Full wwPDB X-ray Structure Validation Report (i)

Apr 10, 2023 – 09:10 PM EDT

PDB ID	:	1GFF
Title	:	THE ATOMIC STRUCTURE OF THE DEGRADED PROCAPSID PARTICLE OF THE BACTERIOPHAGE G4: INDUCED STRUCTURAL CHANGES IN THE PRESENCE OF CALCIUM IONS AND FUNCTIONAL IMPLICATIONS
Authors	:	Rossmann, M.G.
Deposited on	:	1995-11-06
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

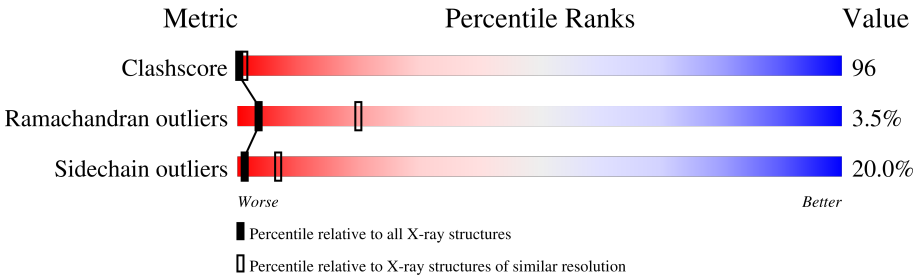
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	426	30% 48% 17%
2	2	177	20% 54% 24%
3	3	25	20% 20% 52%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4779 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 BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	417	3357	2144	571	623	19	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	378	ASP	GLU	conflict	UNP P03642

- Molecule 2 is a protein called BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	177	1325	840	229	252	4	0	0	0

- Molecule 3 is a protein called BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	3	12	97	64	17	16	0	0	0

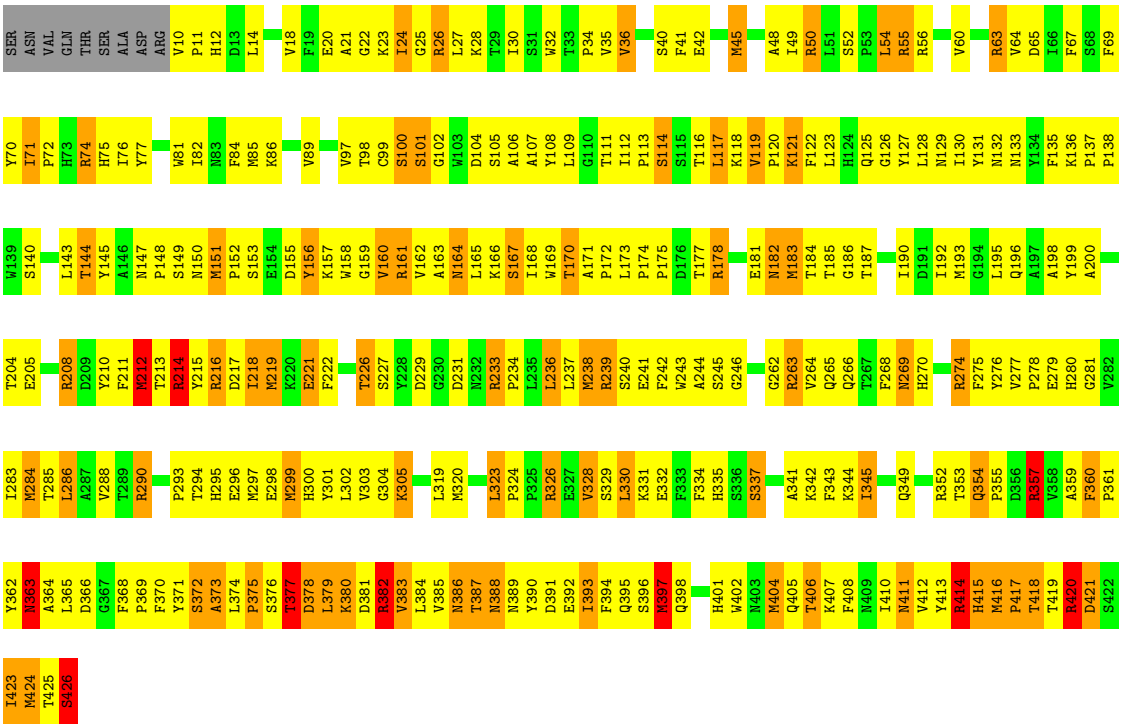
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

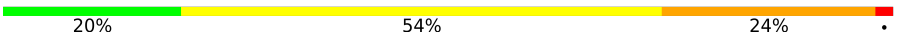
• Molecule 1: BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ

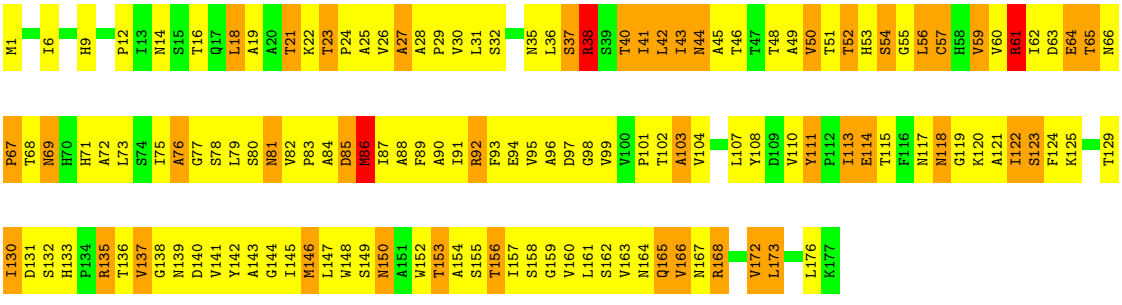
Chain 1:



• Molecule 2: BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ

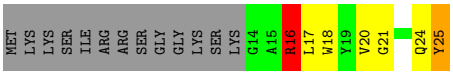
Chain 2:





• Molecule 3: BACTERIOPHAGE G4 CAPSID PROTEINS GPF, GPG, GPJ

Chain 3:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	414.20Å 414.20Å 263.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.352 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4779	wwPDB-VP
Average B, all atoms (Å^2)	0.0	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	1	0.93	0/3461	1.30	40/4713 (0.8%)
2	2	0.90	0/1354	1.40	10/1859 (0.5%)
3	3	1.23	0/100	1.47	1/135 (0.7%)
All	All	0.93	0/4915	1.33	51/6707 (0.8%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	214	ARG	NE-CZ-NH2	7.95	124.27	120.30
1	1	357	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	1	55	ARG	NE-CZ-NH2	7.73	124.17	120.30
2	2	61	ARG	NE-CZ-NH2	7.71	124.16	120.30
1	1	208	ARG	NE-CZ-NH2	7.67	124.13	120.30
2	2	168	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	1	216	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	1	414	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	1	326	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	1	74	ARG	NE-CZ-NH2	7.47	124.04	120.30
1	1	50	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	1	290	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	1	382	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	2	38	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	1	161	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	1	420	ARG	NE-CZ-NH2	7.38	123.99	120.30
2	2	135	ARG	NE-CZ-NH2	7.37	123.99	120.30
3	3	16	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	1	26	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	1	274	ARG	NE-CZ-NH2	7.30	123.95	120.30
2	2	92	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	1	233	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	1	63	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	1	178	ARG	NE-CZ-NH2	6.87	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	263	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	1	239	ARG	NE-CZ-NH2	6.71	123.65	120.30
2	2	41	ILE	CB-CG1-CD1	-6.69	95.17	113.90
1	1	352	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	1	284	MET	CG-SD-CE	6.32	110.31	100.20
1	1	404	MET	CG-SD-CE	6.27	110.22	100.20
1	1	56	ARG	NE-CZ-NH2	6.25	123.42	120.30
2	2	1	MET	CG-SD-CE	6.18	110.09	100.20
1	1	238	MET	CG-SD-CE	6.17	110.07	100.20
1	1	416	MET	CG-SD-CE	6.16	110.05	100.20
1	1	299	MET	CG-SD-CE	6.14	110.02	100.20
2	2	146	MET	CG-SD-CE	6.14	110.02	100.20
1	1	424	MET	CG-SD-CE	6.14	110.02	100.20
1	1	85	MET	CG-SD-CE	6.13	110.01	100.20
1	1	397	MET	CG-SD-CE	6.13	110.00	100.20
1	1	151	MET	CG-SD-CE	6.11	109.97	100.20
1	1	320	MET	CG-SD-CE	6.09	109.94	100.20
1	1	297	MET	CG-SD-CE	6.07	109.91	100.20
1	1	183	MET	CG-SD-CE	6.01	109.81	100.20
1	1	45	MET	CG-SD-CE	6.00	109.81	100.20
2	2	86	MET	CG-SD-CE	6.00	109.79	100.20
1	1	193	MET	CG-SD-CE	5.87	109.58	100.20
1	1	426	SER	CA-C-O	-5.68	108.16	120.10
1	1	219	MET	CG-SD-CE	5.66	109.25	100.20
1	1	212	MET	CG-SD-CE	5.61	109.18	100.20
2	2	64	GLU	CB-CA-C	-5.41	99.58	110.40
1	1	199	TYR	CB-CG-CD1	5.28	124.17	121.00

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	1	3357	0	3220	557	0
2	2	1325	0	1334	350	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	97	0	89	41	0
All	All	4779	0	4643	904	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 96.

