12	1:C:466:LEU:HD23	1.81	0.62
1:B:438:PRO:HG2	1:B:439:VAL:H	1.65	0.61
1:B:86:LYS:HE3	1:B:107:ASP:CG	2.20	0.61
1:C:466:LEU:O	1:C:468:LYS:N	2.33	0.61
1:C:90:ILE:O	1:C:99:MET:HB2	1.98	0.61
1:C:86:LYS:HE3	1:C:107:ASP:CG	2.20	0.61
1:C:181:MET:HE1	1:C:196:GLY:HA3	1.80	0.61
1:B:100:LYS:HE2	1:B:130:TRP:HE1	1.65	0.61
1:C:323:GLN:OE1	1:C:325:LEU:HD21	2.00	0.61
1:B:412:SER:O	1:B:416:GLN:HG3	1.99	0.61
1:B:454:GLU:HB3	1:B:456:LYS:HZ1	1.65	0.61
1:A:106:ASP:N	1:A:106:ASP:OD2	2.34	0.61
1:A:197:HIS:HD2	1:A:221:ARG:H	1.48	0.61
1:A:204:PHE:CZ	1:A:288:GLU:HB2	2.36	0.61
1:A:370:ALA:O	1:A:374:GLN:HG3	2.00	0.61
1:C:106:ASP:N	1:C:106:ASP:OD2	2.33	0.61
1:A:442:GLN:HB2	1:A:444:ARG:HH12	1.65	0.61
1:C:145:HIS:ND1	1:C:146:SER:N	2.49	0.61
1:C:253:PRO:HD2	1:C:256:ALA:HB3	1.82	0.61
1:C:99:MET:O	1:C:100:LYS:HB2	2.01	0.61
1:C:16:GLN:NE2	1:C:22:PRO:HG3	2.15	0.61
1:A:449:GLU:O	1:A:453:LYS:HE3	2.01	0.60
1:A:176:ARG:HG2	1:A:177:VAL:HG23	1.83	0.60
1:B:166:LEU:HD22	1:B:216:PHE:CE1	2.36	0.60
1:A:429:LYS:HG3	1:A:458:GLU:OE2	2.01	0.60
1:A:99:MET:O	1:A:100:LYS:HB2	2.00	0.60
1:C:227:LYS:HD3	1:C:249:ASP:HA	1.81	0.60
1:C:438:PRO:HA	1:C:441:GLN:HE21	1.66	0.60
1:B:211:GLU:CB	1:B:237:PRO:HG2	2.31	0.60
1:C:407:GLN:NE2	1:C:408:PRO:O	2.34	0.60
1:C:438:PRO:C	1:C:441:GLN:HB2	2.21	0.60
1:A:102:HIS:CE1	1:A:138:PRO:HD2	2.36	0.60
1:B:197:HIS:CD2	1:B:221:ARG:H	2.19	0.60
1:C:462:GLU:O	1:C:463:LEU:C	2.40	0.60
1:B:166:LEU:CD2	1:B:216:PHE:HE1	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:HIS:ND1	1:A:146:SER:N	2.50	0.60
1:B:99:MET:O	1:B:100:LYS:HB2	2.01	0.60
1:A:188:ARG:O	1:A:190:VAL:HG23	2.01	0.60
1:C:102:HIS:CE1	1:C:138:PRO:HD2	2.37	0.60
1:C:91:PHE:HE2	1:C:96:LYS:HE2	1.66	0.60
1:B:106:ASP:N	1:B:106:ASP:OD2	2.35	0.60
1:B:253:PRO:HD2	1:B:256:ALA:CB	2.31	0.60
1:C:385:ALA:C	1:C:386:ASN:HD22	2.05	0.60
1:A:410:GLN:N	1:A:410:GLN:CD	2.55	0.59
1:A:24:ASN:HD22	1:A:42:GLU:CG	2.12	0.59
1:A:440:LEU:HD12	1:A:466:LEU:HD23	1.85	0.59
1:C:188:ARG:O	1:C:190:VAL:HG23	2.02	0.59
1:C:204:PHE:CZ	1:C:288:GLU:HB2	2.37	0.59
1:A:471:ASP:OD1	1:A:472:PRO:HD2	2.02	0.59
1:C:404:VAL:CG2	1:C:405:PRO:HD2	2.31	0.59
1:B:86:LYS:HE3	1:B:107:ASP:OD1	2.02	0.59
1:C:367:LYS:O	1:C:370:ALA:HB3	2.02	0.59
1:C:272:VAL:HG11	1:C:284:LEU:HD13	1.83	0.59
1:A:338:ILE:HA	1:A:342:LEU:HB2	1.85	0.59
1:B:211:GLU:HB2	1:B:237:PRO:HG2	1.85	0.59
1:B:373:ALA:HB3	1:B:374:GLN:NE2	2.17	0.59
1:A:477:SER:HB2	1:C:152:GLN:OE1	2.02	0.59
1:C:197:HIS:CD2	1:C:221:ARG:H	2.21	0.59
1:B:16:GLN:NE2	1:B:22:PRO:HG3	2.18	0.59
1:C:413:PRO:HA	1:C:416:GLN:CB	2.31	0.59
1:B:181:MET:CE	1:B:196:GLY:HA3	2.33	0.59
1:B:472:PRO:O	1:B:492:PHE:CE2	2.56	0.59
1:B:248:VAL:HG21	1:B:290:GLY:O	2.02	0.58
1:C:371:LEU:O	1:C:374:GLN:HB3	2.02	0.58
1:A:170:ILE:HB	1:A:177:VAL:CG1	2.32	0.58
1:A:216:PHE:CD2	1:A:231:ILE:HD11	2.35	0.58
1:B:216:PHE:CD2	1:B:231:ILE:HD11	2.36	0.58
1:B:453:LYS:C	1:B:455:ASP:N	2.56	0.58
1:A:128:TYR:N	1:A:128:TYR:CD1	2.71	0.58
1:A:244:PRO:O	1:A:246:LYS:HD2	2.04	0.58
1:C:221:ARG:HA	1:C:226:GLY:HA2	1.85	0.58
1:A:16:GLN:OE1	1:A:22:PRO:HB3	2.04	0.58
1:A:463:LEU:O	1:A:467:VAL:HG23	2.04	0.58
1:A:421:LEU:HB3	1:A:427:LEU:HD23	1.84	0.58
1:B:208:GLY:C	1:B:209:ASN:HD22	2.07	0.58
1:B:437:ARG:O	1:B:441:GLN:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:TYR:CD1	1:C:128:TYR:N	2.70	0.58
1:C:208:GLY:C	1:C:209:ASN:HD22	2.06	0.58
1:B:181:MET:HE1	1:B:218:PHE:CD1	2.39	0.58
1:C:360:ALA:O	1:C:364:PHE:HB2	2.03	0.58
1:A:398:ILE:HD12	1:A:430:TYR:HD2	1.63	0.57
1:B:188:ARG:O	1:B:190:VAL:HG23	2.03	0.57
1:C:244:PRO:O	1:C:246:LYS:HD2	2.04	0.57
1:C:361:GLU:N	1:C:361:GLU:CD	2.49	0.57
1:A:454:GLU:O	1:A:455:ASP:HB2	2.04	0.57
1:A:197:HIS:CD2	1:A:221:ARG:H	2.21	0.57
1:B:244:PRO:O	1:B:246:LYS:HD2	2.03	0.57
1:B:1:MET:SD	1:C:1:MET:CG	2.90	0.57
1:C:297:ARG:NH2	1:C:300:GLY:HA2	2.19	0.57
1:C:367:LYS:O	1:C:371:LEU:HD12	2.04	0.57
1:C:381:ALA:HB2	1:C:401:PHE:CZ	2.39	0.57
1:A:461:GLU:HG3	1:A:484:VAL:CG1	2.34	0.57
1:C:12:HIS:CD2	1:C:326:SER:HB3	2.39	0.57
1:C:372:PHE:CD1	1:C:377:TYR:HD2	2.22	0.57
1:B:428:ASN:O	1:B:458:GLU:HB3	2.05	0.57
1:C:402:GLN:O	1:C:404:VAL:N	2.32	0.57
1:A:455:ASP:HB3	1:C:69:ASP:OD1	2.04	0.57
1:B:145:HIS:ND1	1:B:147:SER:OG	2.36	0.57
1:B:482:ALA:O	1:B:483:ASN:HB3	2.04	0.57
1:A:297:ARG:NH2	1:A:300:GLY:HA2	2.20	0.57
1:B:9:PHE:HD2	1:C:5:LEU:HD23	1.67	0.57
1:C:231:ILE:O	1:C:231:ILE:HG12	2.03	0.57
1:C:364:PHE:C	1:C:366:ARG:N	2.57	0.57
1:A:190:VAL:CG1	1:A:191:SER:N	2.68	0.56
1:B:475:ALA:HB3	1:B:492:PHE:HZ	1.69	0.56
1:A:476:LEU:HD21	1:C:170:ILE:CD1	2.34	0.56
1:B:114:ILE:O	1:B:115:SER:HB3	2.05	0.56
1:B:171:SER:CB	1:B:173:GLN:NE2	2.68	0.56
1:B:471:ASP:CB	1:B:474:LEU:HB2	2.34	0.56
1:C:485:PRO:C	1:C:487:LYS:H	2.06	0.56
1:A:454:GLU:CB	1:A:456:LYS:HD2	2.35	0.56
1:A:73:MET:HE2	1:A:80:ILE:HG13	1.87	0.56
1:C:12:HIS:NE2	1:C:326:SER:HB3	2.20	0.56
1:C:377:TYR:CE1	1:C:405:PRO:HG2	2.40	0.56
