Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:47 PM GMT

PDB ID	:	1CD3
Title	:	PROCAPSID OF BACTERIOPHAGE PHIX174
Authors	:	Rossmann, M.G.; Dokland, T.
Deposited on	:	1999-03-05
Resolution	:	3.50 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

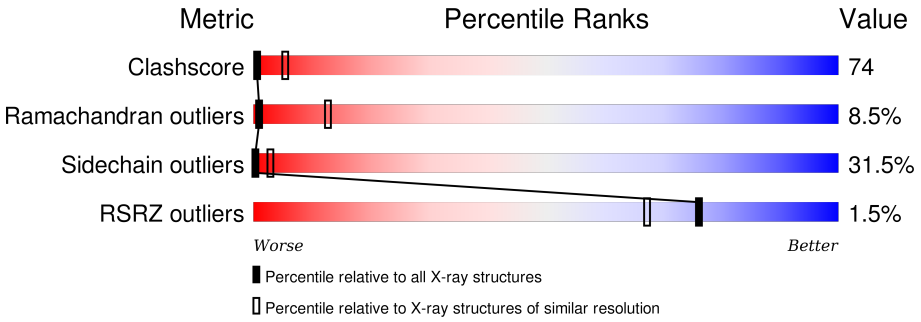
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	152	3% 22% 46% 23% • 6%
1	2	152	% 10% 51% 26% • 11%
1	3	152	3% 16% 50% 22% 5% 8%
1	4	152	2% 18% 49% 24% • •
2	F	426	20% 52% 26% •
3	G	175	22% 54% 21% •
4	B	120	3% 13% 29% 11% • 43%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9851 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 (SCAFFOLDING PROTEIN GPD).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	143	Total	C	N	O	S	0	0	0
			1125	716	194	211	4			
1	2	135	Total	C	N	O	S	0	0	0
			1057	675	177	201	4			
1	3	140	Total	C	N	O	S	0	0	0
			1099	699	187	209	4			
1	4	146	Total	C	N	O	S	0	0	0
			1145	728	197	215	5			

- Molecule 2 is a protein called PROTEIN (CAPSID PROTEIN GPF).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	426	Total	C	N	O	S	0	0	0
			3415	2173	590	638	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	216	ARG	HIS	CONFLICT	UNP P03641

- Molecule 3 is a protein called PROTEIN (SPIKE PROTEIN GPG).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	175	Total	C	N	O	S	0	0	0
			1340	856	221	255	8			

- Molecule 4 is a protein called PROTEIN (SCAFFOLDING PROTEIN GPB).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	68	Total	C	N	O	S	0	0	0
			574	358	105	108	3			

- Molecule 5 is water.

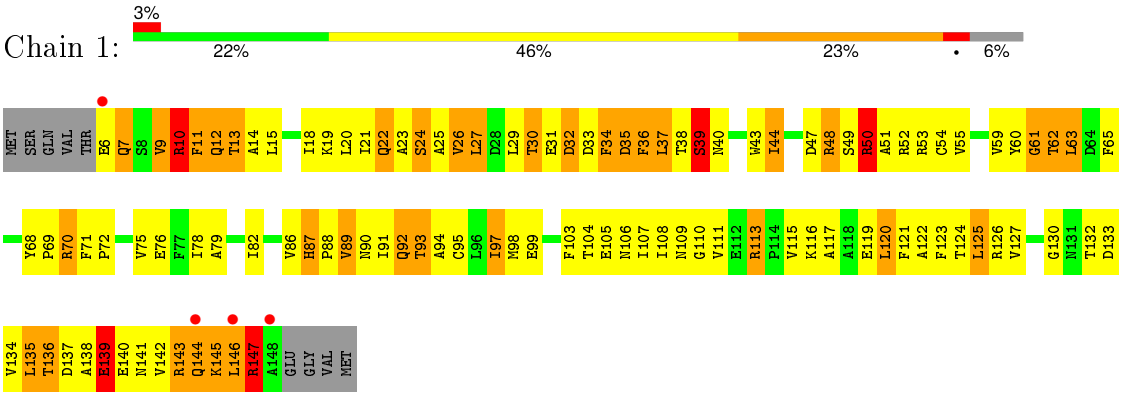
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1	13	Total O 13 13	0	0
5	2	9	Total O 9 9	0	0
5	3	14	Total O 14 14	0	0
5	4	9	Total O 9 9	0	0
5	B	18	Total O 18 18	0	0
5	F	25	Total O 25 25	0	0
5	G	8	Total O 8 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