All (904) 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)
2:2:18:LEU:HD23	2:2:41:ILE:CD1	1.26	1.60
1:1:138:PRO:HG2	3:3:20:VAL:CG1	1.20	1.57
2:2:18:LEU:CB	2:2:43:ILE:HG22	1.19	1.57
1:1:138:PRO:CG	3:3:20:VAL:HG12	1.13	1.56
2:2:18:LEU:CD2	2:2:41:ILE:HD11	1.32	1.53
2:2:82:VAL:CG1	2:2:86:MET:SD	2.05	1.44
2:2:82:VAL:HG11	2:2:86:MET:SD	1.61	1.39
1:1:328:VAL:HG12	1:1:332:GLU:OE1	1.23	1.38
1:1:138:PRO:CG	3:3:20:VAL:CG1	1.79	1.38
2:2:26:VAL:CA	2:2:54:SER:OG	1.70	1.37
2:2:21:THR:HA	2:2:46:THR:CG2	1.56	1.36
1:1:108:TYR:CE1	1:1:109:LEU:HD21	1.60	1.35
1:1:419:THR:O	1:1:423:ILE:CD1	1.73	1.35
2:2:118:ASN:CG	2:2:119:GLY:H	1.22	1.35
2:2:26:VAL:N	2:2:54:SER:OG	1.58	1.33
1:1:138:PRO:CD	3:3:20:VAL:CG1	2.06	1.33
2:2:49:ALA:HA	2:2:152:TRP:O	1.21	1.30
1:1:138:PRO:CD	3:3:20:VAL:HG11	1.59	1.30
1:1:419:THR:O	1:1:423:ILE:HD12	1.19	1.29
2:2:40:THR:HG23	2:2:162:SER:OG	1.11	1.29
2:2:18:LEU:CB	2:2:43:ILE:CG2	2.10	1.28
2:2:21:THR:CA	2:2:46:THR:HG22	1.63	1.28
1:1:296:GLU:OE1	1:1:363:ASN:HA	1.33	1.22
2:2:43:ILE:O	2:2:45:ALA:N	1.72	1.21
2:2:164:ASN:OD1	2:2:165:GLN:N	1.73	1.20
2:2:94:GLU:OE2	2:2:135:ARG:N	1.76	1.18
1:1:295:HIS:NE2	1:1:373:ALA:O	1.76	1.18
1:1:357:ARG:HH11	1:1:357:ARG:CG	1.57	1.18
1:1:420:ARG:CA	1:1:423:ILE:HD11	1.73	1.18
2:2:40:THR:CG2	2:2:162:SER:OG	1.90	1.18
1:1:18:VAL:CG1	1:1:406:THR:HG23	1.74	1.15
2:2:82:VAL:HG13	2:2:86:MET:SD	1.85	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:175:PRO:HG3	1:1:379:LEU:HD23	1.23	1.15
1:1:390:TYR:O	1:1:393:ILE:HG23	1.44	1.15
1:1:10:VAL:O	1:1:12:HIS:HD2	1.28	1.15
2:2:49:ALA:CA	2:2:152:TRP:O	1.93	1.15
2:2:21:THR:CA	2:2:46:THR:CG2	2.23	1.15
2:2:21:THR:HB	2:2:46:THR:CG2	1.77	1.15
1:1:145:TYR:CD2	1:1:151:MET:HG2	1.82	1.14
1:1:138:PRO:HD2	3:3:20:VAL:CG1	1.75	1.14
2:2:43:ILE:O	2:2:43:ILE:HG12	1.42	1.13
2:2:18:LEU:HB3	2:2:43:ILE:CG2	1.71	1.13
1:1:108:TYR:CE1	1:1:109:LEU:CD2	2.32	1.12
1:1:424:MET:O	1:1:426:SER:OG	1.68	1.11
2:2:40:THR:CG2	2:2:162:SER:CB	2.28	1.11
2:2:12:PRO:HG3	2:2:38:ARG:HB2	1.31	1.11
1:1:213:THR:HG22	3:3:21:GLY:O	1.49	1.11
2:2:42:LEU:O	2:2:42:LEU:HG	1.42	1.11
2:2:118:ASN:ND2	2:2:119:GLY:H	1.49	1.10
1:1:63:ARG:NE	1:1:241:GLU:OE2	1.83	1.10
2:2:18:LEU:CD2	2:2:32:SER:HB2	1.82	1.10
1:1:269:ASN:HD22	1:1:270:HIS:N	1.49	1.09
2:2:32:SER:HB2	2:2:41:ILE:HD11	1.24	1.09
1:1:368:PHE:HB3	1:1:370:PHE:CD2	1.87	1.09
2:2:18:LEU:CG	2:2:43:ILE:HG22	1.83	1.09
2:2:18:LEU:HB3	2:2:43:ILE:HG22	1.14	1.08
2:2:21:THR:CB	2:2:46:THR:CG2	2.31	1.08
1:1:418:THR:HG22	1:1:421:ASP:HB2	1.32	1.08
1:1:418:THR:CG2	1:1:421:ASP:HB2	1.82	1.08
2:2:26:VAL:N	2:2:54:SER:CB	2.17	1.08
2:2:118:ASN:CG	2:2:119:GLY:N	1.99	1.08
2:2:18:LEU:HB2	2:2:43:ILE:HG22	1.13	1.07
1:1:386:ASN:ND2	1:1:386:ASN:O	1.87	1.07
1:1:18:VAL:HG13	1:1:406:THR:HG23	1.34	1.06
1:1:10:VAL:CG2	1:1:11:PRO:HD2	1.85	1.06
2:2:18:LEU:HB3	2:2:43:ILE:CB	1.85	1.06
2:2:40:THR:HG23	2:2:162:SER:CB	1.84	1.06
1:1:359:ALA:C	1:1:361:PRO:HD2	1.77	1.05
2:2:94:GLU:HG2	2:2:141:VAL:HG12	1.33	1.05
1:1:420:ARG:HA	1:1:423:ILE:CD1	1.86	1.04
1:1:10:VAL:O	1:1:12:HIS:CD2	2.10	1.04
2:2:21:THR:HB	2:2:46:THR:HG21	1.04	1.04
1:1:10:VAL:HG23	1:1:11:PRO:HD2	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:63:ARG:CZ	1:1:241:GLU:OE2	2.06	1.03
1:1:300:HIS:O	1:1:303:VAL:HG12	1.57	1.03
2:2:31:LEU:HG	2:2:57:CYS:O	1.59	1.02
1:1:175:PRO:HG3	1:1:379:LEU:CD2	1.89	1.02
2:2:26:VAL:CB	2:2:54:SER:OG	2.07	1.02
1:1:71:ILE:CD1	1:1:126:GLY:HA2	1.88	1.01
1:1:242:PHE:CZ	1:1:268:PHE:HB3	1.94	1.01
2:2:21:THR:CB	2:2:46:THR:HG21	1.87	1.01
1:1:390:TYR:O	1:1:393:ILE:CG2	2.09	1.01
1:1:71:ILE:CD1	1:1:76:ILE:HD11	1.89	1.00
1:1:386:ASN:C	1:1:386:ASN:HD22	1.60	1.00
1:1:49:ILE:CG2	1:1:266:GLN:HB3	1.92	0.99
1:1:108:TYR:HE1	1:1:109:LEU:HD21	1.22	0.99
2:2:50:VAL:HG12	2:2:152:TRP:HB2	1.44	0.99
2:2:18:LEU:HD21	2:2:32:SER:HB2	1.40	0.98
1:1:319:LEU:O	1:1:323:LEU:CD2	2.11	0.98
1:1:357:ARG:NH1	1:1:357:ARG:HG2	1.58	0.98
1:1:70:TYR:HB2	1:1:237:LEU:HD11	1.46	0.97
1:1:133:ASN:O	1:1:214:ARG:NH2	1.98	0.97
2:2:28:ALA:CB	2:2:55:GLY:O	2.12	0.97
1:1:18:VAL:HG12	1:1:406:THR:O	1.65	0.96
1:1:357:ARG:HH11	1:1:357:ARG:HG2	0.79	0.96
1:1:363:ASN:O	1:1:363:ASN:ND2	1.99	0.95
1:1:269:ASN:HD22	1:1:270:HIS:H	1.06	0.95
1:1:319:LEU:O	1:1:323:LEU:HD22	1.64	0.95
1:1:416:MET:SD	1:1:417:PRO:HD2	2.07	0.95
1:1:98:THR:HG22	1:1:147:ASN:ND2	1.82	0.94
2:2:25:ALA:C	2:2:54:SER:HB3	1.86	0.94
2:2:32:SER:HB2	2:2:41:ILE:CD1	1.96	0.94
2:2:86:MET:CE	2:2:147:LEU:HD22	1.97	0.94
1:1:178:ARG:HH22	1:1:205:GLU:CD	1.52	0.94
2:2:36:LEU:HD13	2:2:61:ARG:HH21	1.32	0.94
1:1:244:ALA:HA	1:1:266:GLN:HG2	1.47	0.93
2:2:9:HIS:CE1	2:2:162:SER:HB3	2.03	0.93
1:1:108:TYR:CZ	1:1:151:MET:HE1	2.03	0.93
2:2:82:VAL:CG1	2:2:86:MET:CG	2.47	0.93
1:1:132:ASN:HD21	1:1:143:LEU:H	0.98	0.92
2:2:94:GLU:OE1	2:2:135:ARG:HB2	1.68	0.92
2:2:18:LEU:HD12	2:2:19:ALA:H	1.35	0.92
2:2:26:VAL:HB	2:2:54:SER:OG	1.68	0.92
1:1:238:MET:HE3	1:1:239:ARG:H	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:59:VAL:HG23	2:2:143:ALA:O	1.69	0.92
1:1:132:ASN:ND2	1:1:143:LEU:H	1.67	0.92
2:2:136:THR:O	2:2:139:ASN:OD1	1.88	0.91
2:2:69:ASN:C	2:2:69:ASN:HD22	1.74	0.91
2:2:57:CYS:SG	2:2:91:ILE:HD11	2.09	0.91
1:1:323:LEU:CD2	1:1:323:LEU:H	1.84	0.91
1:1:71:ILE:HD11	1:1:76:ILE:HD11	1.50	0.91
1:1:363:ASN:HD22	1:1:363:ASN:C	1.72	0.91
2:2:136:THR:HB	2:2:139:ASN:HD21	1.34	0.91
2:2:95:VAL:O	2:2:139:ASN:HB2	1.70	0.90
1:1:323:LEU:CD2	1:1:323:LEU:N	2.34	0.90
2:2:40:THR:CG2	2:2:162:SER:HB2	2.01	0.90
1:1:239:ARG:NH1	3:3:25:TYR:HE1	1.68	0.90
2:2:18:LEU:CG	2:2:43:ILE:CG2	2.46	0.90
1:1:178:ARG:NH2	1:1:205:GLU:CD	2.21	0.90
2:2:50:VAL:N	2:2:152:TRP:O	2.04	0.90
1:1:30:ILE:HD12	1:1:45:MET:HE3	1.52	0.89
1:1:242:PHE:CZ	1:1:268:PHE:CB	2.54	0.89
1:1:328:VAL:CG1	1:1:332:GLU:OE1	2.17	0.89
2:2:79:LEU:HD23	2:2:159:GLY:HA3	1.52	0.89
2:2:92:ARG:HD2	2:2:130:ILE:HG13	1.54	0.89
1:1:296:GLU:OE1	1:1:363:ASN:CA	2.20	0.89
1:1:323:LEU:HD22	1:1:323:LEU:N	1.86	0.89
2:2:64:GLU:OE2	2:2:140:ASP:OD1	1.90	0.89
2:2:97:ASP:CB	2:2:138:GLY:O	2.21	0.89
2:2:97:ASP:N	2:2:139:ASN:HA	1.87	0.89
2:2:40:THR:HG22	2:2:162:SER:HB2	1.53	0.89
1:1:368:PHE:HB3	1:1:370:PHE:CE2	2.08	0.88
2:2:61:ARG:HG3	2:2:142:TYR:CE1	2.09	0.88
1:1:420:ARG:HA	1:1:423:ILE:HD11	0.92	0.88
2:2:28:ALA:HA	2:2:55:GLY:O	1.72	0.88
2:2:118:ASN:ND2	2:2:121:ALA:H	1.71	0.88
2:2:18:LEU:HB2	2:2:41:ILE:HG12	1.52	0.88
1:1:99:CYS:SG	1:1:148:PRO:HG2	2.12	0.88
1:1:138:PRO:HD2	3:3:20:VAL:HG11	1.41	0.87
1:1:221:GLU:O	1:1:221:GLU:HG3	1.74	0.87
2:2:56:LEU:O	2:2:56:LEU:HD12	1.73	0.87
2:2:43:ILE:O	2:2:44:ASN:C	2.03	0.87
2:2:79:LEU:O	2:2:121:ALA:HA	1.74	0.87
1:1:245:SER:H	1:1:266:GLN:HE21	1.20	0.87
1:1:49:ILE:HG22	1:1:266:GLN:HB3	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:104:ASP:OD2	1:1:157:LYS:HE2	1.73	0.87
1:1:128:LEU:HD22	1:1:143:LEU:O	1.75	0.87
2:2:18:LEU:HD23	2:2:41:ILE:CG1	2.04	0.87
2:2:153:THR:HG23	2:2:154:ALA:N	1.87	0.86
1:1:420:ARG:O	1:1:424:MET:HG2	1.75	0.86
2:2:97:ASP:HB3	2:2:138:GLY:O	1.76	0.86
1:1:21:ALA:O	1:1:28:LYS:NZ	2.09	0.86
1:1:172:PRO:HG2	1:1:379:LEU:HD11	1.58	0.85
1:1:18:VAL:HG11	1:1:406:THR:HG23	1.56	0.85
2:2:37:SER:C	2:2:38:ARG:HD3	1.95	0.85
2:2:9:HIS:HE1	2:2:162:SER:HB3	1.39	0.85
1:1:161:ARG:O	1:1:384:LEU:HD22	1.75	0.85
1:1:167:SER:H	1:1:170:THR:HG22	1.41	0.85
2:2:28:ALA:CA	2:2:55:GLY:O	2.24	0.85
1:1:377:THR:O	1:1:382:ARG:NH1	2.09	0.85
2:2:52:THR:CG2	2:2:52:THR:O	2.23	0.85
1:1:138:PRO:HD2	3:3:20:VAL:HG13	1.59	0.85
2:2:26:VAL:HA	2:2:54:SER:OG	1.72	0.85
1:1:138:PRO:CG	3:3:20:VAL:HG11	1.83	0.84
2:2:41:ILE:HG23	2:2:43:ILE:HG23	1.56	0.84
2:2:69:ASN:HD21	2:2:131:ASP:HB2	1.40	0.84
2:2:40:THR:HG23	2:2:162:SER:HG	0.88	0.84
1:1:423:ILE:HD13	1:1:423:ILE:H	1.43	0.84
2:2:95:VAL:O	2:2:139:ASN:CB	2.27	0.83
1:1:145:TYR:CG	1:1:151:MET:HG2	2.13	0.83
1:1:18:VAL:HG22	1:1:20:GLU:CG	2.07	0.83