1:C:412:SER:HB3	1:C:415:LEU:HD23	1.86	0.56
1:A:148:LEU:CD2	1:A:167:LEU:HD23	2.35	0.56
1:C:386:ASN:N	1:C:386:ASN:ND2	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:HG22	1:A:222:GLY:H	1.69	0.56
1:B:190:VAL:CG1	1:B:191:SER:N	2.69	0.56
1:C:412:SER:O	1:C:416:GLN:N	2.37	0.56
1:A:73:MET:CE	1:A:80:ILE:CB	2.82	0.56
1:B:21:ASN:HD21	1:B:23:ALA:CB	2.02	0.56
1:B:354:ARG:HG2	1:B:355:ASN:ND2	2.20	0.56
1:C:148:LEU:HD22	1:C:167:LEU:HD23	1.87	0.56
1:C:227:LYS:HA	1:C:249:ASP:HA	1.88	0.56
1:A:199:ALA:HB2	1:A:218:PHE:CB	2.36	0.56
1:A:231:ILE:O	1:A:231:ILE:HG12	2.05	0.56
1:A:412:SER:OG	1:A:415:LEU:CD2	2.54	0.56
1:B:204:PHE:CZ	1:B:288:GLU:HB2	2.41	0.56
1:C:164:TRP:CD2	1:C:233:VAL:HG13	2.39	0.56
1:C:372:PHE:C	1:C:374:GLN:H	2.09	0.56
1:A:426:GLN:HG3	1:A:427:LEU:N	2.20	0.56
1:A:444:ARG:HG2	1:A:446:GLN:OE1	2.06	0.56
1:B:486:ASN:O	1:B:489:ILE:N	2.37	0.56
1:C:449:GLU:HG2	1:C:474:LEU:HD21	1.87	0.56
1:C:484:VAL:HB	1:C:485:PRO:HD2	1.88	0.56
1:A:166:LEU:HD22	1:A:216:PHE:CE1	2.38	0.56
1:A:454:GLU:HB3	1:A:456:LYS:HD2	1.87	0.56
1:B:145:HIS:ND1	1:B:146:SER:N	2.53	0.56
1:C:309:HIS:CD2	1:C:312:THR:HG23	2.40	0.56
1:C:368:PHE:CD2	1:C:400:ARG:CZ	2.88	0.56
1:C:442:GLN:HG2	1:C:444:ARG:NH1	2.21	0.56
1:C:462:GLU:C	1:C:464:GLY:N	2.58	0.56
1:C:164:TRP:HZ2	1:C:234:GLY:CA	2.19	0.55
1:A:21:ASN:HD21	1:A:23:ALA:CB	2.08	0.55
1:A:440:LEU:HD11	1:A:467:VAL:HG22	1.89	0.55
1:A:479:TYR:O	1:A:483:ASN:N	2.37	0.55
1:A:71:ALA:HB1	1:A:80:ILE:HD11	1.88	0.55
1:A:95:MET:HG3	1:A:97:SER:OG	2.06	0.55
1:C:47:GLN:HG3	1:C:48:ALA:N	2.22	0.55
1:A:199:ALA:HB2	1:A:218:PHE:HB2	1.88	0.55
1:C:199:ALA:HB2	1:C:218:PHE:HB2	1.88	0.55
1:C:448:LEU:HG	1:C:449:GLU:N	2.20	0.55
1:B:13:LEU:HD11	1:B:15:LEU:CD2	2.37	0.55
1:A:221:ARG:HA	1:A:226:GLY:HA2	1.88	0.55
1:B:99:MET:O	1:B:100:LYS:CB	2.55	0.55
1:C:216:PHE:CD2	1:C:231:ILE:HD11	2.39	0.55
1:C:379:GLU:HA	1:C:379:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:GLU:O	1:C:464:GLY:N	2.39	0.55
1:C:57:ASP:CG	1:C:60:ASN:HD22	2.09	0.55
1:A:173:GLN:NE2	1:A:178:VAL:HG21	2.21	0.55
1:C:24:ASN:HD22	1:C:42:GLU:CG	2.18	0.55
1:A:69:ASP:HB2	1:A:83:LYS:HZ2	1.72	0.55
1:C:438:PRO:CA	1:C:441:GLN:NE2	2.68	0.55
1:C:86:LYS:HE3	1:C:107:ASP:OD1	2.06	0.55
1:A:456:LYS:NZ	1:A:456:LYS:HB3	2.21	0.55
1:B:274:PHE:CD2	1:B:284:LEU:HD22	2.42	0.55
1:C:188:ARG:NH2	2:C:501:HOH:O	2.34	0.55
1:C:407:GLN:NE2	1:C:410:GLN:HG2	2.22	0.55
1:B:74:ASN:HD22	1:B:77:SER:H	1.55	0.54
1:A:164:TRP:CD2	1:A:233:VAL:HG13	2.42	0.54
1:B:454:GLU:HB3	1:B:456:LYS:NZ	2.21	0.54
1:B:89:GLN:OE1	1:B:98:LYS:HD2	2.08	0.54
1:B:8:ARG:HE	1:B:10:GLN:NE2	2.05	0.54
1:C:190:VAL:HG12	1:C:191:SER:N	2.22	0.54
1:A:309:HIS:CD2	1:A:312:THR:OG1	2.51	0.54
1:C:199:ALA:HB2	1:C:218:PHE:CB	2.38	0.54
1:C:13:LEU:HD11	1:C:58:PRO:CB	2.33	0.54
1:C:188:ARG:O	1:C:190:VAL:N	2.40	0.54
1:C:377:TYR:O	1:C:413:PRO:HB3	2.07	0.54
1:B:137:GLN:HB3	1:B:138:PRO:HD2	1.89	0.54
1:C:442:GLN:OE1	1:C:444:ARG:NH1	2.41	0.54
1:A:128:TYR:O	1:A:129:HIS:HD2	1.91	0.54
1:B:209:ASN:HD22	1:B:209:ASN:N	2.06	0.54
1:A:100:LYS:CE	1:A:130:TRP:HE1	2.18	0.54
1:A:16:GLN:NE2	1:A:22:PRO:HG3	2.23	0.54
1:A:449:GLU:CG	1:A:474:LEU:HD11	2.35	0.54
1:A:139:VAL:O	1:A:139:VAL:HG12	2.06	0.54
1:A:141:MET:O	1:A:142:PHE:HB3	2.07	0.54
1:A:176:ARG:HH22	1:A:221:ARG:HD3	1.71	0.54
1:A:253:PRO:HD2	1:A:256:ALA:CB	2.38	0.54
1:C:402:GLN:C	1:C:404:VAL:N	2.62	0.54
1:B:140:LYS:NZ	1:B:143:ASP:OD2	2.41	0.54
1:C:137:GLN:HB3	1:C:138:PRO:HD2	1.90	0.54
1:C:465:ASP:OD1	1:C:479:TYR:OH	2.18	0.54
1:C:222:GLY:C	1:C:224:ALA:N	2.60	0.53
1:C:468:LYS:HD3	1:C:475:ALA:CB	2.38	0.53
1:C:65:PRO:O	1:C:66:ILE:HG13	2.09	0.53
1:A:99:MET:O	1:A:100:LYS:CB	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:TYR:N	1:B:128:TYR:CD1	2.76	0.53
1:C:411:THR:O	1:C:416:GLN:NE2	2.42	0.53
1:A:114:ILE:O	1:A:115:SER:HB3	2.09	0.53
1:A:166:LEU:CD2	1:A:216:PHE:HE1	2.20	0.53
1:C:173:GLN:OE1	1:C:173:GLN:CA	2.37	0.53
1:B:1:MET:HG3	1:C:1:MET:HA	1.88	0.53
1:A:3:GLN:HB2	1:A:341:VAL:HG22	1.90	0.53
1:A:433:LEU:HD13	1:A:463:LEU:HB2	1.91	0.53
1:B:335:ILE:HB	1:B:336:PRO:HD3	1.90	0.53
1:A:437:ARG:HB3	1:A:438:PRO:CD	2.38	0.53
1:B:158:THR:CG2	1:B:159:ASP:O	2.56	0.53
1:C:100:LYS:HE2	1:C:130:TRP:HE1	1.74	0.53
1:C:137:GLN:HB3	1:C:138:PRO:CD	2.38	0.53
1:C:420:ILE:O	1:C:424:GLN:HG3	2.09	0.53
1:B:12:HIS:NE2	1:B:326:SER:CB	2.72	0.53
1:C:347:LEU:CD1	1:C:351:MET:HE3	2.39	0.53
1:C:123:THR:HB	1:C:126:ALA:O	2.09	0.53
1:C:222:GLY:C	1:C:224:ALA:H	2.12	0.53
1:B:92:ASN:OD1	1:B:92:ASN:C	2.48	0.53
1:C:444:ARG:HD2	1:C:444:ARG:N	2.24	0.53
1:A:12:HIS:CD2	1:A:326:SER:HB3	2.43	0.52
1:B:461:GLU:HG3	1:B:484:VAL:HG12	1.91	0.52
1:C:164:TRP:C	1:C:165:LEU:HD23	2.29	0.52
1:A:248:VAL:HG21	1:A:290:GLY:O	2.10	0.52
1:A:4:ILE:CG2	1:A:337:TYR:HB2	2.39	0.52
1:A:47:GLN:HG3	1:A:48:ALA:N	2.25	0.52
1:B:454:GLU:CB	1:B:456:LYS:HE3	2.38	0.52
1:C:111:TRP:O	1:C:112:LYS:CB	2.52	0.52
1:C:211:GLU:CB	1:C:237:PRO:HG2	2.38	0.52