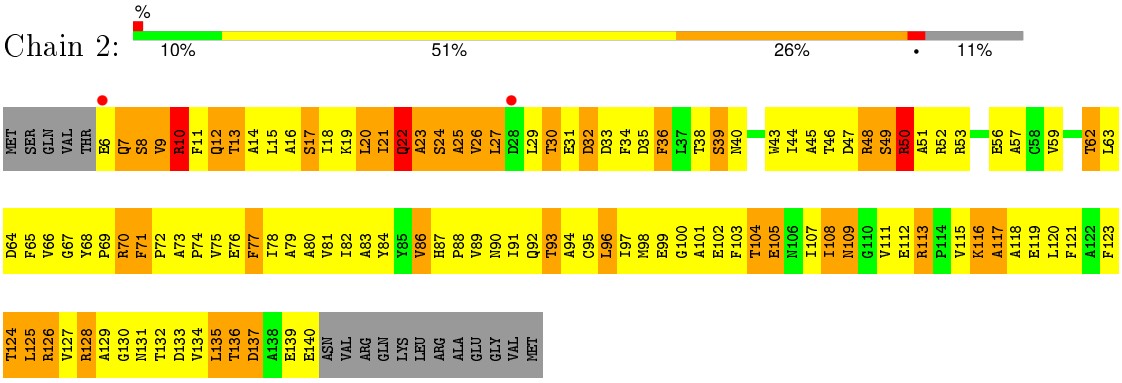
- Molecule 1: PROTEIN (SCAFFOLDING PROTEIN GPD)

Chain 1:



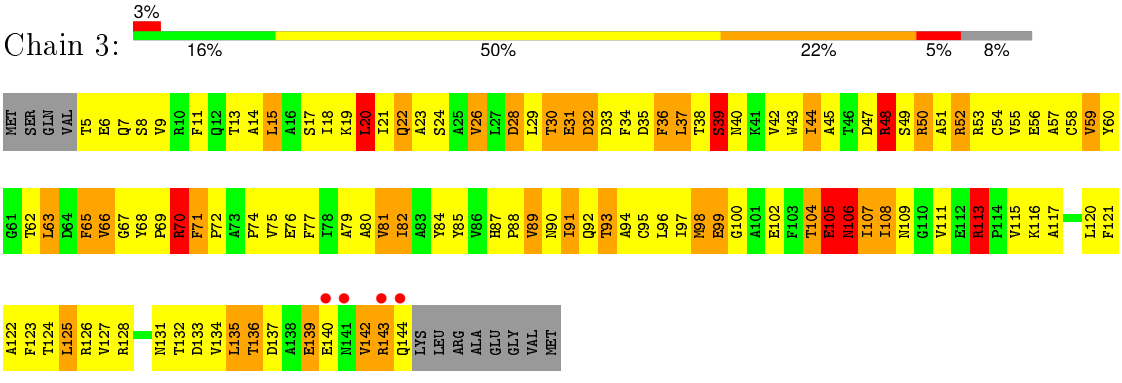
- Molecule 1: PROTEIN (SCAFFOLDING PROTEIN GPD)

Chain 2:



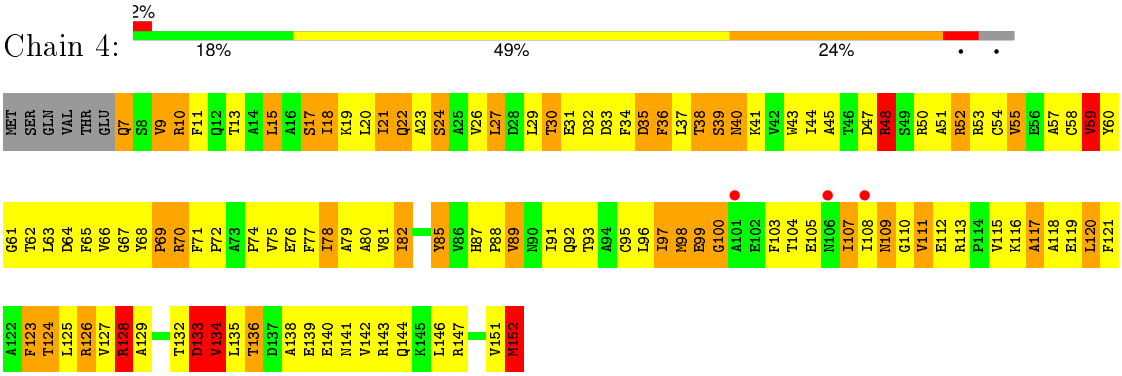
- Molecule 1: PROTEIN (SCAFFOLDING PROTEIN GPD)