1:1:120:PRO:HG2	1:1:123:LEU:HD12	1.58	0.83
1:1:368:PHE:HB3	1:1:370:PHE:HD2	1.42	0.83
2:2:44:ASN:HD22	2:2:158:SER:HB2	1.42	0.83
2:2:82:VAL:HG12	2:2:86:MET:HG3	1.59	0.83
1:1:353:THR:HG22	1:1:354:GLN:N	1.93	0.83
2:2:73:LEU:HD12	2:2:164:ASN:O	1.78	0.83
2:2:153:THR:CG2	2:2:154:ALA:N	2.42	0.82
1:1:71:ILE:HD13	1:1:126:GLY:HA2	1.62	0.82
1:1:52:SER:HB2	1:1:394:PHE:CD2	2.15	0.82
1:1:269:ASN:ND2	1:1:270:HIS:N	2.28	0.82
1:1:144:THR:O	1:1:144:THR:HG23	1.78	0.82
1:1:360:PHE:N	1:1:361:PRO:CD	2.42	0.82
2:2:23:THR:HA	2:2:48:THR:CG2	2.10	0.82
2:2:36:LEU:O	2:2:61:ARG:O	1.98	0.81
1:1:108:TYR:CD1	1:1:109:LEU:CD2	2.64	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:163:ALA:O	1:1:290:ARG:NH1	2.12	0.81
1:1:30:ILE:CD1	1:1:45:MET:HE3	2.11	0.81
1:1:386:ASN:ND2	1:1:386:ASN:C	2.31	0.81
1:1:210:TYR:O	3:3:21:GLY:HA2	1.82	0.80
1:1:372:SER:H	1:1:389:ASN:HD21	1.28	0.80
1:1:360:PHE:N	1:1:361:PRO:HD2	1.95	0.80
1:1:387:THR:HG22	1:1:388:ASN:N	1.96	0.80
1:1:120:PRO:HG2	1:1:123:LEU:CD1	2.11	0.80
1:1:363:ASN:ND2	1:1:363:ASN:C	2.31	0.80
1:1:239:ARG:NH1	3:3:25:TYR:CE1	2.50	0.80
2:2:52:THR:O	2:2:52:THR:HG23	1.81	0.80
2:2:95:VAL:CG1	2:2:142:TYR:HE2	1.94	0.79
1:1:162:VAL:C	1:1:384:LEU:HD23	2.03	0.79
2:2:9:HIS:HB3	2:2:125:LYS:HE2	1.63	0.79
2:2:157:ILE:HG13	2:2:157:ILE:O	1.83	0.79
1:1:164:ASN:ND2	1:1:385:VAL:HB	1.98	0.79
2:2:118:ASN:ND2	2:2:119:GLY:N	2.23	0.79
2:2:23:THR:HA	2:2:48:THR:HG22	1.64	0.79
2:2:37:SER:HB3	2:2:38:ARG:CD	2.12	0.79
2:2:130:ILE:HG12	2:2:131:ASP:N	1.98	0.79
1:1:372:SER:N	1:1:389:ASN:HD21	1.79	0.79
1:1:216:ARG:HA	1:1:226:THR:HG21	1.65	0.78
1:1:420:ARG:CA	1:1:423:ILE:CD1	2.55	0.78
1:1:133:ASN:C	1:1:214:ARG:NH2	2.36	0.78
1:1:387:THR:CG2	1:1:388:ASN:N	2.46	0.78
1:1:417:PRO:O	1:1:418:THR:HB	1.84	0.78
1:1:238:MET:CE	1:1:239:ARG:H	1.96	0.78
2:2:77:GLY:O	2:2:123:SER:HA	1.83	0.78
2:2:37:SER:HB3	2:2:38:ARG:NH1	1.99	0.78
2:2:101:PRO:HD3	2:2:142:TYR:CZ	2.19	0.78
2:2:82:VAL:HG12	2:2:86:MET:CG	2.14	0.78
2:2:165:GLN:OE1	2:2:167:ASN:OD1	2.02	0.78
2:2:63:ASP:OD1	2:2:65:THR:HG23	1.82	0.78
2:2:36:LEU:HD13	2:2:61:ARG:NH2	2.00	0.77
1:1:71:ILE:HD13	1:1:126:GLY:CA	2.15	0.77
2:2:101:PRO:CD	2:2:142:TYR:CZ	2.67	0.77
1:1:345:ILE:HD11	1:1:349:GLN:HB3	1.67	0.77
1:1:416:MET:SD	1:1:417:PRO:CD	2.72	0.77
1:1:97:VAL:CG2	1:1:121:LYS:HA	2.14	0.77
2:2:44:ASN:HD22	2:2:158:SER:CB	1.98	0.77
2:2:86:MET:HE1	2:2:147:LEU:HD22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:319:LEU:O	1:1:323:LEU:HD21	1.84	0.76
2:2:18:LEU:HB3	2:2:43:ILE:CA	2.15	0.76
2:2:18:LEU:HD21	2:2:32:SER:CB	2.15	0.76
1:1:125:GLN:OE1	1:1:129:ASN:ND2	2.17	0.76
1:1:10:VAL:HG22	1:1:11:PRO:HD2	1.67	0.76
1:1:145:TYR:CD2	1:1:151:MET:CG	2.68	0.76
1:1:136:LYS:O	1:1:136:LYS:HG3	1.85	0.76
2:2:49:ALA:CB	2:2:153:THR:HA	2.15	0.76
2:2:153:THR:HG23	2:2:154:ALA:H	1.49	0.75
1:1:170:THR:HG23	1:1:170:THR:O	1.85	0.75
2:2:94:GLU:OE2	2:2:135:ARG:CB	2.34	0.75
2:2:26:VAL:C	2:2:28:ALA:H	1.88	0.75
2:2:43:ILE:O	2:2:43:ILE:CG1	2.21	0.75
1:1:166:LYS:CD	3:3:18:TRP:CD1	2.69	0.75
2:2:137:VAL:HG13	2:2:138:GLY:N	2.01	0.75
1:1:132:ASN:HD21	1:1:143:LEU:N	1.81	0.75
2:2:86:MET:HE2	2:2:147:LEU:HB3	1.69	0.75
2:2:38:ARG:HD3	2:2:38:ARG:N	2.02	0.74
2:2:18:LEU:HG	2:2:43:ILE:CG2	2.15	0.74
2:2:82:VAL:CG1	2:2:86:MET:HG3	2.16	0.74
1:1:323:LEU:HD22	1:1:323:LEU:H	1.50	0.74
1:1:231:ASP:CG	1:1:233:ARG:HH11	1.91	0.73
1:1:166:LYS:HD3	3:3:18:TRP:CD1	2.23	0.73
2:2:69:ASN:HA	2:2:133:HIS:CE1	2.22	0.73
1:1:268:PHE:CZ	1:1:404:MET:CE	2.71	0.73
1:1:18:VAL:HG21	1:1:20:GLU:OE2	1.89	0.73
1:1:108:TYR:CZ	1:1:151:MET:CE	2.71	0.73
1:1:162:VAL:CG1	1:1:290:ARG:HD3	2.17	0.73
1:1:387:THR:HG22	1:1:388:ASN:HD22	1.53	0.73
1:1:213:THR:CG2	3:3:21:GLY:O	2.34	0.73
1:1:156:TYR:CD1	1:1:156:TYR:C	2.62	0.73
2:2:118:ASN:HD21	2:2:121:ALA:H	1.34	0.73
1:1:323:LEU:H	1:1:323:LEU:HD23	1.54	0.73
2:2:40:THR:HG22	2:2:162:SER:CB	2.09	0.72
2:2:21:THR:HA	2:2:46:THR:HG22	0.77	0.72
1:1:299:MET:SD	1:1:304:GLY:HA3	2.30	0.72
2:2:18:LEU:HD21	2:2:41:ILE:HD11	1.61	0.72
2:2:26:VAL:N	2:2:54:SER:HB3	1.94	0.72
2:2:94:GLU:CD	2:2:135:ARG:HB2	2.10	0.72
1:1:63:ARG:NH2	1:1:241:GLU:CD	2.43	0.72
1:1:379:LEU:O	1:1:383:VAL:HG13	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:18:VAL:CG1	1:1:406:THR:CG2	2.64	0.72
2:2:165:GLN:CD	2:2:167:ASN:OD1	2.28	0.71
1:1:71:ILE:CD1	1:1:126:GLY:CA	2.65	0.71
1:1:300:HIS:O	1:1:303:VAL:CG1	2.38	0.71
1:1:359:ALA:CB	1:1:361:PRO:HD2	2.20	0.71
1:1:72:PRO:O	1:1:75:HIS:HB2	1.90	0.71
2:2:95:VAL:HG11	2:2:142:TYR:HE2	1.53	0.71
1:1:55:ARG:NH1	1:1:392:GLU:O	2.23	0.71
1:1:397:MET:O	2:2:68:THR:OG1	2.08	0.71
2:2:9:HIS:HE1	2:2:162:SER:CB	2.03	0.71
2:2:29:PRO:HA	2:2:103:ALA:HB2	1.72	0.71
1:1:63:ARG:HH21	1:1:241:GLU:CD	1.94	0.71
2:2:28:ALA:HB1	2:2:55:GLY:O	1.89	0.71
2:2:90:ALA:O	2:2:91:ILE:CG2	2.39	0.71
1:1:30:ILE:HD12	1:1:45:MET:CE	2.19	0.71
2:2:36:LEU:CD1	2:2:61:ARG:HH21	2.03	0.71
2:2:115:THR:OG1	2:2:122:ILE:HD11	1.90	0.71
1:1:329:SER:C	1:1:331:LYS:H	1.94	0.70
1:1:63:ARG:HE	1:1:241:GLU:CD	1.95	0.70
1:1:138:PRO:HD3	3:3:20:VAL:HG11	1.70	0.70
2:2:81:ASN:O	2:2:157:ILE:HG22	1.91	0.70
2:2:137:VAL:HG13	2:2:138:GLY:H	1.56	0.70
1:1:12:HIS:CE1	1:1:416:MET:HG3	2.27	0.70
1:1:49:ILE:HG23	1:1:266:GLN:HB3	1.72	0.70
1:1:295:HIS:CE1	1:1:373:ALA:O	2.45	0.70
2:2:18:LEU:CD2	2:2:41:ILE:CD1	2.17	0.70
2:2:59:VAL:HA	2:2:144:GLY:HA3	1.74	0.70
2:2:65:THR:O	2:2:65:THR:OG1	2.09	0.70
1:1:100:SER:O	1:1:105:SER:CB	2.39	0.70
1:1:353:THR:CG2	1:1:354:GLN:N	2.54	0.70
2:2:24:PRO:HB3	2:2:56:LEU:HG	1.72	0.70
1:1:108:TYR:CD1	1:1:109:LEU:HD23	2.25	0.70
2:2:86:MET:HE2	2:2:147:LEU:HD22	1.74	0.70
2:2:89:PHE:CE1	2:2:110:VAL:HG12	2.27	0.70
2:2:37:SER:C	2:2:38:ARG:CD	2.60	0.70
1:1:335:HIS:CG	1:1:335:HIS:O	2.45	0.69
1:1:246:GLY:HA3	1:1:263:ARG:O	1.92	0.69
1:1:65:ASP:HB2	1:1:288:VAL:CG1	2.21	0.69
1:1:144:THR:O	1:1:144:THR:CG2	2.40	0.69
1:1:30:ILE:CD1	1:1:45:MET:CE	2.70	0.69
1:1:63:ARG:NE	1:1:241:GLU:CD	2.44	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:71:ILE:CG1	1:1:76:ILE:HD11	2.21	0.69
1:1:98:THR:O	1:1:148:PRO:HD2	1.93	0.69
1:1:116:THR:HB	1:1:118:LYS:NZ	2.08	0.69
2:2:37:SER:HB3	2:2:38:ARG:HD3	1.74	0.69
1:1:97:VAL:HG23	1:1:121:LYS:HA	1.74	0.68
1:1:268:PHE:CZ	1:1:404:MET:HE1	2.28	0.68
1:1:24:ILE:HG12	1:1:401:HIS:HD2	1.57	0.68
1:1:98:THR:HG22	1:1:147:ASN:HD22	1.55	0.68
1:1:301:TYR:HE1	1:1:332:GLU:OE1	1.76	0.68
2:2:172:VAL:HG23	2:2:173:LEU:N	2.08	0.68
2:2:32:SER:CB	2:2:41:ILE:CD1	2.69	0.68
1:1:164:ASN:HD21	1:1:385:VAL:HB	1.55	0.68
1:1:196:GLN:NE2	1:1:196:GLN:HA	2.07	0.68
1:1:240:SER:CB	1:1:270:HIS:HD1	2.06	0.68
2:2:26:VAL:HG13	2:2:27:ALA:H	1.57	0.68
1:1:300:HIS:CD2	1:1:302:LEU:HB2	2.29	0.68
1:1:357:ARG:CG	1:1:357:ARG:NH1	2.29	0.68
1:1:133:ASN:C	1:1:214:ARG:HH21	1.95	0.68
1:1:387:THR:HG22	1:1:388:ASN:H	1.56	0.68
1:1:10:VAL:CG2	1:1:11:PRO:CD	2.69	0.68
1:1:208:ARG:NH1	1:1:218:ILE:HD12	2.10	0.67
1:1:368:PHE:CD1	1:1:370:PHE:HE2	2.12	0.67
1:1:18:VAL:HG22	1:1:20:GLU:HG2	1.74	0.67
1:1:323:LEU:HB2	1:1:324:PRO:HD2	1.75	0.67
1:1:349:GLN:HE21	1:1:349:GLN:HA	1.59	0.67
2:2:41:ILE:CG2	2:2:43:ILE:HG23	2.24	0.67
1:1:101:SER:HA	1:1:117:LEU:HD21	1.77	0.67
2:2:86:MET:HB2	2:2:117:ASN:HD22	1.60	0.67
1:1:22:GLY:HA2	1:1:158:TRP:CE3	2.30	0.67
1:1:182:ASN:N	1:1:182:ASN:HD22	1.92	0.67
2:2:32:SER:CB	2:2:41:ILE:HD11	2.15	0.66
1:1:353:THR:CG2	1:1:354:GLN:H	2.09	0.66
1:1:98:THR:H	1:1:147:ASN:HD22	1.44	0.66
1:1:108:TYR:CE2	1:1:151:MET:HE1	2.30	0.66
1:1:162:VAL:O	1:1:385:VAL:HG13	1.95	0.66
1:1:100:SER:O	1:1:105:SER:OG	2.14	0.66
1:1:97:VAL:HG23	1:1:121:LYS:CA	2.26	0.66
1:1:162:VAL:HG13	1:1:290:ARG:HD3	1.78	0.66
1:1:387:THR:HG22	1:1:388:ASN:ND2	2.10	0.66
1:1:108:TYR:CE2	1:1:151:MET:CE	2.79	0.66
1:1:156:TYR:HD1	1:1:156:TYR:O	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:12:PRO:CG	2:2:38:ARG:HB2	2.19	0.66