1:A:176:ARG:CG	1:A:177:VAL:N	2.72	0.52
1:A:372:PHE:HZ	1:A:400:ARG:O	1.93	0.52
1:B:71:ALA:HB1	1:B:80:ILE:HD11	1.90	0.52
1:C:437:ARG:O	1:C:441:GLN:HG3	2.09	0.52
1:A:442:GLN:HB3	1:A:444:ARG:NH1	2.24	0.52
1:B:376:ASN:OD1	1:B:379:GLU:HB2	2.09	0.52
1:C:173:GLN:CG	1:C:178:VAL:HG21	2.36	0.52
1:A:144:ARG:HD3	1:A:167:LEU:HD21	1.91	0.52
1:A:454:GLU:HB3	1:A:456:LYS:CG	2.40	0.52
1:A:57:ASP:CG	1:A:60:ASN:HD22	2.12	0.52
1:A:91:PHE:CZ	1:A:96:LYS:HA	2.44	0.52
1:B:1:MET:CG	1:B:2:ALA:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLY:C	1:A:209:ASN:HD22	2.13	0.52
1:C:394:THR:O	1:C:398:ILE:HD12	2.10	0.52
1:B:353:VAL:HG23	1:B:364:PHE:CZ	2.45	0.52
1:C:312:THR:O	1:C:313:ALA:HB3	2.10	0.52
1:C:52:ILE:HD13	1:C:73:MET:HE3	1.91	0.52
1:A:111:TRP:O	1:A:112:LYS:CB	2.55	0.52
1:A:395:PRO:HB3	1:A:430:TYR:CZ	2.45	0.52
1:B:227:LYS:HD3	1:B:249:ASP:HA	1.92	0.52
1:C:209:ASN:HD22	1:C:209:ASN:N	2.07	0.52
1:A:123:THR:CG2	1:A:124:ASP:N	2.73	0.51
1:A:47:GLN:NE2	1:A:65:PRO:HB3	2.25	0.51
1:C:413:PRO:HA	1:C:416:GLN:CG	2.40	0.51
1:C:448:LEU:HD21	1:C:474:LEU:CG	2.39	0.51
1:C:485:PRO:O	1:C:487:LYS:N	2.43	0.51
1:A:253:PRO:HD2	1:A:256:ALA:HB3	1.91	0.51
1:A:211:GLU:CB	1:A:237:PRO:HG2	2.41	0.51
1:B:338:ILE:HA	1:B:342:LEU:HB2	1.93	0.51
1:C:374:GLN:HG2	1:C:375:GLY:N	2.16	0.51
1:C:437:ARG:O	1:C:441:GLN:N	2.43	0.51
1:A:140:LYS:NZ	1:A:143:ASP:OD2	2.42	0.51
1:A:412:SER:HG	1:A:415:LEU:CD2	2.23	0.51
1:B:16:GLN:CD	1:B:22:PRO:HG3	2.31	0.51
1:B:445:LYS:HG2	1:B:449:GLU:OE2	2.11	0.51
1:B:376:ASN:O	1:B:379:GLU:N	2.43	0.51
1:B:227:LYS:HA	1:B:249:ASP:HA	1.93	0.51
1:B:323:GLN:OE1	1:B:325:LEU:HD21	2.10	0.51
1:C:383:VAL:HG12	1:C:384:ALA:N	2.25	0.51
1:C:73:MET:CE	1:C:80:ILE:HB	2.25	0.51
1:B:139:VAL:HG12	1:B:139:VAL:O	2.09	0.51
1:A:476:LEU:HD11	1:C:177:VAL:CG2	2.41	0.51
1:B:437:ARG:HB3	1:B:438:PRO:CD	2.41	0.51
1:C:345:PRO:HA	1:C:348:ALA:CB	2.38	0.51
1:C:484:VAL:HG13	1:C:484:VAL:CG2	2.38	0.51
1:B:376:ASN:O	1:B:377:TYR:C	2.48	0.50
1:A:83:LYS:O	1:A:83:LYS:HG2	2.10	0.50
1:C:429:LYS:HE3	1:C:459:CYS:O	2.11	0.50
1:A:279:TYR:N	1:A:279:TYR:CD2	2.79	0.50
1:B:69:ASP:CB	1:B:83:LYS:HZ2	2.24	0.50
1:C:144:ARG:HD3	1:C:167:LEU:HD21	1.92	0.50
1:C:237:PRO:HD2	1:C:240:ASN:OD1	2.12	0.50
1:C:253:PRO:HD2	1:C:256:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:OE1	1:A:178:VAL:HG11	2.11	0.50
1:A:362:GLU:O	1:A:366:ARG:HB2	2.11	0.50
1:B:475:ALA:O	1:B:478:VAL:N	2.45	0.50
1:B:13:LEU:HD23	1:B:58:PRO:CB	2.41	0.50
1:C:335:ILE:HB	1:C:336:PRO:HD3	1.94	0.50
1:C:391:ILE:HG23	1:C:392:LEU:N	2.26	0.50
1:A:73:MET:HE2	1:A:80:ILE:CG1	2.42	0.50
1:B:253:PRO:HD2	1:B:256:ALA:HB3	1.93	0.50
1:C:221:ARG:HG3	1:C:252:PHE:CE1	2.46	0.50
1:C:372:PHE:CD1	1:C:377:TYR:CD2	2.99	0.50
1:C:89:GLN:NE2	1:C:98:LYS:CD	2.70	0.50
1:A:440:LEU:HD21	1:A:448:LEU:HD22	1.92	0.50
1:B:144:ARG:HD3	1:B:167:LEU:HD21	1.94	0.50
1:B:258:ASN:N	1:B:258:ASN:OD1	2.44	0.50
1:B:472:PRO:O	1:B:475:ALA:HB3	2.11	0.50
1:B:461:GLU:HG3	1:B:484:VAL:CG1	2.42	0.50
1:C:258:ASN:N	1:C:258:ASN:OD1	2.44	0.50
1:C:248:VAL:HG21	1:C:290:GLY:O	2.11	0.50
1:A:227:LYS:HA	1:A:249:ASP:HA	1.93	0.50
1:A:384:ALA:HA	1:A:392:LEU:HD12	1.94	0.50
1:B:487:LYS:O	1:B:487:LYS:HD2	2.12	0.50
1:C:54:ASP:O	1:C:56:ASN:N	2.45	0.50
1:A:69:ASP:CB	1:A:83:LYS:HZ2	2.24	0.50
1:B:148:LEU:CD2	1:B:167:LEU:HD23	2.42	0.50
1:B:188:ARG:O	1:B:190:VAL:N	2.45	0.50
1:C:164:TRP:NE1	1:C:233:VAL:HG13	2.25	0.50
1:A:353:VAL:HG23	1:A:364:PHE:CZ	2.46	0.49
1:B:111:TRP:O	1:B:112:LYS:CB	2.58	0.49
1:B:47:GLN:HG3	1:B:48:ALA:N	2.25	0.49
1:C:181:MET:HE1	1:C:218:PHE:CD1	2.47	0.49
1:C:358:ALA:N	1:C:389:LYS:HZ1	2.10	0.49
1:C:356:ASN:O	1:C:389:LYS:NZ	2.45	0.49
1:B:129:HIS:CD2	1:B:141:MET:HG3	2.47	0.49
1:B:279:TYR:N	1:B:279:TYR:CD2	2.77	0.49
1:B:353:VAL:HG23	1:B:364:PHE:HZ	1.76	0.49
1:B:376:ASN:ND2	1:B:378:SER:OG	2.45	0.49
1:B:377:TYR:HB3	1:B:413:PRO:HB3	1.93	0.49
1:C:166:LEU:HD22	1:C:216:PHE:CE1	2.45	0.49
1:A:377:TYR:CB	1:A:413:PRO:HB3	2.36	0.49
1:B:439:VAL:HA	1:B:444:ARG:HD2	1.93	0.49
1:C:245:LYS:O	1:C:245:LYS:HG3	2.08	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HB	1:A:336:PRO:HD3	1.93	0.49
1:B:111:TRP:HA	1:B:120:ALA:O	2.13	0.49
1:B:373:ALA:O	1:B:374:GLN:C	2.50	0.49
1:C:372:PHE:CD2	1:C:400:ARG:HD2	2.48	0.49
1:C:372:PHE:C	1:C:374:GLN:N	2.66	0.49
1:A:164:TRP:HZ2	1:A:234:GLY:CA	2.25	0.49
1:A:173:GLN:HG3	1:A:178:VAL:HG21	1.93	0.49
1:A:168:THR:HG23	1:A:181:MET:HG2	1.94	0.49
1:A:454:GLU:HB3	1:A:456:LYS:CD	2.42	0.49
1:B:398:ILE:HG23	1:B:414:LEU:HD11	1.95	0.49
1:B:91:PHE:CZ	1:B:96:LYS:HA	2.47	0.49
1:C:352:ALA:HA	1:C:357:LEU:HB2	1.93	0.49
1:A:181:MET:HE1	1:A:218:PHE:CD1	2.48	0.49
1:A:407:GLN:CD	1:A:407:GLN:C	2.71	0.49
1:A:123:THR:HB	1:A:126:ALA:O	2.12	0.49
1:A:412:SER:OG	1:A:415:LEU:HB2	2.12	0.49
1:B:13:LEU:HD11	1:B:15:LEU:HD23	1.93	0.49
1:C:361:GLU:HA	1:C:391:ILE:CD1	2.40	0.49
1:A:427:LEU:O	1:A:458:GLU:HB2	2.13	0.49
1:B:137:GLN:HB3	1:B:138:PRO:CD	2.43	0.49