Chain 3:



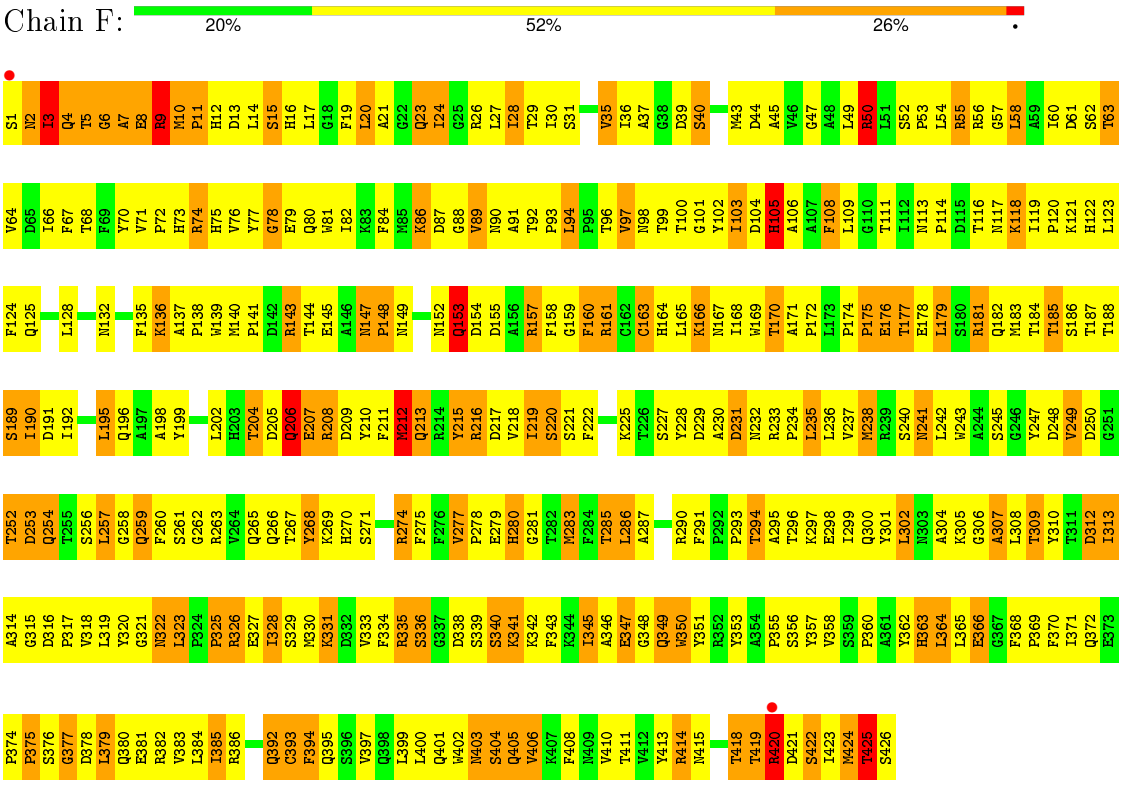
- Molecule 1: PROTEIN (SCAFFOLDING PROTEIN GPD)

Chain 4:



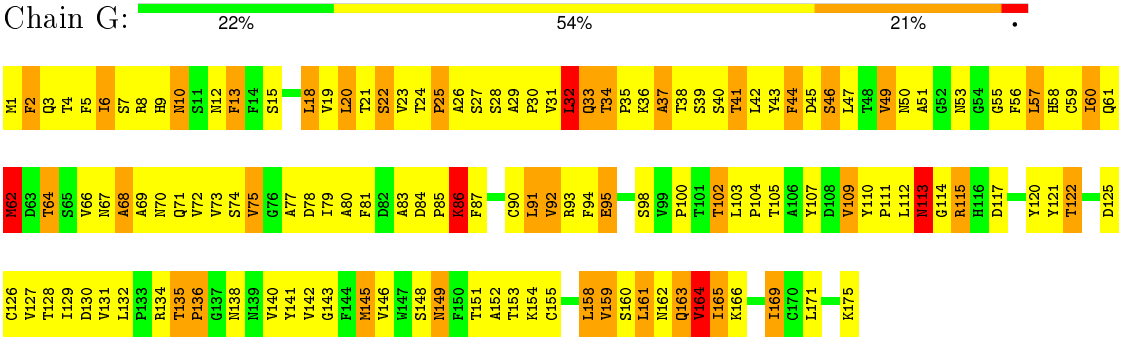
- Molecule 2: PROTEIN (CAPSID PROTEIN GPF)