1:1:45:MET:HE3	1:1:408:PHE:CZ	2.31	0.65
2:2:49:ALA:HA	2:2:152:TRP:C	2.13	0.65
2:2:49:ALA:C	2:2:152:TRP:O	2.34	0.65
2:2:90:ALA:O	2:2:91:ILE:HG23	1.95	0.65
1:1:24:ILE:HG12	1:1:401:HIS:CD2	2.32	0.65
1:1:268:PHE:CE2	1:1:404:MET:SD	2.89	0.65
1:1:268:PHE:HZ	1:1:404:MET:CE	2.09	0.65
2:2:50:VAL:HG12	2:2:152:TRP:CB	2.23	0.65
1:1:70:TYR:CE1	1:1:277:VAL:HG13	2.32	0.65
1:1:376:SER:O	1:1:378:ASP:N	2.29	0.65
1:1:242:PHE:HE2	1:1:266:GLN:HG3	1.62	0.65
1:1:70:TYR:OH	1:1:277:VAL:HG13	1.97	0.65
1:1:167:SER:HB3	1:1:170:THR:HB	1.77	0.65
1:1:360:PHE:CD1	1:1:360:PHE:C	2.70	0.64
1:1:167:SER:OG	1:1:168:ILE:N	2.30	0.64
2:2:18:LEU:CD2	2:2:41:ILE:CG1	2.70	0.64
2:2:85:ASP:OD1	2:2:85:ASP:C	2.35	0.64
2:2:12:PRO:HG3	2:2:38:ARG:CB	2.20	0.64
1:1:63:ARG:HE	1:1:241:GLU:CG	2.11	0.64
2:2:37:SER:HB3	2:2:38:ARG:HH11	1.60	0.64
1:1:227:SER:C	1:1:229:ASP:H	1.99	0.64
1:1:359:ALA:C	1:1:361:PRO:CD	2.61	0.64
1:1:97:VAL:HG21	1:1:121:LYS:HA	1.80	0.64
2:2:78:SER:HA	2:2:122:ILE:O	1.98	0.64
2:2:94:GLU:OE2	2:2:135:ARG:CA	2.46	0.64
1:1:70:TYR:CZ	1:1:277:VAL:HG13	2.33	0.63
1:1:116:THR:CB	1:1:118:LYS:NZ	2.62	0.63
2:2:59:VAL:CG2	2:2:60:VAL:N	2.61	0.63
2:2:87:ILE:HG22	2:2:148:TRP:O	1.98	0.63
1:1:126:GLY:C	1:1:284:MET:HE3	2.19	0.63
1:1:63:ARG:CZ	1:1:241:GLU:CD	2.66	0.63
1:1:214:ARG:O	1:1:217:ASP:HB2	1.99	0.63
1:1:153:SER:O	1:1:157:LYS:HG3	1.97	0.63
1:1:156:TYR:C	1:1:156:TYR:HD1	2.01	0.63
1:1:389:ASN:OD1	1:1:389:ASN:O	2.17	0.63
2:2:89:PHE:CD1	2:2:110:VAL:HG12	2.33	0.63
1:1:63:ARG:HE	1:1:241:GLU:HG3	1.62	0.63
1:1:45:MET:HE3	1:1:408:PHE:HZ	1.62	0.63
1:1:240:SER:OG	1:1:270:HIS:ND1	1.90	0.63
1:1:420:ARG:O	1:1:424:MET:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:ALA:HB2	2:2:153:THR:HA	1.80	0.63
2:2:18:LEU:CD2	2:2:32:SER:CB	2.69	0.63
1:1:166:LYS:CG	3:3:18:TRP:CD1	2.82	0.62
1:1:238:MET:CE	1:1:239:ARG:O	2.47	0.62
2:2:18:LEU:HD23	2:2:41:ILE:HD11	0.63	0.62
1:1:23:LYS:O	1:1:402:TRP:CD1	2.53	0.62
1:1:82:ILE:O	1:1:86:LYS:HG3	1.98	0.62
1:1:239:ARG:HH11	3:3:25:TYR:HE1	1.43	0.62
1:1:419:THR:C	1:1:423:ILE:CD1	2.65	0.62
2:2:69:ASN:C	2:2:69:ASN:ND2	2.45	0.62
1:1:67:PHE:HB3	1:1:69:PHE:CE2	2.34	0.62
1:1:133:ASN:CA	1:1:214:ARG:HH21	2.13	0.62
2:2:59:VAL:HB	2:2:144:GLY:HA3	1.81	0.62
1:1:359:ALA:HB1	1:1:361:PRO:HD2	1.82	0.62
1:1:26:ARG:NE	1:1:159:GLY:O	2.31	0.62
1:1:127:TYR:N	1:1:284:MET:HE1	2.14	0.62
2:2:26:VAL:C	2:2:28:ALA:N	2.53	0.62
2:2:26:VAL:HG13	2:2:27:ALA:N	2.15	0.62
2:2:94:GLU:OE2	2:2:135:ARG:HB2	1.99	0.62
1:1:294:THR:HG21	1:1:370:PHE:CD1	2.35	0.62
1:1:71:ILE:HG13	1:1:76:ILE:HD11	1.82	0.61
1:1:294:THR:CG2	1:1:370:PHE:HD1	2.13	0.61
1:1:226:THR:O	1:1:233:ARG:NH2	2.26	0.61
1:1:414:ARG:CG	1:1:415:HIS:H	2.13	0.61
1:1:102:GLY:O	1:1:105:SER:HB3	2.00	0.61
1:1:295:HIS:HA	1:1:371:TYR:HB2	1.82	0.61
1:1:300:HIS:HD2	1:1:302:LEU:HB2	1.65	0.61
2:2:37:SER:CB	2:2:38:ARG:HD3	2.30	0.61
2:2:50:VAL:O	2:2:50:VAL:CG1	2.47	0.61
1:1:116:THR:CB	1:1:118:LYS:HZ3	2.13	0.61
1:1:238:MET:HE2	1:1:239:ARG:O	2.00	0.61
1:1:242:PHE:CE1	1:1:268:PHE:HB2	2.36	0.61
1:1:138:PRO:HG3	3:3:20:VAL:CG1	2.19	0.61
1:1:60:VAL:HG13	1:1:369:PRO:HG2	1.83	0.61
1:1:102:GLY:O	1:1:105:SER:CB	2.49	0.61
1:1:240:SER:HG	1:1:270:HIS:CE1	2.07	0.61
2:2:36:LEU:CD1	2:2:61:ARG:NH2	2.63	0.61
1:1:77:TYR:HB2	1:1:81:TRP:HB2	1.81	0.61
2:2:51:THR:HG23	2:2:51:THR:O	2.00	0.61
1:1:305:LYS:O	1:1:305:LYS:HG3	2.01	0.60
1:1:137:PRO:O	1:1:140:SER:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:133:ASN:HA	1:1:214:ARG:HH21	1.66	0.60
1:1:329:SER:C	1:1:331:LYS:N	2.55	0.60
1:1:204:THR:O	1:1:208:ARG:HG3	2.02	0.60
1:1:383:VAL:CG2	1:1:384:LEU:N	2.64	0.60
1:1:420:ARG:O	1:1:424:MET:CG	2.47	0.60
1:1:18:VAL:HG22	1:1:20:GLU:HG3	1.83	0.60
1:1:162:VAL:C	1:1:384:LEU:CD2	2.71	0.60
1:1:418:THR:HG22	1:1:421:ASP:CB	2.20	0.60
2:2:92:ARG:HG2	2:2:92:ARG:HH11	1.65	0.60
1:1:153:SER:HA	1:1:156:TYR:CE2	2.37	0.59
2:2:95:VAL:HG12	2:2:142:TYR:HE2	1.67	0.59
2:2:97:ASP:HB2	2:2:138:GLY:O	2.01	0.59
1:1:69:PHE:CE1	1:1:236:LEU:HG	2.37	0.59
1:1:185:THR:HG23	1:1:186:GLY:O	2.02	0.59
1:1:245:SER:N	1:1:266:GLN:HE21	1.96	0.59
1:1:397:MET:HG2	2:2:68:THR:HG1	1.68	0.59
2:2:38:ARG:CD	2:2:38:ARG:N	2.65	0.59
1:1:11:PRO:HG3	1:1:413:TYR:CE1	2.38	0.59
2:2:94:GLU:OE1	2:2:135:ARG:CB	2.45	0.59
2:2:94:GLU:CD	2:2:135:ARG:HG3	2.23	0.59
1:1:26:ARG:HB3	1:1:159:GLY:O	2.03	0.58
1:1:120:PRO:CG	1:1:123:LEU:HD12	2.31	0.58
1:1:163:ALA:N	1:1:384:LEU:HD23	2.17	0.58
2:2:95:VAL:HG12	2:2:142:TYR:CE2	2.39	0.58
2:2:90:ALA:C	2:2:91:ILE:HG23	2.23	0.58
2:2:118:ASN:HD21	2:2:120:LYS:H	1.50	0.58
1:1:231:ASP:OD1	1:1:233:ARG:NH1	2.35	0.58
1:1:349:GLN:HA	1:1:349:GLN:NE2	2.19	0.58
1:1:164:ASN:ND2	1:1:385:VAL:CB	2.67	0.58
1:1:166:LYS:CD	3:3:18:TRP:HD1	2.15	0.58
1:1:397:MET:HG2	2:2:68:THR:OG1	2.03	0.58
1:1:155:ASP:O	1:1:159:GLY:HA2	2.04	0.58
1:1:166:LYS:HD3	3:3:18:TRP:HD1	1.69	0.58
1:1:173:LEU:HB2	1:1:344:LYS:O	2.04	0.58
2:2:30:VAL:HG23	2:2:103:ALA:HA	1.86	0.58
2:2:156:THR:HG22	2:2:156:THR:O	2.04	0.58
1:1:63:ARG:NH2	1:1:241:GLU:OE1	2.37	0.57
1:1:128:LEU:CD2	1:1:143:LEU:O	2.51	0.57
2:2:79:LEU:HD23	2:2:159:GLY:CA	2.29	0.57
1:1:165:LEU:HB2	1:1:293:PRO:HD3	1.85	0.57
1:1:383:VAL:CG2	1:1:384:LEU:H	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:94:GLU:OE1	2:2:135:ARG:HG3	2.05	0.57
2:2:95:VAL:CG1	2:2:142:TYR:CE2	2.82	0.57
2:2:137:VAL:CG1	2:2:138:GLY:H	2.17	0.57
2:2:165:GLN:O	2:2:167:ASN:N	2.37	0.57
1:1:18:VAL:HG11	1:1:406:THR:CG2	2.31	0.57
1:1:70:TYR:OH	1:1:279:GLU:O	2.21	0.57
1:1:166:LYS:HB3	3:3:18:TRP:NE1	2.19	0.57
1:1:166:LYS:HG2	3:3:18:TRP:CG	2.39	0.57
1:1:167:SER:O	3:3:18:TRP:CH2	2.57	0.57
2:2:137:VAL:CG1	2:2:138:GLY:N	2.68	0.57
1:1:27:LEU:O	1:1:159:GLY:HA3	2.04	0.57
1:1:277:VAL:HG12	1:1:279:GLU:O	2.05	0.57
1:1:14:LEU:HD12	1:1:412:VAL:HG21	1.86	0.56
1:1:106:ALA:O	1:1:109:LEU:N	2.29	0.56
1:1:170:THR:O	1:1:170:THR:CG2	2.52	0.56
2:2:18:LEU:HB2	2:2:43:ILE:CG2	2.04	0.56
2:2:156:THR:O	2:2:156:THR:CG2	2.53	0.56
1:1:335:HIS:O	1:1:335:HIS:CD2	2.57	0.56
1:1:40:SER:OG	1:1:413:TYR:HB2	2.06	0.56
1:1:135:PHE:CE1	3:3:25:TYR:HB3	2.40	0.56
1:1:268:PHE:CZ	1:1:404:MET:SD	2.98	0.56
1:1:378:ASP:O	1:1:382:ARG:HD2	2.05	0.56
2:2:37:SER:HB3	2:2:38:ARG:CZ	2.36	0.56
2:2:101:PRO:HD3	2:2:142:TYR:OH	2.03	0.56
2:2:101:PRO:HG3	2:2:142:TYR:CE2	2.40	0.56
1:1:362:TYR:O	1:1:364:ALA:N	2.39	0.56
2:2:18:LEU:HB3	2:2:43:ILE:HB	1.85	0.56
1:1:242:PHE:CE1	1:1:268:PHE:CB	2.89	0.56
1:1:300:HIS:HB3	1:1:303:VAL:HG12	1.87	0.56
1:1:376:SER:O	1:1:377:THR:C	2.44	0.56
1:1:276:TYR:O	1:1:278:PRO:HD3	2.06	0.56
2:2:59:VAL:HG23	2:2:143:ALA:C	2.26	0.56
2:2:94:GLU:CD	2:2:135:ARG:CB	2.74	0.56
1:1:178:ARG:HD3	1:1:181:GLU:OE1	2.06	0.56
2:2:98:GLY:N	2:2:140:ASP:OD2	2.27	0.56
1:1:227:SER:C	1:1:229:ASP:N	2.58	0.55
1:1:12:HIS:CE1	1:1:416:MET:HB2	2.41	0.55
1:1:71:ILE:HD11	1:1:76:ILE:CD1	2.31	0.55
1:1:167:SER:O	3:3:18:TRP:CZ3	2.59	0.55
2:2:92:ARG:HH22	2:2:141:VAL:HG11	1.70	0.55
1:1:11:PRO:HG3	1:1:413:TYR:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:45:MET:SD	1:1:408:PHE:CE1	3.00	0.55
1:1:69:PHE:CD1	1:1:236:LEU:HA	2.41	0.55
2:2:101:PRO:HD3	2:2:142:TYR:CE2	2.42	0.55
2:2:50:VAL:O	2:2:50:VAL:HG13	2.05	0.55
1:1:14:LEU:HD12	1:1:412:VAL:CG2	2.36	0.55
1:1:382:ARG:O	1:1:382:ARG:HG2	2.02	0.55
2:2:97:ASP:OD1	2:2:140:ASP:OD1	2.23	0.55
1:1:135:PHE:CE1	3:3:25:TYR:CB	2.90	0.55
1:1:171:ALA:N	1:1:172:PRO:HD3	2.22	0.55
2:2:18:LEU:HG	2:2:43:ILE:HG21	1.87	0.55
1:1:70:TYR:OH	1:1:277:VAL:CG1	2.55	0.55
1:1:119:VAL:HG13	1:1:120:PRO:HD2	1.89	0.55
2:2:160:VAL:HG22	2:2:161:LEU:N	2.22	0.55
2:2:18:LEU:CG	2:2:43:ILE:HG21	2.36	0.55
1:1:166:LYS:HB3	3:3:18:TRP:CD1	2.41	0.54
2:2:59:VAL:HG23	2:2:60:VAL:N	2.21	0.54
2:2:26:VAL:CA	2:2:54:SER:CB	2.76	0.54
1:1:383:VAL:HG22	1:1:384:LEU:H	1.72	0.54
2:2:40:THR:HA	2:2:161:LEU:O	2.06	0.54
1:1:50:ARG:NH1	1:1:265:GLN:OE1	2.35	0.54
1:1:387:THR:CG2	1:1:388:ASN:HD22	2.19	0.54