1:B:445:LYS:HE3	1:B:449:GLU:OE1	2.13	0.49
1:C:356:ASN:HA	1:C:388:PRO:HB3	1.95	0.49
1:A:16:GLN:CD	1:A:22:PRO:HG3	2.34	0.49
1:A:451:TRP:O	1:A:456:LYS:HG3	2.12	0.49
1:C:188:ARG:O	1:C:188:ARG:CG	2.60	0.49
1:C:404:VAL:HG22	1:C:405:PRO:HD2	1.94	0.49
1:C:401:PHE:HB3	1:C:414:LEU:CD1	2.43	0.49
1:B:100:LYS:NZ	1:B:133:GLU:O	2.45	0.48
1:C:184:TYR:HD1	1:C:191:SER:HB2	1.77	0.48
1:C:279:TYR:CD2	1:C:279:TYR:N	2.80	0.48
1:C:415:LEU:HD22	1:C:415:LEU:N	2.28	0.48
1:C:433:LEU:HD21	1:C:462:GLU:CB	2.43	0.48
1:C:462:GLU:O	1:C:465:ASP:N	2.46	0.48
1:A:170:ILE:HA	1:A:178:VAL:O	2.12	0.48
1:A:35:ASP:OD1	1:A:36:LYS:HD3	2.14	0.48
1:C:102:HIS:CE1	1:C:138:PRO:CD	2.97	0.48
1:C:217:CYS:HA	1:C:229:HIS:O	2.14	0.48
1:C:401:PHE:O	1:C:404:VAL:CB	2.47	0.48
1:A:4:ILE:HG12	1:A:333:ASN:HB3	1.95	0.48
1:C:362:GLU:C	1:C:364:PHE:H	2.15	0.48
1:C:438:PRO:HA	1:C:441:GLN:CD	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CG	1:A:2:ALA:H	2.27	0.48
1:A:65:PRO:O	1:A:66:ILE:HG13	2.14	0.48
1:B:211:GLU:HB3	1:B:237:PRO:HG2	1.96	0.48
1:C:274:PHE:CD2	1:C:284:LEU:HD22	2.48	0.48
1:C:445:LYS:HD3	1:C:449:GLU:CD	2.33	0.48
1:C:114:ILE:O	1:C:115:SER:HB3	2.14	0.48
1:C:188:ARG:O	1:C:188:ARG:HG3	2.13	0.48
1:C:466:LEU:C	1:C:468:LYS:H	2.16	0.48
1:B:12:HIS:CD2	1:B:326:SER:HB3	2.49	0.48
1:B:16:GLN:O	1:B:19:GLY:N	2.42	0.48
1:B:421:LEU:HB3	1:B:427:LEU:HD11	1.96	0.48
1:B:438:PRO:O	1:B:441:GLN:N	2.45	0.48
1:A:407:GLN:OE1	1:A:408:PRO:O	2.32	0.48
1:C:347:LEU:HD11	1:C:351:MET:HE3	1.95	0.48
1:A:110:PHE:CD2	1:A:111:TRP:N	2.82	0.48
1:A:456:LYS:CB	1:A:456:LYS:NZ	2.77	0.48
1:B:472:PRO:O	1:B:492:PHE:HE2	1.96	0.48
1:C:199:ALA:HB1	1:C:217:CYS:O	2.13	0.48
1:C:35:ASP:OD1	1:C:36:LYS:HD3	2.13	0.48
1:C:372:PHE:HD1	1:C:377:TYR:HD2	1.60	0.48
1:C:363:LEU:HA	1:C:366:ARG:HB2	1.96	0.48
1:C:426:GLN:HA	1:C:456:LYS:O	2.14	0.48
1:C:466:LEU:C	1:C:468:LYS:N	2.66	0.48
1:A:188:ARG:O	1:A:188:ARG:HG3	2.14	0.47
1:B:123:THR:CG2	1:B:124:ASP:N	2.77	0.47
1:B:250:VAL:HG22	1:B:250:VAL:O	2.13	0.47
1:B:338:ILE:O	1:B:342:LEU:HB2	2.13	0.47
1:C:347:LEU:HD12	1:C:347:LEU:C	2.35	0.47
1:C:421:LEU:O	1:C:424:GLN:HB2	2.14	0.47
1:C:484:VAL:HG23	1:C:484:VAL:O	2.13	0.47
1:B:459:CYS:SG	1:B:478:VAL:CG1	3.02	0.47
1:C:459:CYS:SG	1:C:478:VAL:HG13	2.54	0.47
1:C:99:MET:O	1:C:100:LYS:CB	2.57	0.47
1:A:258:ASN:OD1	1:A:258:ASN:N	2.47	0.47
1:A:286:ASP:OD2	1:A:289:THR:HG23	2.13	0.47
1:A:78:LYS:HB3	1:A:78:LYS:HE3	1.56	0.47
1:B:65:PRO:O	1:B:66:ILE:CG1	2.62	0.47
1:A:356:ASN:HA	1:A:388:PRO:HB3	1.96	0.47
1:B:181:MET:HE1	1:B:196:GLY:HA3	1.95	0.47
1:B:199:ALA:HB2	1:B:218:PHE:HB2	1.97	0.47
1:B:250:VAL:HG22	1:B:252:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLN:CD	1:C:22:PRO:HG3	2.35	0.47
1:C:391:ILE:HG12	1:C:392:LEU:HD23	1.96	0.47
1:C:393:ARG:NH2	1:C:431:GLU:OE1	2.48	0.47
1:A:465:ASP:OD1	1:A:479:TYR:OH	2.22	0.47
1:A:54:ASP:O	1:A:56:ASN:N	2.47	0.47
1:B:116:LEU:O	1:B:132:MET:HE2	2.15	0.47
1:B:35:ASP:OD1	1:B:36:LYS:HD3	2.15	0.47
1:C:152:GLN:O	1:C:169:GLY:HA2	2.14	0.47
1:C:227:LYS:HD3	1:C:249:ASP:CA	2.44	0.47
1:C:347:LEU:HD11	1:C:351:MET:CE	2.45	0.47
1:A:363:LEU:HD23	1:A:366:ARG:NH1	2.29	0.47
1:A:8:ARG:HE	1:A:10:GLN:NE2	2.12	0.47
1:B:459:CYS:SG	1:B:478:VAL:HG13	2.54	0.47
1:C:57:ASP:N	1:C:58:PRO:CD	2.78	0.47
1:B:485:PRO:HD2	1:B:488:VAL:HG23	1.97	0.47
1:C:211:GLU:HB2	1:C:237:PRO:HG2	1.96	0.47
1:C:351:MET:HB2	1:C:351:MET:HE3	1.76	0.47
1:A:110:PHE:CD2	1:A:110:PHE:C	2.88	0.47
1:A:173:GLN:CG	1:A:178:VAL:HG21	2.45	0.47
1:B:116:LEU:CD2	1:B:116:LEU:H	2.26	0.47
1:B:69:ASP:HB2	1:B:83:LYS:HZ2	1.79	0.47
1:A:245:LYS:O	1:A:245:LYS:HG3	2.14	0.47
1:C:371:LEU:HD13	1:C:380:ALA:CA	2.40	0.47
1:C:47:GLN:NE2	1:C:65:PRO:HB3	2.30	0.47
1:C:78:LYS:HE3	1:C:78:LYS:HB3	1.44	0.47
1:B:100:LYS:HG2	1:B:130:TRP:CZ2	2.50	0.47
1:A:227:LYS:HD3	1:A:249:ASP:CA	2.42	0.46
1:A:26:GLY:O	1:A:30:LEU:N	2.38	0.46
1:B:12:HIS:O	1:B:13:LEU:HB3	2.15	0.46
1:B:447:LEU:O	1:B:447:LEU:HD12	2.15	0.46
1:B:78:LYS:HB3	1:B:78:LYS:HE3	1.53	0.46
1:C:117:ASN:HB2	1:C:132:MET:CG	2.43	0.46
1:A:170:ILE:CB	1:A:177:VAL:HG12	2.43	0.46
1:A:188:ARG:O	1:A:188:ARG:CG	2.62	0.46
1:B:371:LEU:CD1	1:B:379:GLU:HG3	2.44	0.46
1:B:43:LYS:HA	1:B:47:GLN:O	2.15	0.46
1:B:478:VAL:HA	1:B:481:ARG:HG3	1.98	0.46
1:C:154:ILE:HD13	1:C:170:ILE:HG12	1.96	0.46
1:C:472:PRO:O	1:C:475:ALA:N	2.49	0.46
1:A:112:LYS:HE2	1:A:155:ASN:OD1	2.15	0.46
1:B:157:ARG:NH1	1:B:200:SER:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:CD2	1:C:216:PHE:HE1	2.25	0.46
1:C:265:GLN:HG3	1:C:315:ILE:HG13	1.97	0.46
1:A:297:ARG:HH21	1:A:300:GLY:HA2	1.81	0.46
1:C:297:ARG:HH21	1:C:300:GLY:HA2	1.80	0.46
1:C:413:PRO:N	1:C:416:GLN:HE21	2.14	0.46
1:C:158:THR:CG2	1:C:159:ASP:O	2.62	0.46
1:A:176:ARG:HD3	1:A:177:VAL:HG23	1.98	0.46
1:B:184:TYR:HD1	1:B:191:SER:HB2	1.80	0.46
1:B:199:ALA:HB2	1:B:218:PHE:CB	2.46	0.46
1:A:485:PRO:HA	1:C:320:ARG:NH1	2.30	0.46
1:A:184:TYR:HD1	1:A:191:SER:HB2	1.81	0.46