Chain F:



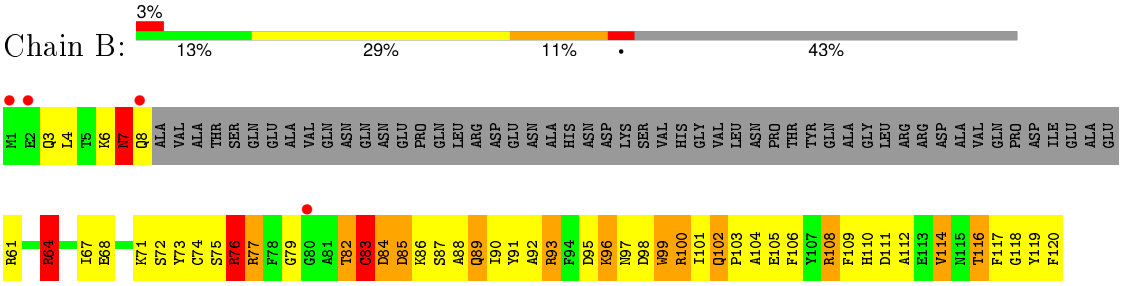
- Molecule 3: PROTEIN (SPIKE PROTEIN GPG)

Chain G:



• Molecule 4: PROTEIN (SCAFFOLDING PROTEIN GPB)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α, β, γ	774.00Å 774.00Å 774.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 44.84 – 3.50	Depositor EDS
% Data completeness (in resolution range)	67.2 (8.00-3.50) 66.3 (44.84-3.50)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.275 , (Not available) 0.477 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	78.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.3	EDS
Estimated twinning fraction	0.023 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	6 of 631903 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.21	EDS
Total number of atoms	9851	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.79	0/1145	1.05	4/1557 (0.3%)
1	2	0.78	0/1077	1.05	4/1467 (0.3%)
1	3	0.87	1/1119 (0.1%)	1.10	6/1524 (0.4%)
1	4	0.79	0/1165	1.03	6/1582 (0.4%)
2	F	0.85	0/3511	1.05	11/4777 (0.2%)
3	G	0.75	0/1372	1.01	2/1872 (0.1%)
4	B	0.84	0/586	1.24	6/779 (0.8%)
All	All	0.82	1/9975 (0.0%)	1.06	39/13558 (0.3%)

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	3	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	50	ARG	CZ-NH1	6.50	1.41	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	64	ARG	NE-CZ-NH2	8.72	124.66	120.30
4	B	61	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	1	50	ARG	NE-CZ-NH2	7.71	124.16	120.30
2	F	161	ARG	NE-CZ-NH2	7.63	124.12	120.30
1	3	70	ARG	NE-CZ-NH2	7.63	124.11	120.30
1	2	50	ARG	NE-CZ-NH2	7.49	124.05	120.30
4	B	77	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	4	128	ARG	NE-CZ-NH2	7.37	123.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	50	ARG	NE-CZ-NH2	7.37	123.98	120.30
2	F	420	ARG	NE-CZ-NH2	7.35	123.98	120.30
1	1	10	ARG	NE-CZ-NH2	7.31	123.96	120.30
2	F	290	ARG	NE-CZ-NH2	7.28	123.94	120.30
2	F	157	ARG	NE-CZ-NH2	7.16	123.88	120.30
2	F	143	ARG	NE-CZ-NH2	7.15	123.88	120.30
4	B	93	ARG	NE-CZ-NH2	7.14	123.87	120.30
4	B	76	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	3	113	ARG	NE-CZ-NH2	7.03	123.81	120.30
4	B	108	ARG	NE-CZ-NH1	6.99	123.80	120.30
2	F	9	ARG	NE-CZ-NH2	6.97	123.78	120.30
1	2	10	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	3	48	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	4	70	ARG	NE-CZ-NH2	6.93	123.76	120.30
1	2	113	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	1	113	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	3	128	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	1	147	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	4	10	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	4	152	MET	CG-SD-CE	6.13	110.01	100.20
3	G	62	MET	CG-SD-CE	6.13	110.00	100.20
3	G	145	MET	CG-SD-CE	6.12	109.99	100.20
2	F	424	MET	CG-SD-CE	6.11	109.97	100.20
1	4	98	MET	CG-SD-CE	6.09	109.95	100.20
2	F	212	MET	CG-SD-CE	5.94	109.70	100.20
1	2	70	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	3	50	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	3	48	ARG	CD-NE-CZ	5.62	131.46	123.60
1	4	85	TYR	CB-CG-CD2	-5.60	117.64	121.00
2	F	238	MET	CG-SD-CE	5.52	109.04	100.20
2	F	335	ARG	NE-CZ-NH2	5.21	122.90	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	48	ARG	Sidechain
1	3	52	ARG	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	1	1125	0	1121	182	0
1	2	1057	0	1043	212	0
1	3	1099	0	1086	187	0
1	4	1145	0	1142	201	0
2	F	3415	0	3305	422	0
3	G	1340	0	1323	194	0
4	B	574	0	538	93	0
5	1	13	0	0	0	0
5	2	9	0	0	3	0
5	3	14	0	0	0	0
5	4	9	0	0	0	0
5	B	18	0	0	1	0
5	F	25	0	0	0	0
5	G	8	0	0	0	0
All	All	9851	0	9558	1426	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 74.