2:2:18:LEU:HB3	2:2:43:ILE:HA	1.89	0.54
2:2:23:THR:O	2:2:23:THR:OG1	2.21	0.54
2:2:117:ASN:OD1	2:2:118:ASN:N	2.40	0.54
1:1:299:MET:SD	1:1:304:GLY:CA	2.96	0.54
1:1:35:VAL:HG22	1:1:281:GLY:O	2.07	0.54
1:1:97:VAL:HG12	1:1:148:PRO:HD2	1.89	0.54
2:2:41:ILE:HG12	2:2:43:ILE:CG2	2.37	0.54
2:2:84:ALA:HB2	2:2:119:GLY:O	2.08	0.54
1:1:18:VAL:CG2	1:1:20:GLU:HG2	2.38	0.54
1:1:359:ALA:CA	1:1:361:PRO:HD2	2.38	0.54
1:1:25:GLY:HA3	1:1:385:VAL:HG21	1.90	0.53
1:1:108:TYR:CE1	1:1:109:LEU:CG	2.91	0.53
1:1:182:ASN:N	1:1:182:ASN:ND2	2.55	0.53
1:1:242:PHE:CE2	1:1:266:GLN:HG3	2.41	0.53
1:1:331:LYS:HG3	1:1:337:SER:O	2.08	0.53
2:2:59:VAL:CG2	2:2:143:ALA:O	2.51	0.53
1:1:60:VAL:CG1	1:1:369:PRO:HG2	2.38	0.53
1:1:326:ARG:O	1:1:345:ILE:HG22	2.08	0.53
2:2:96:ALA:C	2:2:139:ASN:HA	2.29	0.53
1:1:18:VAL:CG2	1:1:20:GLU:OE2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:80:SER:HA	2:2:120:LYS:O	2.09	0.53
1:1:152:PRO:HG2	1:1:155:ASP:OD2	2.08	0.53
1:1:372:SER:H	1:1:389:ASN:ND2	2.02	0.53
1:1:216:ARG:HD3	1:1:231:ASP:OD2	2.08	0.53
1:1:238:MET:HG3	1:1:270:HIS:CE1	2.43	0.53
1:1:420:ARG:O	1:1:424:MET:CB	2.57	0.53
1:1:362:TYR:C	1:1:364:ALA:H	2.13	0.53
1:1:418:THR:HG23	1:1:421:ASP:H	1.74	0.53
1:1:101:SER:HA	1:1:117:LEU:CD2	2.40	0.52
2:2:52:THR:O	2:2:52:THR:HG22	2.07	0.52
2:2:111:TYR:N	2:2:111:TYR:CD1	2.77	0.52
1:1:55:ARG:HH11	1:1:366:ASP:HB3	1.73	0.52
1:1:398:GLN:HB2	2:2:66:ASN:HD21	1.74	0.52
2:2:26:VAL:O	2:2:28:ALA:N	2.25	0.52
2:2:59:VAL:HB	2:2:144:GLY:CA	2.39	0.52
2:2:69:ASN:HD21	2:2:131:ASP:CB	2.17	0.52
1:1:67:PHE:O	1:1:285:THR:HA	2.10	0.52
2:2:44:ASN:HA	2:2:158:SER:HA	1.91	0.52
2:2:59:VAL:CG2	2:2:60:VAL:O	2.57	0.52
1:1:120:PRO:HD2	1:1:123:LEU:HD12	1.92	0.52
1:1:163:ALA:HA	1:1:384:LEU:HA	1.92	0.52
1:1:63:ARG:NH2	1:1:241:GLU:OE2	2.39	0.52
1:1:65:ASP:HB2	1:1:288:VAL:HG12	1.90	0.52
1:1:127:TYR:N	1:1:284:MET:CE	2.72	0.52
2:2:94:GLU:CD	2:2:135:ARG:CG	2.78	0.52
1:1:294:THR:CG2	1:1:370:PHE:CD1	2.91	0.51
2:2:44:ASN:ND2	2:2:158:SER:OG	2.42	0.51
2:2:63:ASP:H	2:2:165:GLN:HE22	1.56	0.51
2:2:97:ASP:N	2:2:138:GLY:O	2.40	0.51
1:1:208:ARG:HG2	1:1:212:MET:CE	2.41	0.51
1:1:244:ALA:HA	1:1:266:GLN:CG	2.32	0.51
1:1:21:ALA:HA	1:1:402:TRP:O	2.11	0.51
1:1:63:ARG:HB2	1:1:243:TRP:CZ3	2.45	0.51
2:2:160:VAL:CG2	2:2:161:LEU:N	2.73	0.51
1:1:10:VAL:HG23	1:1:11:PRO:CD	2.27	0.51
1:1:359:ALA:HB1	1:1:361:PRO:CD	2.40	0.51
2:2:25:ALA:CA	2:2:54:SER:HB3	2.40	0.51
2:2:37:SER:CA	2:2:38:ARG:HD3	2.41	0.51
1:1:345:ILE:CD1	1:1:349:GLN:HB3	2.38	0.51
1:1:231:ASP:OD1	1:1:233:ARG:HG2	2.09	0.51
1:1:48:ALA:HA	1:1:266:GLN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:210:TYR:C	3:3:21:GLY:HA2	2.31	0.51
1:1:50:ARG:HA	1:1:264:VAL:O	2.11	0.51
1:1:131:TYR:CE2	1:1:136:LYS:HB3	2.46	0.51
2:2:37:SER:CB	2:2:38:ARG:NH1	2.74	0.51
1:1:404:MET:HG2	1:1:406:THR:HG22	1.93	0.51
2:2:108:TYR:CD1	2:2:108:TYR:C	2.84	0.51
2:2:59:VAL:HG23	2:2:60:VAL:O	2.11	0.51
1:1:161:ARG:C	1:1:384:LEU:HD22	2.31	0.50
1:1:353:THR:HG22	1:1:354:GLN:H	1.64	0.50
2:2:92:ARG:CD	2:2:130:ILE:HG13	2.33	0.50
1:1:67:PHE:CE2	3:3:25:TYR:CE2	2.99	0.50
1:1:71:ILE:HG13	1:1:76:ILE:CD1	2.40	0.50
1:1:174:PRO:O	1:1:177:THR:OG1	2.21	0.50
2:2:59:VAL:CG2	2:2:143:ALA:C	2.80	0.50
1:1:166:LYS:HD3	3:3:18:TRP:HB2	1.93	0.50
1:1:380:LYS:O	1:1:383:VAL:HG22	2.11	0.50
1:1:390:TYR:O	1:1:393:ILE:HG22	2.07	0.50
2:2:41:ILE:HG12	2:2:43:ILE:HG22	1.93	0.50
1:1:167:SER:N	1:1:170:THR:HG22	2.20	0.50
1:1:238:MET:HE3	1:1:239:ARG:N	2.14	0.50
2:2:59:VAL:HB	2:2:144:GLY:N	2.27	0.50
1:1:414:ARG:HG2	1:1:415:HIS:H	1.77	0.50
2:2:85:ASP:OD1	2:2:85:ASP:O	2.29	0.50
1:1:210:TYR:O	3:3:21:GLY:CA	2.58	0.50
2:2:110:VAL:C	2:2:111:TYR:CD1	2.85	0.50
2:2:69:ASN:O	2:2:132:SER:HB3	2.11	0.50
1:1:12:HIS:CE1	1:1:416:MET:CB	2.95	0.50
2:2:32:SER:CB	2:2:41:ILE:HD12	2.41	0.50
1:1:386:ASN:O	1:1:386:ASN:CG	2.46	0.49
1:1:50:ARG:NH1	1:1:265:GLN:HG2	2.27	0.49
1:1:55:ARG:NH1	1:1:366:ASP:HB3	2.26	0.49
1:1:76:ILE:CG2	1:1:121:LYS:HG2	2.43	0.49
1:1:240:SER:OG	1:1:270:HIS:CE1	2.62	0.49
2:2:79:LEU:HB2	2:2:82:VAL:HG21	1.94	0.49
1:1:23:LYS:O	1:1:402:TRP:NE1	2.45	0.49
1:1:127:TYR:OH	1:1:160:VAL:HG12	2.12	0.49
1:1:156:TYR:CD1	1:1:156:TYR:O	2.61	0.49
1:1:237:LEU:HD22	1:1:275:PHE:CD1	2.47	0.49
2:2:26:VAL:CG1	2:2:27:ALA:H	2.23	0.49
1:1:300:HIS:HB3	1:1:303:VAL:CG1	2.43	0.49
1:1:70:TYR:CE2	1:1:278:PRO:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:126:GLY:HA3	1:1:284:MET:HE3	1.95	0.49
1:1:208:ARG:HG2	1:1:212:MET:HE2	1.95	0.49
1:1:368:PHE:CB	1:1:370:PHE:HD2	2.20	0.49
1:1:30:ILE:HD11	1:1:45:MET:CE	2.43	0.49
1:1:329:SER:O	1:1:331:LYS:N	2.46	0.49
2:2:145:ILE:CD1	2:2:163:VAL:HG23	2.43	0.49
1:1:45:MET:SD	1:1:408:PHE:CZ	3.06	0.49
1:1:383:VAL:HG23	1:1:384:LEU:N	2.28	0.49
2:2:18:LEU:HD12	2:2:19:ALA:N	2.16	0.49
1:1:215:TYR:HA	1:1:218:ILE:HG23	1.94	0.49
1:1:397:MET:O	1:1:397:MET:CG	2.61	0.49
2:2:96:ALA:HA	2:2:139:ASN:HB3	1.95	0.49
1:1:423:ILE:CD1	1:1:423:ILE:H	2.21	0.48
2:2:30:VAL:HG23	2:2:103:ALA:N	2.27	0.48
2:2:42:LEU:O	2:2:42:LEU:CG	2.33	0.48
2:2:86:MET:SD	2:2:122:ILE:HG21	2.53	0.48
2:2:28:ALA:HB2	2:2:55:GLY:O	2.10	0.48
1:1:172:PRO:HG2	1:1:379:LEU:CD1	2.37	0.48
2:2:59:VAL:CA	2:2:144:GLY:HA3	2.41	0.48
2:2:76:ALA:HA	2:2:124:PHE:O	2.13	0.48
2:2:157:ILE:O	2:2:157:ILE:CG1	2.58	0.48
2:2:21:THR:CB	2:2:46:THR:HG23	2.37	0.48
2:2:85:ASP:OD2	2:2:150:ASN:N	2.45	0.48
1:1:120:PRO:HG2	1:1:123:LEU:CG	2.43	0.48
1:1:296:GLU:CD	1:1:363:ASN:HA	2.24	0.48
1:1:382:ARG:O	1:1:382:ARG:CG	2.62	0.48
2:2:57:CYS:SG	2:2:91:ILE:CD1	2.92	0.48
2:2:86:MET:CE	2:2:147:LEU:HD13	2.43	0.48
1:1:130:ILE:O	1:1:130:ILE:HG22	2.14	0.48
2:2:102:THR:O	2:2:103:ALA:HB2	2.14	0.48
1:1:168:ILE:HG23	1:1:169:TRP:N	2.28	0.48
2:2:118:ASN:HD21	2:2:120:LYS:N	2.12	0.48
1:1:40:SER:HA	1:1:275:PHE:O	2.14	0.48
1:1:237:LEU:HD21	1:1:275:PHE:CE1	2.49	0.48
1:1:299:MET:CE	1:1:335:HIS:HA	2.44	0.48
1:1:360:PHE:CD1	1:1:360:PHE:O	2.66	0.48
1:1:69:PHE:CE1	1:1:236:LEU:CG	2.97	0.47
1:1:410:ILE:HG22	1:1:411:ASN:N	2.28	0.47
2:2:61:ARG:HG3	2:2:142:TYR:CD1	2.50	0.47
2:2:89:PHE:HD1	2:2:90:ALA:O	1.97	0.47
2:2:118:ASN:HD21	2:2:121:ALA:N	2.06	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:94:GLU:OE2	2:2:135:ARG:CG	2.62	0.47
2:2:97:ASP:HA	2:2:140:ASP:OD2	2.14	0.47
2:2:30:VAL:HG23	2:2:103:ALA:CA	2.43	0.47
2:2:45:ALA:HB3	2:2:157:ILE:HG13	1.97	0.47
1:1:12:HIS:CE1	1:1:416:MET:CG	2.98	0.47
1:1:171:ALA:N	1:1:172:PRO:CD	2.77	0.47
1:1:175:PRO:O	1:1:344:LYS:NZ	2.40	0.47
1:1:195:LEU:O	1:1:198:ALA:HB3	2.14	0.47
1:1:208:ARG:HH12	1:1:218:ILE:HD12	1.78	0.47
1:1:219:MET:O	1:1:222:PHE:HB2	2.14	0.47
2:2:68:THR:O	2:2:71:HIS:CE1	2.67	0.47
1:1:71:ILE:HD13	1:1:126:GLY:HA3	1.95	0.47
1:1:126:GLY:CA	1:1:284:MET:HE3	2.44	0.47
1:1:130:ILE:HA	1:1:234:PRO:HG2	1.97	0.47
1:1:218:ILE:O	1:1:222:PHE:HD2	1.97	0.47
1:1:379:LEU:O	1:1:380:LYS:C	2.52	0.47
1:1:379:LEU:HA	1:1:382:ARG:HD3	1.96	0.47
1:1:419:THR:O	1:1:423:ILE:HD13	1.96	0.47
1:1:301:TYR:CE1	1:1:332:GLU:OE1	2.63	0.47
2:2:95:VAL:HG11	2:2:142:TYR:CE2	2.41	0.47
1:1:162:VAL:HG11	1:1:290:ARG:HD3	1.95	0.47
1:1:330:LEU:HB3	1:1:337:SER:OG	2.15	0.47
1:1:394:PHE:HE1	1:1:401:HIS:CD2	2.33	0.47
1:1:113:PRO:O	1:1:114:SER:O	2.32	0.47
1:1:135:PHE:CD1	3:3:25:TYR:HB2	2.50	0.47
1:1:137:PRO:HA	1:1:138:PRO:HD3	1.78	0.47
2:2:75:ILE:HG22	2:2:163:VAL:HG22	1.96	0.47
2:2:85:ASP:OD1	2:2:149:SER:HA	2.09	0.47
1:1:300:HIS:C	1:1:303:VAL:HG12	2.29	0.46
1:1:323:LEU:N	1:1:323:LEU:HD23	2.22	0.46
1:1:71:ILE:HD12	1:1:126:GLY:HA2	1.87	0.46
1:1:377:THR:CG2	1:1:378:ASP:N	2.78	0.46
1:1:419:THR:O	1:1:423:ILE:HD11	1.89	0.46
2:2:66:ASN:C	2:2:68:THR:H	2.18	0.46
2:2:73:LEU:CD2	2:2:143:ALA:HB1	2.45	0.46
1:1:416:MET:SD	1:1:417:PRO:HD3	2.54	0.46
1:1:133:ASN:CA	1:1:214:ARG:NH2	2.77	0.46
1:1:391:ASP:OD1	1:1:401:HIS:HE1	1.98	0.46
1:1:120:PRO:O	1:1:123:LEU:HB2	2.16	0.46