1:A:37:PHE:HA	1:A:53:ILE:O	2.16	0.46
1:B:401:PHE:HD2	1:B:413:PRO:HB2	1.79	0.46
1:B:486:ASN:HB3	1:B:490:GLN:OE1	2.16	0.46
1:C:145:HIS:ND1	1:C:147:SER:OG	2.44	0.46
1:C:145:HIS:CD2	1:C:193:PRO:HG3	2.50	0.46
1:A:158:THR:CG2	1:A:159:ASP:O	2.61	0.46
1:C:100:LYS:HG2	1:C:130:TRP:CZ2	2.51	0.46
1:A:473:THR:CG2	1:C:171:SER:HA	2.41	0.46
1:C:369:ASN:CG	1:C:400:ARG:HH12	2.19	0.46
1:A:250:VAL:HG22	1:A:252:PHE:CE1	2.51	0.46
1:A:266:ILE:HG12	1:A:273:VAL:HG22	1.97	0.46
1:A:349:LEU:HD21	1:A:363:LEU:HB2	1.98	0.46
1:B:86:LYS:HE2	1:B:106:ASP:HA	1.98	0.46
1:B:206:MET:SD	1:B:243:PHE:HB2	2.56	0.46
1:B:164:TRP:HZ2	1:B:234:GLY:CA	2.29	0.46
1:B:362:GLU:O	1:B:366:ARG:HB2	2.15	0.46
1:C:74:ASN:OD1	1:C:113:TRP:CZ3	2.69	0.46
1:C:445:LYS:HG3	1:C:446:GLN:N	2.29	0.46
1:A:485:PRO:HB2	1:A:487:LYS:CG	2.46	0.45
1:A:57:ASP:N	1:A:58:PRO:CD	2.79	0.45
1:C:102:HIS:NE2	1:C:138:PRO:HG2	2.31	0.45
1:C:110:PHE:C	1:C:110:PHE:CD2	2.89	0.45
1:C:2:ALA:C	1:C:4:ILE:H	2.20	0.45
1:C:301:GLU:HG3	1:C:321:LYS:HE2	1.99	0.45
1:C:421:LEU:CA	1:C:424:GLN:HB2	2.44	0.45
1:A:338:ILE:HG22	1:A:344:ASN:O	2.17	0.45
1:A:396:ASP:N	1:A:396:ASP:OD2	2.49	0.45
1:B:109:THR:N	1:B:122:VAL:O	2.44	0.45
1:B:250:VAL:CG2	1:B:250:VAL:O	2.62	0.45
1:C:374:GLN:NE2	1:C:376:ASN:CB	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:VAL:HG23	1:C:405:PRO:HD2	1.97	0.45
1:A:444:ARG:HH11	1:A:444:ARG:CG	2.27	0.45
1:B:489:ILE:O	1:B:492:PHE:HB2	2.16	0.45
1:C:372:PHE:CE2	1:C:400:ARG:HB3	2.52	0.45
1:A:16:GLN:O	1:A:19:GLY:N	2.46	0.45
1:C:211:GLU:HB3	1:C:237:PRO:HG2	1.98	0.45
1:C:280:GLY:HA3	1:C:299:SER:O	2.16	0.45
1:A:438:PRO:HG2	1:A:439:VAL:H	1.80	0.45
1:B:14:GLN:HE21	1:B:16:GLN:H	1.65	0.45
1:B:192:GLN:HA	1:B:193:PRO:HD3	1.73	0.45
1:B:47:GLN:NE2	1:B:65:PRO:HB3	2.32	0.45
1:C:480:LEU:HD23	1:C:480:LEU:C	2.36	0.45
1:C:52:ILE:CD1	1:C:73:MET:HE3	2.47	0.45
1:A:218:PHE:CZ	1:A:229:HIS:CD2	3.05	0.45
1:B:44:VAL:N	1:B:47:GLN:O	2.49	0.45
1:C:164:TRP:CZ2	1:C:234:GLY:CA	2.99	0.45
1:C:57:ASP:CG	1:C:60:ASN:ND2	2.69	0.45
1:A:216:PHE:HD2	1:A:231:ILE:CD1	2.23	0.45
1:C:190:VAL:CG1	1:C:191:SER:N	2.79	0.45
1:C:227:LYS:HD3	1:C:249:ASP:HB3	1.97	0.45
1:C:395:PRO:C	1:C:397:THR:N	2.68	0.45
1:C:396:ASP:CG	1:C:399:ARG:HH12	2.20	0.45
1:A:474:LEU:O	1:A:478:VAL:HG23	2.16	0.45
1:A:92:ASN:C	1:A:92:ASN:OD1	2.55	0.45
1:B:102:HIS:CE1	1:B:138:PRO:HD2	2.51	0.45
1:B:339:THR:O	1:B:343:GLN:HA	2.16	0.45
1:C:438:PRO:HB3	1:C:441:GLN:NE2	2.32	0.45
1:C:442:GLN:CG	1:C:444:ARG:NH1	2.80	0.45
1:C:468:LYS:HZ3	1:C:479:TYR:HE1	1.64	0.45
1:A:455:ASP:CB	1:C:69:ASP:OD1	2.64	0.45
1:A:211:GLU:HB3	1:A:237:PRO:HG2	1.99	0.45
1:A:356:ASN:O	1:A:356:ASN:CG	2.53	0.45
1:B:454:GLU:HB3	1:B:456:LYS:HE3	1.98	0.45
1:C:167:LEU:O	1:C:181:MET:HA	2.17	0.45
1:C:392:LEU:O	1:C:394:THR:N	2.44	0.45
1:C:396:ASP:CA	1:C:399:ARG:NH1	2.75	0.45
1:A:211:GLU:HB2	1:A:237:PRO:HG2	1.99	0.45
1:A:265:GLN:HG3	1:A:315:ILE:HG13	1.98	0.45
1:A:398:ILE:HD12	1:A:430:TYR:HE2	1.73	0.45
1:B:145:HIS:CE1	1:B:147:SER:OG	2.70	0.45
1:B:475:ALA:HB1	1:B:479:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:HIS:CE1	1:C:147:SER:OG	2.70	0.45
1:A:91:PHE:CZ	1:A:96:LYS:C	2.90	0.44
1:B:186:VAL:HG12	1:B:187:ASP:N	2.32	0.44
1:B:446:GLN:HA	1:B:449:GLU:OE2	2.16	0.44
1:C:438:PRO:HA	1:C:441:GLN:CG	2.47	0.44
1:C:463:LEU:HD12	1:C:463:LEU:HA	1.77	0.44
1:C:57:ASP:OD1	1:C:60:ASN:ND2	2.50	0.44
1:A:407:GLN:HA	1:A:408:PRO:HD2	1.63	0.44
1:A:89:GLN:NE2	1:A:98:LYS:CD	2.76	0.44
1:B:199:ALA:HB1	1:B:217:CYS:O	2.17	0.44
1:B:57:ASP:N	1:B:58:PRO:CD	2.78	0.44
1:C:163:LYS:O	1:C:186:VAL:HB	2.18	0.44
1:C:253:PRO:O	1:C:256:ALA:HB3	2.16	0.44
1:A:86:LYS:HG3	1:A:107:ASP:OD1	2.18	0.44
1:C:279:TYR:O	1:C:297:ARG:NH2	2.50	0.44
1:C:339:THR:HG23	1:C:345:PRO:HG3	1.99	0.44
1:A:109:THR:O	1:A:109:THR:HG23	2.16	0.44
1:A:167:LEU:O	1:A:181:MET:HA	2.18	0.44
1:A:471:ASP:HA	1:A:472:PRO:HD3	1.79	0.44
1:B:197:HIS:HD2	1:B:221:ARG:N	2.13	0.44
1:C:145:HIS:CE1	1:C:147:SER:HG	2.34	0.44
1:C:3:GLN:HB2	1:C:341:VAL:HG22	1.99	0.44
1:A:13:LEU:HD13	1:A:58:PRO:HB2	1.99	0.44
1:B:396:ASP:N	1:B:396:ASP:OD1	2.50	0.44
1:B:442:GLN:O	1:B:444:ARG:HG3	2.17	0.44
1:C:16:GLN:O	1:C:19:GLY:N	2.47	0.44
1:A:476:LEU:CD1	1:C:177:VAL:HG22	2.44	0.44
1:C:415:LEU:HD13	1:C:415:LEU:HA	1.67	0.44
1:A:176:ARG:NH2	1:A:221:ARG:HD3	2.33	0.44
1:B:57:ASP:N	1:B:58:PRO:HD3	2.33	0.44
1:C:407:GLN:OE1	1:C:410:GLN:HG3	2.18	0.44
1:A:145:HIS:ND1	1:A:147:SER:OG	2.47	0.44
1:A:445:LYS:HB2	1:A:445:LYS:HE2	1.65	0.44
1:A:91:PHE:CE2	1:A:96:LYS:HA	2.53	0.44
1:B:449:GLU:O	1:B:453:LYS:HE3	2.18	0.44
1:B:454:GLU:HB3	1:B:456:LYS:CE	2.48	0.44
1:B:73:MET:HE3	1:B:93:ILE:HG13	2.00	0.44
1:C:95:MET:HG3	1:C:97:SER:OG	2.18	0.44
1:A:176:ARG:CD	1:A:177:VAL:H	2.30	0.44
1:A:217:CYS:HA	1:A:229:HIS:O	2.18	0.44
1:A:471:ASP:OD1	1:A:472:PRO:CD	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:PRO:HD2	1:B:256:ALA:HB2	2.00	0.44
1:C:158:THR:CG2	1:C:159:ASP:N	2.81	0.44