All (1426) 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)
4:B:64:ARG:O	4:B:67:ILE:HG22	1.27	1.31
2:F:23:GLN:NE2	2:F:401:GLN:HG3	1.57	1.19
1:2:71:PHE:CD2	1:2:72:PRO:HD3	1.78	1.19
3:G:62:MET:HG3	3:G:131:VAL:HG12	1.29	1.11
4:B:64:ARG:O	4:B:67:ILE:CG2	2.00	1.09
1:4:128:ARG:HH11	1:4:128:ARG:HG3	1.11	1.09
1:3:48:ARG:HH11	1:3:48:ARG:HG3	1.05	1.08
2:F:23:GLN:HA	2:F:23:GLN:HE21	1.02	1.08
1:3:26:VAL:HG13	1:3:65:PHE:HD2	0.96	1.07
1:3:26:VAL:HG13	1:3:65:PHE:CD2	1.88	1.07
2:F:68:THR:HG23	2:F:285:THR:HB	1.35	1.05
2:F:375:PRO:HB2	2:F:382:ARG:HG2	1.36	1.05
1:1:29:LEU:HD22	1:1:33:ASP:HB3	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:379:LEU:HG	2:F:379:LEU:O	1.57	1.04
3:G:60:ILE:HD13	3:G:161:LEU:HB3	1.36	1.04
4:B:6:LYS:HB2	4:B:82:THR:HB	1.09	1.04
1:4:108:ILE:HD11	1:4:111:VAL:HG23	1.36	1.02
1:2:71:PHE:HB3	1:2:72:PRO:HD3	1.38	1.01
2:F:23:GLN:HE22	2:F:401:GLN:CG	1.74	1.00
1:2:71:PHE:HB3	1:2:72:PRO:CD	1.90	1.00
1:4:80:ALA:HB2	1:4:135:LEU:HD11	1.44	0.99
1:4:15:LEU:HD23	1:4:62:THR:HG21	1.44	0.99
1:1:146:LEU:HD23	1:1:147:ARG:CG	1.93	0.99
2:F:328:ILE:HD12	2:F:345:ILE:HD12	1.45	0.98
1:3:36:PHE:HA	1:3:39:SER:CB	1.94	0.98
1:3:36:PHE:HA	1:3:39:SER:HB3	0.98	0.98
1:3:30:THR:HG23	1:3:33:ASP:OD2	1.64	0.97
2:F:172:PRO:HG2	2:F:379:LEU:HD11	1.44	0.97
1:4:68:TYR:HB3	1:4:71:PHE:HE2	1.27	0.97
3:G:84:ASP:CG	3:G:86:LYS:HE3	1.83	0.97
4:B:64:ARG:C	4:B:67:ILE:HG22	1.85	0.97
1:3:93:THR:O	1:3:97:ILE:HD12	1.64	0.97
1:2:71:PHE:CD2	1:2:72:PRO:CD	2.46	0.96
2:F:23:GLN:HE22	2:F:401:GLN:HG3	0.82	0.95
1:3:98:MET:O	1:3:99:GLU:O	1.81	0.95
2:F:23:GLN:HA	2:F:23:GLN:NE2	1.78	0.95
2:F:328:ILE:CD1	2:F:345:ILE:HD12	1.95	0.95
1:2:71:PHE:CB	1:2:72:PRO:HD3	1.97	0.95
2:F:60:ILE:HD11	2:F:370:PHE:CE2	2.00	0.95
1:4:88:PRO:HA	1:4:91:ILE:HD12	1.47	0.94
3:G:20:LEU:HD11	3:G:22:SER:O	1.68	0.94
1:3:36:PHE:CA	1:3:39:SER:HB3	1.94	0.94
4:B:7:ASN:HA	4:B:110:HIS:O	1.68	0.94
1:2:71:PHE:HD2	1:2:72:PRO:HD3	1.27	0.93
1:1:32:ASP:O	1:1:35:ASP:HB2	1.68	0.93
4:B:3:GLN:OE1	4:B:90:ILE:HB	1.69	0.93
2:F:20:LEU:HD22	2:F:30:ILE:CG2	1.97	0.93
4:B:72:SER:HB3	4:B:88:ALA:HB1	1.50	0.92