1:1:330:LEU:HD13	1:1:341:ALA:CB	2.46	0.46
2:2:104:VAL:HG23	2:2:104:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:163:ALA:HB1	3:3:24:GLN:NE2	2.31	0.46
1:1:242:PHE:CE2	1:1:268:PHE:HB3	2.47	0.46
1:1:106:ALA:HB3	1:1:111:THR:O	2.16	0.46
1:1:200:ALA:O	1:1:204:THR:HG23	2.16	0.46
1:1:133:ASN:HA	1:1:214:ARG:NH2	2.28	0.46
1:1:323:LEU:HB2	1:1:324:PRO:CD	2.43	0.46
3:3:16:ARG:O	3:3:17:LEU:HD23	2.16	0.46
1:1:155:ASP:O	1:1:159:GLY:CA	2.64	0.45
2:2:16:THR:O	2:2:16:THR:HG23	2.16	0.45
1:1:165:LEU:O	1:1:170:THR:HG21	2.15	0.45
1:1:242:PHE:CZ	1:1:268:PHE:CG	3.04	0.45
1:1:329:SER:OG	1:1:331:LYS:CB	2.64	0.45
2:2:96:ALA:HB3	2:2:99:VAL:HG21	1.98	0.45
1:1:150:ASN:N	1:1:150:ASN:HD22	2.14	0.45
1:1:354:GLN:HE21	1:1:354:GLN:HB2	1.61	0.45
2:2:72:ALA:O	2:2:166:VAL:HG23	2.17	0.45
1:1:120:PRO:CD	1:1:123:LEU:HD12	2.47	0.45
1:1:67:PHE:HE2	3:3:25:TYR:CZ	2.35	0.45
2:2:94:GLU:OE1	2:2:135:ARG:CG	2.64	0.45
1:1:149:SER:C	1:1:150:ASN:HD22	2.20	0.45
2:2:26:VAL:CG1	2:2:27:ALA:N	2.80	0.45
2:2:63:ASP:H	2:2:165:GLN:NE2	2.14	0.45
2:2:90:ALA:O	2:2:91:ILE:HG22	2.17	0.45
2:2:136:THR:CB	2:2:139:ASN:HD21	2.17	0.45
1:1:166:LYS:CB	3:3:18:TRP:CD1	2.99	0.45
2:2:49:ALA:HB1	2:2:153:THR:HA	1.97	0.45
1:1:24:ILE:HG22	1:1:25:GLY:N	2.31	0.45
1:1:216:ARG:CA	1:1:226:THR:HG21	2.43	0.45
1:1:390:TYR:C	1:1:393:ILE:CG2	2.83	0.45
1:1:392:GLU:H	1:1:392:GLU:HG2	1.56	0.45
2:2:41:ILE:CD1	2:2:43:ILE:CG2	2.95	0.45
2:2:56:LEU:O	2:2:56:LEU:CD1	2.56	0.45
1:1:97:VAL:CG2	1:1:121:LYS:HB2	2.47	0.44
1:1:100:SER:O	1:1:105:SER:HB2	2.17	0.44
1:1:323:LEU:CB	1:1:324:PRO:HD2	2.45	0.44
2:2:117:ASN:HB2	2:2:122:ILE:HG13	1.98	0.44
1:1:388:ASN:C	1:1:390:TYR:H	2.20	0.44
1:1:394:PHE:CE1	1:1:401:HIS:CD2	3.05	0.44
2:2:101:PRO:HG3	2:2:142:TYR:CD2	2.53	0.44
1:1:133:ASN:C	1:1:214:ARG:HH22	2.20	0.44
2:2:77:GLY:N	2:2:124:PHE:CE1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:45:MET:CE	1:1:408:PHE:CZ	2.98	0.44
1:1:288:VAL:O	1:1:288:VAL:HG13	2.18	0.44
2:2:90:ALA:C	2:2:91:ILE:CG2	2.83	0.44
1:1:18:VAL:HG13	1:1:18:VAL:O	2.18	0.44
1:1:286:LEU:N	1:1:286:LEU:HD12	2.33	0.44
2:2:73:LEU:CD2	2:2:143:ALA:CB	2.95	0.44
2:2:118:ASN:OD1	2:2:119:GLY:N	2.42	0.44
1:1:18:VAL:CG2	1:1:20:GLU:CG	2.86	0.44
1:1:50:ARG:NH2	1:1:265:GLN:OE1	2.49	0.44
2:2:18:LEU:CD2	2:2:43:ILE:CG2	2.95	0.44
2:2:95:VAL:O	2:2:139:ASN:HB3	2.13	0.44
1:1:116:THR:O	1:1:117:LEU:HB2	2.18	0.44
1:1:126:GLY:C	1:1:284:MET:CE	2.86	0.44
1:1:420:ARG:C	1:1:423:ILE:CD1	2.86	0.44
2:2:41:ILE:HG21	2:2:41:ILE:HD13	1.35	0.44
1:1:334:PHE:CD2	1:1:375:PRO:HG3	2.53	0.43
2:2:9:HIS:CE1	2:2:162:SER:CB	2.84	0.43
2:2:86:MET:HE1	2:2:147:LEU:HD13	2.00	0.43
2:2:23:THR:HA	2:2:48:THR:HG21	1.97	0.43
1:1:30:ILE:CD1	1:1:45:MET:HE1	2.47	0.43
1:1:64:VAL:O	1:1:241:GLU:HA	2.18	0.43
1:1:98:THR:HG22	1:1:147:ASN:CG	2.34	0.43
1:1:165:LEU:O	1:1:293:PRO:CG	2.66	0.43
1:1:368:PHE:O	1:1:370:PHE:N	2.49	0.43
1:1:70:TYR:HB2	1:1:237:LEU:CD1	2.33	0.43
2:2:41:ILE:HD13	2:2:43:ILE:HG21	2.01	0.43
1:1:76:ILE:HD12	1:1:76:ILE:N	2.33	0.43
1:1:298:GLU:HB2	1:1:334:PHE:CE1	2.53	0.43
1:1:97:VAL:CG2	1:1:121:LYS:CA	2.88	0.43
2:2:18:LEU:HD13	2:2:18:LEU:HA	1.78	0.43
2:2:89:PHE:CE1	2:2:110:VAL:CG1	3.00	0.43
1:1:97:VAL:HG11	1:1:148:PRO:HD3	2.01	0.43
1:1:416:MET:CB	1:1:417:PRO:HD2	2.47	0.43
2:2:83:PRO:C	2:2:85:ASP:H	2.21	0.43
1:1:268:PHE:HZ	1:1:404:MET:HE3	1.84	0.43
1:1:328:VAL:HG23	1:1:343:PHE:O	2.19	0.43
2:2:113:ILE:HB	2:2:114:GLU:H	1.67	0.43
1:1:41:PHE:CD1	1:1:41:PHE:C	2.93	0.42
1:1:97:VAL:HG13	1:1:147:ASN:ND2	2.33	0.42
1:1:107:ALA:CB	1:1:157:LYS:O	2.67	0.42
1:1:330:LEU:HD22	1:1:341:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:32:SER:HB3	2:2:41:ILE:HD12	2.01	0.42
2:2:69:ASN:O	2:2:132:SER:N	2.36	0.42
2:2:91:ILE:HD13	2:2:146:MET:HB2	2.01	0.42
1:1:54:LEU:HD11	1:1:262:GLY:HA3	2.01	0.42
1:1:97:VAL:HG12	1:1:98:THR:N	2.35	0.42
1:1:135:PHE:CZ	3:3:25:TYR:CD2	3.08	0.42
1:1:145:TYR:CG	1:1:151:MET:CG	2.96	0.42
2:2:22:LYS:HD2	2:2:29:PRO:HB2	2.00	0.42
2:2:25:ALA:C	2:2:54:SER:CB	2.61	0.42
1:1:45:MET:CG	1:1:408:PHE:CE1	3.03	0.42
1:1:330:LEU:HD13	1:1:341:ALA:O	2.17	0.42
1:1:36:VAL:HG13	1:1:414:ARG:HH11	1.84	0.42
1:1:162:VAL:HG11	1:1:288:VAL:CG2	2.49	0.42
1:1:12:HIS:HE1	1:1:416:MET:CB	2.33	0.42
2:2:145:ILE:CD1	2:2:163:VAL:CG2	2.98	0.42
1:1:130:ILE:O	1:1:130:ILE:CG2	2.67	0.42
1:1:242:PHE:HE2	1:1:266:GLN:CG	2.30	0.42
1:1:63:ARG:NH2	1:1:239:ARG:NH2	2.67	0.42
1:1:71:ILE:CG1	1:1:71:ILE:O	2.67	0.42
1:1:374:LEU:O	1:1:375:PRO:O	2.37	0.42
1:1:65:ASP:HB2	1:1:288:VAL:HG13	2.01	0.42
1:1:122:PHE:O	1:1:126:GLY:HA3	2.20	0.42
1:1:242:PHE:CZ	1:1:268:PHE:HB2	2.48	0.42
1:1:298:GLU:OE2	1:1:355:PRO:HB3	2.20	0.42
2:2:18:LEU:CD2	2:2:43:ILE:HG22	2.46	0.42
2:2:86:MET:HE2	2:2:147:LEU:CB	2.47	0.42
1:1:32:TRP:CE3	1:1:34:PRO:HD3	2.55	0.41
1:1:71:ILE:O	1:1:71:ILE:HG12	2.20	0.41
1:1:11:PRO:CG	1:1:413:TYR:CE1	3.01	0.41
1:1:12:HIS:NE2	1:1:416:MET:HB2	2.35	0.41
1:1:18:VAL:HG12	1:1:406:THR:C	2.37	0.41
1:1:67:PHE:HE2	3:3:25:TYR:CE2	2.38	0.41
2:2:41:ILE:CG1	2:2:43:ILE:CG2	2.98	0.41
2:2:88:ALA:O	2:2:113:ILE:HD11	2.20	0.41
1:1:30:ILE:HD11	1:1:45:MET:HE3	1.97	0.41
1:1:165:LEU:O	1:1:293:PRO:HG3	2.21	0.41
1:1:397:MET:O	1:1:397:MET:HG2	2.19	0.41
2:2:66:ASN:O	2:2:68:THR:N	2.53	0.41
2:2:101:PRO:CD	2:2:142:TYR:OH	2.65	0.41
2:2:93:PHE:CZ	2:2:142:TYR:HB2	2.55	0.41
2:2:94:GLU:HA	2:2:140:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:101:PRO:HD2	2:2:142:TYR:CZ	2.55	0.41
2:2:18:LEU:HD23	2:2:43:ILE:CG2	2.50	0.41
2:2:41:ILE:HD13	2:2:43:ILE:CG2	2.51	0.41
2:2:101:PRO:CG	2:2:142:TYR:CE2	3.03	0.41
1:1:42:GLU:HB3	1:1:274:ARG:HA	2.02	0.41
1:1:128:LEU:HD21	1:1:143:LEU:HB3	2.02	0.41
1:1:362:TYR:C	1:1:364:ALA:N	2.74	0.41
2:2:92:ARG:HH12	2:2:94:GLU:CG	2.33	0.41
2:2:123:SER:OG	2:2:124:PHE:N	2.53	0.41
1:1:183:MET:SD	1:1:195:LEU:HA	2.61	0.41
1:1:231:ASP:CG	1:1:233:ARG:NH1	2.68	0.41
1:1:328:VAL:O	1:1:342:LYS:HA	2.20	0.41
2:2:25:ALA:O	2:2:28:ALA:HA	2.21	0.41
2:2:82:VAL:HG13	2:2:86:MET:CE	2.49	0.41
1:1:120:PRO:HG2	1:1:123:LEU:HG	2.03	0.41
1:1:237:LEU:CD2	1:1:275:PHE:CE1	3.04	0.41
1:1:323:LEU:CB	1:1:324:PRO:CD	2.98	0.41
2:2:164:ASN:OD1	2:2:165:GLN:CA	2.63	0.41
1:1:12:HIS:N	1:1:412:VAL:O	2.42	0.41
1:1:22:GLY:HA2	1:1:158:TRP:CZ3	2.55	0.41
1:1:36:VAL:HB	1:1:280:HIS:CD2	2.56	0.41
1:1:50:ARG:HH12	1:1:265:GLN:CD	2.23	0.41
1:1:74:ARG:CZ	1:1:74:ARG:HB3	2.51	0.41
1:1:135:PHE:CD1	3:3:25:TYR:CB	3.04	0.41
1:1:174:PRO:O	1:1:177:THR:CB	2.69	0.41
1:1:377:THR:HG22	1:1:378:ASP:N	2.36	0.41
1:1:410:ILE:CG2	1:1:411:ASN:N	2.84	0.41
1:1:420:ARG:HE	1:1:420:ARG:HB3	1.53	0.41
2:2:26:VAL:HA	2:2:54:SER:CB	2.49	0.41
2:2:43:ILE:O	2:2:45:ALA:CA	2.61	0.41
2:2:50:VAL:HG12	2:2:152:TRP:CG	2.56	0.41
2:2:92:ARG:NE	2:2:131:ASP:OD1	2.54	0.41
1:1:10:VAL:HG22	1:1:11:PRO:CD	2.42	0.41
2:2:78:SER:O	2:2:79:LEU:HD23	2.21	0.41
1:1:137:PRO:O	1:1:140:SER:CB	2.66	0.40
1:1:238:MET:CE	1:1:239:ARG:N	2.75	0.40
1:1:330:LEU:HD12	1:1:343:PHE:CE1	2.56	0.40
1:1:410:ILE:HD13	1:1:410:ILE:HG21	1.83	0.40
2:2:59:VAL:HB	2:2:143:ALA:C	2.41	0.40
2:2:86:MET:HB2	2:2:117:ASN:ND2	2.31	0.40
1:1:32:TRP:HA	1:1:283:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:45:MET:HG3	1:1:408:PHE:CE1	2.57	0.40
1:1:109:LEU:HD22	1:1:123:LEU:O	2.20	0.40
2:2:31:LEU:HD23	2:2:31:LEU:HA	1.91	0.40
2:2:66:ASN:ND2	2:2:67:PRO:HD2	2.36	0.40
2:2:145:ILE:HD12	2:2:163:VAL:HG23	2.03	0.40
2:2:89:PHE:HE1	2:2:91:ILE:CG2	2.34	0.40
2:2:92:ARG:NH2	2:2:141:VAL:HG11	2.35	0.40
1:1:81:TRP:O	1:1:84:PHE:HB3	2.22	0.40
1:1:97:VAL:HG23	1:1:121:LYS:CB	2.52	0.40
1:1:380:LYS:HB3	1:1:381:ASP:H	1.75	0.40
2:2:86:MET:HE2	2:2:147:LEU:CD2	2.48	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	1	415/426 (97%)	362 (87%)	40 (10%)	13 (3%)	4 23
2	2	175/177 (99%)	137 (78%)	30 (17%)	8 (5%)	2 14
3	3	10/25 (40%)	7 (70%)	3 (30%)	0	100 100
All	All	600/628 (96%)	506 (84%)	73 (12%)	21 (4%)	3 20