1:C:391:ILE:HD13	1:C:392:LEU:HD21	1.99	0.44
1:A:109:THR:N	1:A:122:VAL:O	2.47	0.43
1:A:173:GLN:HG3	1:A:178:VAL:CG2	2.48	0.43
1:A:379:GLU:HA	1:A:379:GLU:OE1	2.16	0.43
1:A:398:ILE:O	1:A:402:GLN:HG3	2.18	0.43
1:A:445:LYS:H	1:A:445:LYS:HG3	1.19	0.43
1:B:13:LEU:CD2	1:B:58:PRO:HB2	2.48	0.43
1:B:205:LYS:HB2	1:B:205:LYS:HE2	1.67	0.43
1:B:453:LYS:O	1:B:455:ASP:N	2.51	0.43
1:C:69:ASP:HB2	1:C:83:LYS:HZ2	1.83	0.43
1:A:152:GLN:O	1:A:169:GLY:HA2	2.18	0.43
1:A:186:VAL:HG12	1:A:187:ASP:N	2.32	0.43
1:A:356:ASN:OD1	1:A:389:LYS:N	2.50	0.43
1:A:66:ILE:O	1:A:66:ILE:HG22	2.18	0.43
1:B:147:SER:H	1:B:147:SER:HG	1.17	0.43
1:B:476:LEU:O	1:B:480:LEU:HG	2.18	0.43
1:C:205:LYS:HB2	1:C:205:LYS:HE2	1.73	0.43
1:C:433:LEU:HD21	1:C:462:GLU:HB3	2.00	0.43
1:A:44:VAL:N	1:A:47:GLN:O	2.51	0.43
1:A:78:LYS:HB2	1:A:94:GLU:HB2	2.00	0.43
1:B:110:PHE:C	1:B:110:PHE:CD2	2.92	0.43
1:B:429:LYS:HD2	1:B:458:GLU:OE1	2.18	0.43
1:B:73:MET:HE2	1:B:80:ILE:HG13	2.00	0.43
1:B:441:GLN:H	1:B:441:GLN:HG2	1.63	0.43
1:B:475:ALA:HB3	1:B:492:PHE:CZ	2.51	0.43
1:B:54:ASP:O	1:B:56:ASN:N	2.51	0.43
1:C:398:ILE:HD13	1:C:430:TYR:CE2	2.54	0.43
1:A:433:LEU:CD1	1:A:463:LEU:HA	2.48	0.43
1:B:117:ASN:HB2	1:B:132:MET:CG	2.47	0.43
1:B:428:ASN:HB2	1:B:429:LYS:H	1.41	0.43
1:C:192:GLN:HA	1:C:193:PRO:HD3	1.76	0.43
1:B:1:MET:HG3	1:C:1:MET:N	2.33	0.43
1:C:442:GLN:CD	1:C:444:ARG:HH11	2.22	0.43
1:A:372:PHE:CZ	1:A:400:ARG:O	2.71	0.43
1:A:438:PRO:O	1:A:439:VAL:C	2.56	0.43
1:B:447:LEU:HD21	1:B:451:TRP:CH2	2.54	0.43
1:B:349:LEU:HD21	1:B:363:LEU:HB2	2.01	0.43
1:C:356:ASN:O	1:C:389:LYS:HE3	2.19	0.43
1:C:30:LEU:HD22	1:C:40:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:LEU:CD2	1:C:476:LEU:C	2.86	0.43
1:A:407:GLN:HE22	1:A:408:PRO:HG2	1.83	0.43
1:A:460:SER:N	1:A:482:ALA:HB2	2.33	0.43
1:A:74:ASN:HD22	1:A:77:SER:N	2.09	0.43
1:B:13:LEU:HD23	1:B:58:PRO:HB3	2.01	0.43
1:C:335:ILE:HD11	1:C:357:LEU:HD12	2.01	0.43
1:A:129:HIS:CD2	1:A:141:MET:HG3	2.53	0.43
1:A:205:LYS:HB2	1:A:205:LYS:HE2	1.78	0.43
1:A:21:ASN:HA	1:A:22:PRO:HD3	1.85	0.43
1:A:415:LEU:HA	1:A:415:LEU:HD13	1.62	0.43
1:A:467:VAL:O	1:A:468:LYS:C	2.56	0.43
1:B:54:ASP:C	1:B:54:ASP:OD1	2.57	0.43
1:C:128:TYR:O	1:C:129:HIS:HD2	2.01	0.43
1:C:250:VAL:HG22	1:C:252:PHE:CE1	2.53	0.43
1:C:392:LEU:C	1:C:394:THR:H	2.22	0.43
1:C:398:ILE:CG2	1:C:414:LEU:HD11	2.41	0.43
1:B:4:ILE:HG23	1:B:4:ILE:O	2.18	0.42
1:C:164:TRP:O	1:C:165:LEU:HD23	2.19	0.42
1:A:283:HIS:ND1	1:A:295:MET:HG2	2.34	0.42
1:B:454:GLU:CB	1:B:456:LYS:CE	2.97	0.42
1:B:467:VAL:HG11	1:B:474:LEU:HB3	2.00	0.42
1:C:163:LYS:HD3	1:C:163:LYS:HA	1.86	0.42
1:C:427:LEU:HD13	1:C:435:LEU:HD12	2.01	0.42
1:A:54:ASP:C	1:A:54:ASP:OD1	2.57	0.42
1:B:484:VAL:HB	1:B:485:PRO:HD3	2.02	0.42
1:A:199:ALA:HB1	1:A:217:CYS:O	2.19	0.42
1:B:30:LEU:CD1	1:B:38:ILE:HG23	2.49	0.42
1:B:446:GLN:O	1:B:449:GLU:HB2	2.20	0.42
1:C:464:GLY:HA3	1:C:479:TYR:CD2	2.54	0.42
1:C:410:GLN:CA	1:C:410:GLN:OE1	2.67	0.42
1:A:362:GLU:CD	1:A:366:ARG:HH22	2.22	0.42
1:B:309:HIS:CD2	1:B:312:THR:OG1	2.62	0.42
1:C:54:ASP:C	1:C:56:ASN:H	2.22	0.42
1:C:83:LYS:HZ2	1:C:83:LYS:HG2	1.67	0.42
1:A:163:LYS:O	1:A:186:VAL:HB	2.19	0.42
1:B:185:SER:HB3	1:B:188:ARG:HG2	2.01	0.42
1:B:484:VAL:HB	1:B:485:PRO:CD	2.50	0.42
1:C:37:PHE:HA	1:C:53:ILE:O	2.19	0.42
1:C:407:GLN:HA	1:C:408:PRO:HD2	1.44	0.42
1:A:117:ASN:HB2	1:A:132:MET:CG	2.46	0.42
1:A:73:MET:HE3	1:A:93:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLU:HG3	1:B:321:LYS:HE2	1.99	0.42
1:B:362:GLU:CD	1:B:366:ARG:HH22	2.23	0.42
1:C:343:GLN:O	1:C:344:ASN:HB2	2.19	0.42
1:C:374:GLN:CG	1:C:375:GLY:N	2.80	0.42
1:C:410:GLN:N	1:C:410:GLN:CD	2.71	0.42
1:C:440:LEU:HD11	1:C:467:VAL:CG2	2.48	0.42
1:A:461:GLU:CG	1:A:484:VAL:HG11	2.49	0.42
1:B:205:LYS:NZ	1:B:210:ALA:O	2.49	0.42
1:B:376:ASN:C	1:B:378:SER:N	2.71	0.42
1:B:475:ALA:CB	1:B:492:PHE:HZ	2.33	0.42
1:C:197:HIS:HD2	1:C:221:ARG:N	2.14	0.42
1:C:362:GLU:C	1:C:364:PHE:N	2.73	0.42
1:B:163:LYS:O	1:B:186:VAL:HB	2.19	0.42
1:B:398:ILE:HD11	1:B:431:GLU:HG2	2.02	0.42
1:B:475:ALA:O	1:B:478:VAL:HG23	2.19	0.42
1:C:216:PHE:HD2	1:C:231:ILE:CD1	2.25	0.42
1:C:261:PRO:HB3	1:C:275:LEU:HD11	2.01	0.42
1:C:450:LYS:O	1:C:454:GLU:CG	2.62	0.42
1:A:176:ARG:CD	1:A:177:VAL:HG23	2.50	0.41
1:A:197:HIS:HB3	1:A:261:PRO:HB2	2.01	0.41
1:B:116:LEU:HD22	1:B:116:LEU:N	2.30	0.41
1:B:371:LEU:HD13	1:B:379:GLU:HG3	2.02	0.41
1:B:454:GLU:O	1:B:456:LYS:HE3	2.19	0.41
1:C:421:LEU:N	1:C:421:LEU:HD23	2.35	0.41
1:C:486:ASN:O	1:C:487:LYS:HG2	2.19	0.41
1:C:333:ASN:C	1:C:336:PRO:HD2	2.41	0.41
1:C:349:LEU:HD22	1:C:364:PHE:CE2	2.54	0.41
1:C:368:PHE:CD2	1:C:400:ARG:NH2	2.85	0.41
1:C:422:LEU:HA	1:C:422:LEU:HD23	1.69	0.41
1:C:464:GLY:HA3	1:C:479:TYR:CE2	2.55	0.41
1:C:472:PRO:O	1:C:474:LEU:N	2.53	0.41
1:C:95:MET:HE3	1:C:95:MET:HB3	1.97	0.41
1:A:12:HIS:NE2	1:A:326:SER:CB	2.79	0.41
1:A:139:VAL:O	1:A:140:LYS:C	2.56	0.41
1:A:164:TRP:C	1:A:165:LEU:HD23	2.40	0.41