3:G:78:ASP:OD2	3:G:122:THR:HG23	1.70	0.92
1:1:93:THR:O	1:1:97:ILE:HG12	1.69	0.91
1:4:36:PHE:HE1	1:4:50:ARG:HB3	1.34	0.91
2:F:172:PRO:HG2	2:F:379:LEU:CD1	2.00	0.91
4:B:3:GLN:HB3	4:B:91:TYR:OH	1.69	0.91
1:3:24:SER:HA	1:4:89:VAL:HG23	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:106:ASN:HB3	1:3:111:VAL:O	1.69	0.91
1:4:151:VAL:O	1:4:152:MET:SD	2.28	0.91
1:1:88:PRO:HA	1:1:91:ILE:HG12	1.53	0.91
2:F:418:THR:O	2:F:422:SER:HB3	1.71	0.91
1:3:48:ARG:HG3	1:3:48:ARG:NH1	1.76	0.90
4:B:73:TYR:O	4:B:76:ARG:HG3	1.70	0.90
2:F:23:GLN:CA	2:F:23:GLN:HE21	1.84	0.90
3:G:143:GLY:HA2	3:G:161:LEU:HD21	1.54	0.90
1:3:104:THR:HG21	1:4:126:ARG:HH21	1.35	0.90
2:F:44:ASP:OD1	2:F:271:SER:HB3	1.70	0.89
1:1:92:GLN:HA	1:1:121:PHE:CE1	2.07	0.89
1:2:71:PHE:CG	1:2:72:PRO:HD3	2.07	0.89
2:F:13:ASP:OD1	2:F:15:SER:HB3	1.73	0.89
1:4:59:VAL:HG12	1:4:60:TYR:N	1.88	0.89
1:4:36:PHE:CE1	1:4:50:ARG:HB3	2.08	0.88
3:G:62:MET:HG3	3:G:131:VAL:CG1	2.02	0.88
4:B:6:LYS:HB2	4:B:82:THR:CB	2.01	0.88
1:4:34:PHE:O	1:4:38:THR:HG23	1.72	0.88
1:3:104:THR:CG2	1:4:126:ARG:HH21	1.86	0.88
2:F:312:ASP:HA	2:F:350:TRP:CH2	2.09	0.88
3:G:15:SER:HA	3:G:41:THR:HG22	1.55	0.88
1:4:107:ILE:HG22	1:4:108:ILE:H	1.39	0.87
4:B:6:LYS:CB	4:B:82:THR:HB	2.01	0.87
3:G:86:LYS:HD2	3:G:86:LYS:H	1.40	0.87
1:3:34:PHE:CE2	1:3:38:THR:HG21	2.10	0.87
1:2:71:PHE:CB	1:2:72:PRO:CD	2.52	0.87
1:3:79:ALA:HA	1:3:124:THR:HG22	1.54	0.87
2:F:39:ASP:OD2	2:F:414:ARG:NH1	2.08	0.87
2:F:215:TYR:CE2	2:F:219:ILE:HD13	2.10	0.87
4:B:4:LEU:HB2	4:B:110:HIS:HE1	1.40	0.86
1:4:55:VAL:HG11	1:4:98:MET:SD	2.15	0.86
1:1:7:GLN:HA	1:1:10:ARG:HG3	1.57	0.86
1:3:71:PHE:CE1	1:4:96:LEU:HD12	2.11	0.86
1:3:63:LEU:HD13	1:3:69:PRO:O	1.76	0.86
1:1:139:GLU:O	1:1:142:VAL:HG23	1.76	0.85
2:F:172:PRO:CG	2:F:379:LEU:HD11	2.06	0.85
3:G:86:LYS:HD2	3:G:86:LYS:N	1.91	0.85
2:F:50:ARG:HD3	2:F:265:GLN:HG3	1.58	0.85
1:1:146:LEU:HD23	1:1:147:ARG:HG2	1.59	0.85
2:F:286:LEU:N	2:F:286:LEU:HD12	1.92	0.85
2:F:70:TYR:CE2	2:F:72:PRO:HG3	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:HIS:CD2	2:F:232:ASN:HA	2.12	0.84