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	114	SER
1	1	377	THR
1	1	417	PRO
2	2	44	ASN
2	2	166	VAL
1	1	101	SER

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Mol	Chain	Res	Type
1	1	363	ASN
1	1	380	LYS
1	1	418	THR
2	2	27	ALA
2	2	103	ALA
1	1	373	ALA
1	1	379	LEU
2	2	76	ALA
1	1	330	LEU
1	1	395	GLN
1	1	375	PRO
1	1	388	ASN
2	2	67	PRO
2	2	113	ILE
2	2	137	VAL

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	1	369/377 (98%)	308 (84%)	61 (16%)	2 11
2	2	148/148 (100%)	106 (72%)	42 (28%)	0 2
3	3	8/19 (42%)	6 (75%)	2 (25%)	0 3
All	All	525/544 (96%)	420 (80%)	105 (20%)	1 7

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	24	ILE
1	1	36	VAL
1	1	54	LEU
1	1	71	ILE
1	1	89	VAL
1	1	100	SER
1	1	112	ILE

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Mol	Chain	Res	Type
1	1	117	LEU
1	1	119	VAL
1	1	121	LYS
1	1	144	THR
1	1	156	TYR
1	1	160	VAL
1	1	164	ASN
1	1	167	SER
1	1	170	THR
1	1	182	ASN
1	1	184	THR
1	1	187	THR
1	1	190	ILE
1	1	192	ILE
1	1	211	PHE
1	1	212	MET
1	1	214	ARG
1	1	218	ILE
1	1	221	GLU
1	1	226	THR
1	1	236	LEU
1	1	269	ASN
1	1	286	LEU
1	1	305	LYS
1	1	323	LEU
1	1	328	VAL
1	1	337	SER
1	1	345	ILE
1	1	354	GLN
1	1	357	ARG
1	1	360	PHE
1	1	363	ASN
1	1	365	LEU
1	1	372	SER
1	1	377	THR
1	1	378	ASP
1	1	382	ARG
1	1	383	VAL
1	1	386	ASN
1	1	387	THR
1	1	393	ILE
1	1	396	SER