1:B:442:GLN:HE21	1:B:442:GLN:HB2	1.48	0.41
1:B:487:LYS:C	1:B:487:LYS:HD2	2.40	0.41
1:B:57:ASP:CG	1:B:60:ASN:HD22	2.24	0.41
1:C:205:LYS:CG	1:C:205:LYS:O	2.68	0.41
1:C:3:GLN:O	1:C:4:ILE:HB	2.20	0.41
1:C:476:LEU:HD23	1:C:477:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ASN:C	1:C:92:ASN:OD1	2.59	0.41
1:A:164:TRP:CZ2	1:A:234:GLY:CA	3.04	0.41
1:B:265:GLN:HG3	1:B:315:ILE:HG13	2.03	0.41
1:A:221:ARG:HD2	1:A:259:ASP:O	2.21	0.41
1:A:43:LYS:HA	1:A:47:GLN:O	2.21	0.41
1:B:379:GLU:HA	1:B:379:GLU:OE1	2.20	0.41
1:B:421:LEU:CB	1:B:427:LEU:HD11	2.49	0.41
1:C:218:PHE:CZ	1:C:229:HIS:CD2	3.08	0.41
1:A:301:GLU:HG3	1:A:321:LYS:HE2	2.02	0.41
1:A:421:LEU:HB3	1:A:427:LEU:CD2	2.49	0.41
1:B:363:LEU:HD23	1:B:366:ARG:NH1	2.36	0.41
1:C:236:PRO:O	1:C:237:PRO:C	2.59	0.41
1:A:349:LEU:HD22	1:A:364:PHE:CE2	2.55	0.41
1:B:309:HIS:CD2	1:B:312:THR:HG23	2.55	0.41
1:B:447:LEU:HD11	1:B:451:TRP:CZ2	2.55	0.41
1:C:401:PHE:HB3	1:C:414:LEU:HD12	2.03	0.41
1:C:54:ASP:C	1:C:56:ASN:N	2.73	0.41
1:A:144:ARG:HD3	1:A:167:LEU:CD2	2.50	0.41
1:A:354:ARG:NE	1:A:355:ASN:OD1	2.44	0.41
1:A:398:ILE:HG23	1:A:414:LEU:HD11	2.01	0.41
1:A:433:LEU:HD21	1:A:462:GLU:CD	2.41	0.41
1:A:444:ARG:CG	1:A:444:ARG:NH1	2.84	0.41
1:B:21:ASN:HA	1:B:22:PRO:HD3	1.85	0.41
1:B:349:LEU:HD21	1:B:363:LEU:CB	2.51	0.41
1:C:24:ASN:ND2	1:C:42:GLU:CG	2.71	0.41
1:A:133:GLU:OE2	1:A:133:GLU:HA	2.20	0.41
1:A:469:SER:HB2	1:A:470:VAL:H	1.74	0.41
1:B:301:GLU:CG	1:B:321:LYS:HE2	2.51	0.41
1:B:356:ASN:HA	1:B:388:PRO:HB3	2.03	0.41
1:C:25:ILE:HG22	1:C:25:ILE:O	2.21	0.41
1:C:468:LYS:NZ	1:C:479:TYR:CE1	2.89	0.41
1:C:74:ASN:HD22	1:C:77:SER:N	2.08	0.41
1:A:111:TRP:HA	1:A:120:ALA:O	2.21	0.41
1:A:376:ASN:ND2	1:A:379:GLU:HB2	2.36	0.41
1:B:73:MET:CE	1:B:80:ILE:CG1	2.99	0.41
1:C:205:LYS:O	1:C:205:LYS:HG3	2.17	0.41
1:C:474:LEU:O	1:C:478:VAL:HG23	2.21	0.41
1:A:14:GLN:CA	1:A:14:GLN:NE2	2.84	0.41
1:A:192:GLN:HA	1:A:193:PRO:HD3	1.76	0.41
1:A:227:LYS:HD3	1:A:249:ASP:HB3	2.03	0.41
1:B:404:VAL:HA	1:B:405:PRO:HD3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:O	1:B:455:ASP:HA	2.21	0.41
1:B:69:ASP:HB2	1:B:83:LYS:O	2.21	0.41
1:C:218:PHE:CE2	1:C:229:HIS:HB2	2.55	0.41
1:C:371:LEU:HB3	1:C:376:ASN:HB3	2.01	0.41
1:C:447:LEU:HD23	1:C:451:TRP:HZ2	1.80	0.41
1:A:261:PRO:HB3	1:A:275:LEU:HD11	2.02	0.40
1:A:57:ASP:CG	1:A:60:ASN:ND2	2.74	0.40
1:B:170:ILE:HG22	1:B:179:GLY:HA2	2.04	0.40
1:B:205:LYS:HD3	1:B:209:ASN:O	2.21	0.40
1:B:475:ALA:O	1:B:476:LEU:C	2.60	0.40
1:B:83:LYS:HG2	1:B:83:LYS:HZ2	1.75	0.40
1:C:86:LYS:HE2	1:C:106:ASP:HA	2.01	0.40
1:A:176:ARG:HG2	1:A:177:VAL:N	2.33	0.40
1:B:439:VAL:CG1	1:B:444:ARG:HB2	2.43	0.40
1:B:478:VAL:O	1:B:482:ALA:N	2.54	0.40
1:B:66:ILE:HG21	1:B:82:LEU:HD22	2.03	0.40
1:C:18:LEU:HA	1:C:18:LEU:HD23	1.98	0.40
1:C:65:PRO:O	1:C:66:ILE:CG1	2.69	0.40
1:A:205:LYS:NZ	1:A:210:ALA:O	2.52	0.40
1:A:400:ARG:HA	1:A:400:ARG:HD2	1.83	0.40
1:A:412:SER:HG	1:A:415:LEU:HD23	1.79	0.40
1:B:410:GLN:HB3	1:B:411:THR:H	1.77	0.40
1:B:454:GLU:HB2	1:B:456:LYS:HE3	2.03	0.40
1:B:95:MET:O	1:B:97:SER:N	2.54	0.40
1:C:257:GLN:HG2	1:C:257:GLN:H	1.70	0.40
1:C:433:LEU:HG	1:C:437:ARG:HH12	1.86	0.40
1:A:197:HIS:HD2	1:A:221:ARG:N	2.15	0.40
1:A:236:PRO:O	1:A:237:PRO:C	2.58	0.40
1:A:4:ILE:HG23	1:A:337:TYR:HB2	2.03	0.40
1:B:173:GLN:HG3	1:B:178:VAL:HB	2.03	0.40
1:B:415:LEU:HD13	1:B:415:LEU:HA	1.65	0.40
1:B:433:LEU:HD21	1:B:462:GLU:CD	2.42	0.40
1:B:4:ILE:HG12	1:B:333:ASN:HB3	2.04	0.40
1:A:476:LEU:CD2	1:C:170:ILE:HD12	2.48	0.40
1:C:364:PHE:O	1:C:366:ARG:N	2.54	0.40
1:C:422:LEU:HD23	1:C:427:LEU:CD1	2.51	0.40
1:A:273:VAL:HB	1:A:285:TYR:HB2	2.04	0.40
1:A:66:ILE:HG21	1:A:82:LEU:HD22	2.04	0.40
1:C:21:ASN:HA	1:C:22:PRO:HD3	1.90	0.40
1:C:206:MET:SD	1:C:243:PHE:HB2	2.61	0.40
1:C:342:LEU:O	1:C:343:GLN:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:PRO:CD	1:C:416:GLN:HE21	2.33	0.40
1:C:422:LEU:HD23	1:C:427:LEU:HD11	2.02	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	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ARG:NH2	1:B:441:GLN:NE2[2_654]	2.10	0.10

## 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	485/494 (98%)	433 (89%)	36 (7%)	16 (3%)	<b>4</b> <b>6</b>
1	B	491/494 (99%)	435 (89%)	39 (8%)	17 (4%)	<b>3</b> <b>5</b>
1	C	485/494 (98%)	418 (86%)	43 (9%)	24 (5%)	<b>2</b> <b>2</b>
All	All	1461/1482 (99%)	1286 (88%)	118 (8%)	57 (4%)	<b>3</b> <b>4</b>

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	LYS
1	A	470	VAL
1	B	96	LYS
1	B	189	LYS
1	B	257	GLN
1	C	57	ASP
1	C	96	LYS
1	C	173	GLN
1	C	189	LYS
1	C	257	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	486	ASN
1	A	55	MET
1	A	96	LYS
1	A	223	GLN
1	A	257	GLN
1	B	57	ASP
1	B	374	GLN
1	B	377	TYR
1	B	410	GLN
1	B	428	ASN
1	B	459	CYS
1	C	136	SER
1	C	467	VAL
1	C	473	THR
1	A	112	LYS
1	A	469	SER
1	B	66	ILE
1	B	112	LYS
1	B	442	GLN
1	C	55	MET
1	C	112	LYS
1	C	362	GLU
1	C	408	PRO
1	C	418	PHE
1	C	462	GLU