1:2:36:PHE:HZ	5:2:160:HOH:O	1.58	0.84
1:3:37:LEU:HD21	1:3:85:TYR:HB3	1.57	0.84
2:F:315:GLY:HA2	2:F:320:TYR:CE1	2.12	0.84
1:3:71:PHE:HE1	1:4:96:LEU:HD12	1.40	0.84
1:1:32:ASP:O	1:1:35:ASP:N	2.09	0.84
1:1:35:ASP:O	1:1:37:LEU:N	2.10	0.84
1:2:120:LEU:O	1:2:124:THR:HG23	1.77	0.84
1:2:69:PRO:HD3	1:3:96:LEU:HD11	1.60	0.84
2:F:286:LEU:HD12	2:F:286:LEU:H	1.42	0.84
3:G:29:ALA:HA	3:G:55:GLY:O	1.78	0.84
1:4:76:GLU:HG3	1:4:123:PHE:CZ	2.12	0.83
2:F:419:THR:HA	2:F:422:SER:OG	1.76	0.83
2:F:315:GLY:HA2	2:F:320:TYR:HE1	1.41	0.83
1:1:33:ASP:OD2	1:1:53:ARG:NH1	2.12	0.83
1:1:142:VAL:O	1:1:145:LYS:HB3	1.78	0.83
2:F:20:LEU:HD22	2:F:30:ILE:HG22	1.59	0.83
1:1:25:ALA:HB3	1:1:62:THR:HG23	1.58	0.83
2:F:420:ARG:HA	2:F:424:MET:HG2	1.59	0.83
1:3:26:VAL:CG1	1:3:65:PHE:HD2	1.86	0.83
1:3:92:GLN:HB2	1:3:121:PHE:HE2	1.45	0.82
2:F:167:ASN:HB3	2:F:170:THR:HG23	1.62	0.82
1:2:128:ARG:HH11	1:2:128:ARG:HB2	1.45	0.82
1:4:18:ILE:HG22	1:4:85:TYR:OH	1.80	0.82
1:3:71:PHE:HE1	1:4:96:LEU:CG	1.93	0.82
1:2:87:HIS:CE1	1:2:88:PRO:HG2	2.15	0.81
1:1:141:ASN:O	1:1:144:GLN:HG3	1.81	0.81
1:1:143:ARG:HG2	1:1:144:GLN:N	1.94	0.81
3:G:62:MET:CE	3:G:73:VAL:HG21	2.10	0.81
1:3:9:VAL:O	1:3:13:THR:HG23	1.80	0.81
1:1:138:ALA:O	1:1:140:GLU:N	2.14	0.81
3:G:81:PHE:CD1	3:G:155:CYS:HB3	2.16	0.81
1:4:128:ARG:CG	1:4:128:ARG:HH11	1.93	0.81
1:1:9:VAL:O	1:1:13:THR:HG23	1.79	0.81
1:2:75:VAL:HG11	1:2:123:PHE:CE1	2.15	0.81
2:F:208:ARG:HA	2:F:212:MET:HB3	1.62	0.81
1:4:99:GLU:O	1:4:100:GLY:O	1.98	0.81
1:3:71:PHE:HE1	1:4:96:LEU:CD1	1.93	0.81
2:F:99:THR:O	2:F:117:ASN:HB3	1.80	0.81
2:F:29:THR:HG22	2:F:286:LEU:HG	1.64	0.80
1:4:120:LEU:O	1:4:124:THR:HG23	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:27:LEU:HD23	1:2:27:LEU:N	1.96	0.80
3:G:135:THR:HG22	3:G:136:PRO:HD2	1.62	0.79
2:F:20:LEU:HD13	2:F:30:ILE:HG23	1.64	0.79
1:4:108:ILE:HD11	1:4:111:VAL:CG2	2.13	0.79
4:B:86:LYS:HA	4:B:89:GLN:CD	2.03	0.79
1:4:74:PRO:HG2	1:4:77:PHE:CG	2.18	0.79
1:4:132:THR:O	1:4:133:ASP:C	2.20	0.79
1:1:92:GLN:HA	1:1:121:PHE:HE1	1.45	0.79
2:F:26:ARG:HG2	2:F:160:PHE:O	1.81	0.78