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Mol	Chain	Res	Type
1	1	397	MET
1	1	405	GLN
1	1	406	THR
1	1	407	LYS
1	1	411	ASN
1	1	414	ARG
1	1	415	HIS
1	1	420	ARG
1	1	421	ASP
1	1	423	ILE
1	1	425	THR
1	1	426	SER
2	2	6	ILE
2	2	14	ASN
2	2	18	LEU
2	2	21	THR
2	2	23	THR
2	2	35	ASN
2	2	37	SER
2	2	38	ARG
2	2	40	THR
2	2	42	LEU
2	2	43	ILE
2	2	50	VAL
2	2	52	THR
2	2	53	HIS
2	2	54	SER
2	2	56	LEU
2	2	57	CYS
2	2	59	VAL
2	2	61	ARG
2	2	62	ILE
2	2	65	THR
2	2	69	ASN
2	2	81	ASN
2	2	85	ASP
2	2	86	MET
2	2	107	LEU
2	2	111	TYR
2	2	114	GLU
2	2	118	ASN
2	2	122	ILE

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Mol	Chain	Res	Type
2	2	123	SER
2	2	129	THR
2	2	130	ILE
2	2	150	ASN
2	2	153	THR
2	2	155	SER
2	2	156	THR
2	2	165	GLN
2	2	168	ARG
2	2	172	VAL
2	2	173	LEU
2	2	176	LEU
3	3	16	ARG
3	3	25	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	12	HIS
1	1	16	HIS
1	1	79	GLN
1	1	83	ASN
1	1	125	GLN
1	1	129	ASN
1	1	132	ASN
1	1	147	ASN
1	1	150	ASN
1	1	164	ASN
1	1	182	ASN
1	1	196	GLN
1	1	266	GLN
1	1	269	ASN
1	1	300	HIS
1	1	335	HIS
1	1	349	GLN
1	1	354	GLN
1	1	386	ASN
1	1	388	ASN
1	1	389	ASN
1	1	395	GLN
1	1	401	HIS
1	1	411	ASN

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Mol	Chain	Res	Type
2	2	9	HIS
2	2	35	ASN
2	2	44	ASN
2	2	69	ASN
2	2	71	HIS
2	2	81	ASN
2	2	118	ASN
2	2	139	ASN
2	2	165	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.