1	A	100	LYS
1	A	408	PRO
1	A	443	GLY
1	B	55	MET
1	B	136	SER
1	C	102	HIS
1	C	472	PRO
1	A	57	ASP
1	A	66	ILE
1	B	100	LYS
1	B	102	HIS
1	C	66	ILE
1	C	100	LYS
1	C	343	GLN
1	C	391	ILE
1	C	403	SER
1	C	405	PRO

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Mol	Chain	Res	Type
1	C	463	LEU
1	A	102	HIS
1	A	136	SER
1	A	483	ASN
1	B	438	PRO

### 5.3.2 Protein sidechains [i](#)

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	416/422 (99%)	336 (81%)	80 (19%)	1	2
1	B	421/422 (100%)	341 (81%)	80 (19%)	1	2
1	C	416/422 (99%)	326 (78%)	90 (22%)	1	1
All	All	1253/1266 (99%)	1003 (80%)	250 (20%)	1	2

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ILE
1	A	11	GLU
1	A	14	GLN
1	A	16	GLN
1	A	20	ILE
1	A	29	THR
1	A	30	LEU
1	A	36	LYS
1	A	43	LYS
1	A	46	GLU
1	A	49	GLN
1	A	59	SER
1	A	63	ARG
1	A	67	SER
1	A	78	LYS
1	A	83	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	89	GLN
1	A	97	SER
1	A	106	ASP
1	A	109	THR
1	A	111	TRP
1	A	112	LYS
1	A	125	ASN
1	A	128	TYR
1	A	133	GLU
1	A	135	GLU
1	A	136	SER
1	A	144	ARG
1	A	147	SER
1	A	170	ILE
1	A	175	ASN
1	A	176	ARG
1	A	188	ARG
1	A	189	LYS
1	A	191	SER
1	A	194	ILE
1	A	205	LYS
1	A	206	MET
1	A	209	ASN
1	A	221	ARG
1	A	231	ILE
1	A	233	VAL
1	A	245	LYS
1	A	249	ASP
1	A	255	GLU
1	A	257	GLN
1	A	268	GLU
1	A	282	ILE
1	A	284	LEU
1	A	288	GLU
1	A	326	SER
1	A	351	MET
1	A	366	ARG
1	A	376	ASN
1	A	389	LYS
1	A	391	ILE
1	A	396	ASP
1	A	407	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	410	GLN
1	A	415	LEU
1	A	424	GLN
1	A	426	GLN
1	A	428	ASN
1	A	435	LEU
1	A	439	VAL
1	A	441	GLN
1	A	444	ARG
1	A	445	LYS
1	A	448	LEU
1	A	450	LYS
1	A	456	LYS
1	A	458	GLU
1	A	460	SER
1	A	461	GLU
1	A	466	LEU
1	A	474	LEU
1	A	477	SER
1	A	480	LEU
1	A	487	LYS
1	B	1	MET
1	B	3	GLN
1	B	10	GLN
1	B	13	LEU
1	B	16	GLN
1	B	20	ILE
1	B	29	THR
1	B	30	LEU
1	B	36	LYS
1	B	43	LYS
1	B	47	GLN
1	B	49	GLN
1	B	59	SER
1	B	63	ARG
1	B	67	SER
1	B	78	LYS
1	B	83	LYS
1	B	89	GLN
1	B	97	SER
1	B	106	ASP
1	B	109	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	111	TRP
1	B	112	LYS
1	B	125	ASN
1	B	128	TYR
1	B	133	GLU
1	B	135	GLU
1	B	136	SER
1	B	144	ARG
1	B	147	SER
1	B	170	ILE
1	B	171	SER
1	B	173	GLN
1	B	188	ARG
1	B	189	LYS
1	B	191	SER
1	B	205	LYS
1	B	206	MET
1	B	209	ASN
1	B	231	ILE
1	B	233	VAL
1	B	245	LYS
1	B	249	ASP
1	B	257	GLN
1	B	268	GLU
1	B	282	ILE
1	B	288	GLU
1	B	326	SER
1	B	342	LEU
1	B	351	MET
1	B	366	ARG
1	B	372	PHE
1	B	374	GLN
1	B	376	ASN
1	B	391	ILE
1	B	396	ASP
1	B	400	ARG
1	B	404	VAL
1	B	412	SER
1	B	415	LEU
1	B	424	GLN
1	B	426	GLN
1	B	428	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	429	LYS
1	B	435	LEU
1	B	442	GLN
1	B	445	LYS
1	B	446	GLN
1	B	448	LEU
1	B	450	LYS
1	B	455	ASP
1	B	456	LYS
1	B	461	GLU
1	B	466	LEU
1	B	471	ASP
1	B	473	THR
1	B	474	LEU
1	B	478	VAL
1	B	481	ARG
1	B	487	LYS
1	C	1	MET
1	C	3	GLN
1	C	16	GLN
1	C	20	ILE
1	C	29	THR
1	C	30	LEU
1	C	36	LYS
1	C	43	LYS
1	C	46	GLU
1	C	47	GLN
1	C	49	GLN
1	C	59	SER
1	C	63	ARG
1	C	67	SER
1	C	78	LYS
1	C	83	LYS
1	C	89	GLN
1	C	97	SER
1	C	106	ASP
1	C	109	THR
1	C	111	TRP
1	C	112	LYS
1	C	125	ASN
1	C	128	TYR
1	C	133	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	135	GLU
1	C	136	SER
1	C	147	SER
1	C	170	ILE
1	C	173	GLN
1	C	176	ARG
1	C	188	ARG
1	C	189	LYS
1	C	191	SER
1	C	194	ILE
1	C	205	LYS
1	C	206	MET
1	C	209	ASN
1	C	231	ILE
1	C	233	VAL
1	C	245	LYS
1	C	249	ASP
1	C	257	GLN
1	C	268	GLU
1	C	282	ILE
1	C	283	HIS
1	C	284	LEU
1	C	288	GLU
1	C	326	SER
1	C	342	LEU
1	C	347	LEU
1	C	351	MET
1	C	363	LEU
1	C	364	PHE
1	C	367	LYS
1	C	369	ASN
1	C	371	LEU
1	C	372	PHE
1	C	376	ASN
1	C	378	SER
1	C	383	VAL
1	C	386	ASN
1	C	401	PHE
1	C	410	GLN
1	C	411	THR
1	C	421	LEU
1	C	427	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	429	LYS
1	C	433	LEU
1	C	435	LEU
1	C	437	ARG
1	C	442	GLN
1	C	444	ARG
1	C	447	LEU
1	C	448	LEU
1	C	450	LYS
1	C	452	LEU
1	C	453	LYS
1	C	454	GLU
1	C	456	LYS
1	C	460	SER
1	C	461	GLU
1	C	462	GLU
1	C	466	LEU
1	C	473	THR
1	C	474	LEU
1	C	476	LEU
1	C	477	SER
1	C	479	TYR
1	C	484	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	3	GLN
1	A	10	GLN
1	A	14	GLN
1	A	17	ASN
1	A	21	ASN
1	A	24	ASN
1	A	60	ASN
1	A	74	ASN
1	A	89	GLN
1	A	197	HIS
1	A	229	HIS
1	A	257	GLN
1	A	309	HIS
1	A	376	ASN
1	A	407	GLN

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Mol	Chain	Res	Type
1	A	410	GLN
1	A	424	GLN
1	B	14	GLN
1	B	17	ASN
1	B	21	ASN
1	B	24	ASN
1	B	60	ASN
1	B	74	ASN
1	B	173	GLN
1	B	197	HIS
1	B	209	ASN
1	B	257	GLN
1	B	309	HIS
1	B	374	GLN
1	B	376	ASN
1	B	424	GLN
1	B	426	GLN
1	B	442	GLN
1	B	490	GLN
1	C	21	ASN
1	C	24	ASN
1	C	60	ASN
1	C	74	ASN
1	C	89	GLN
1	C	197	HIS
1	C	209	ASN
1	C	229	HIS
1	C	257	GLN
1	C	309	HIS
1	C	374	GLN
1	C	376	ASN
1	C	386	ASN
1	C	407	GLN
1	C	416	GLN
1	C	441	GLN
1	C	486	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	222:GLY	C	223:GLN	N	1.16
1	A	174:GLN	C	175:ASN	N	1.15

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.