3:G:28:SER:O	3:G:102:THR:HG22	1.83	0.78
1:1:35:ASP:O	1:1:36:PHE:C	2.18	0.78
1:3:91:ILE:O	1:3:94:ALA:HB3	1.83	0.78
3:G:66:VAL:HG23	3:G:165:ILE:HD11	1.64	0.78
1:2:67:GLY:O	1:3:48:ARG:NH2	2.16	0.78
1:4:108:ILE:CD1	1:4:111:VAL:HG23	2.12	0.78
4:B:4:LEU:HB2	4:B:110:HIS:CE1	2.18	0.78
1:4:68:TYR:O	1:4:69:PRO:O	2.01	0.78
1:4:15:LEU:CD2	1:4:62:THR:HG21	2.13	0.78
2:F:419:THR:HB	2:F:423:ILE:HD12	1.66	0.78
1:4:44:ILE:HG22	1:4:45:ALA:N	1.96	0.78
1:2:59:VAL:HG12	1:2:63:LEU:HD12	1.65	0.78
2:F:137:ALA:HB3	2:F:140:MET:SD	2.23	0.78
2:F:322:ASN:ND2	2:F:322:ASN:H	1.82	0.77
1:1:106:ASN:HD21	1:1:113:ARG:HE	1.30	0.77
1:4:64:ASP:OD1	1:4:70:ARG:NH1	2.17	0.77
4:B:3:GLN:HB3	4:B:91:TYR:CZ	2.19	0.77
1:1:120:LEU:O	1:1:124:THR:HG23	1.84	0.77
3:G:40:SER:N	3:G:60:ILE:HD11	2.00	0.77
3:G:169:ILE:HD13	3:G:169:ILE:H	1.48	0.77
1:2:17:SER:O	1:2:21:ILE:HD12	1.83	0.77
1:3:96:LEU:O	1:3:96:LEU:HD23	1.83	0.77
2:F:76:VAL:HG22	2:F:125:GLN:HB3	1.67	0.77
1:4:87:HIS:CE1	1:4:89:VAL:H	2.03	0.77
1:2:17:SER:HB2	1:2:66:VAL:CG2	2.15	0.77
1:4:109:ASN:HA	1:4:112:GLU:HG3	1.66	0.77
1:4:128:ARG:NH1	1:4:128:ARG:HG3	1.91	0.77
2:F:211:PHE:O	2:F:212:MET:HB2	1.83	0.77
3:G:32:LEU:HD11	3:G:56:PHE:CD2	2.20	0.77
1:1:33:ASP:C	1:1:35:ASP:H	1.87	0.77
1:3:104:THR:CG2	1:4:126:ARG:NH2	2.47	0.77
1:1:36:PHE:CZ	1:1:50:ARG:HD3	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:79:GLU:HA	2:F:82:ILE:HD13	1.65	0.76
2:F:297:LYS:HG2	2:F:335:ARG:HG2	1.66	0.76
1:3:20:LEU:HD21	1:4:91:ILE:HD13	1.66	0.76
4:B:3:GLN:HG2	4:B:87:SER:HB2	1.66	0.76
3:G:51:ALA:HB2	3:G:152:ALA:H	1.48	0.76
3:G:114:GLY:O	3:G:115:ARG:HD2	1.86	0.76
4:B:82:THR:HG22	4:B:83:CYS:H	1.50	0.75
2:F:268:TYR:OH	2:F:406:VAL:HG11	1.85	0.75
2:F:328:ILE:HD12	2:F:345:ILE:CD1	2.16	0.75
1:1:31:GLU:HA	1:1:145:LYS:HD2	1.68	0.75
1:1:76:GLU:OE1	1:1:104:THR:HG23	1.86	0.75
1:1:134:VAL:CG1	1:1:136:THR:HG23	2.16	0.75
1:2:131:ASN:HA	1:2:134:VAL:CG2	2.16	0.75
4:B:3:GLN:HE22	4:B:104:ALA:HA	1.49	0.75
4:B:88:ALA:HA	4:B:91:TYR:HD1	1.51	0.75
1:4:68:TYR:HB3	1:4:71:PHE:CE2	2.18	0.75
1:4:78:ILE:HG22	1:4:120:LEU:HD11	1.69	0.75
2:F:228:TYR:CZ	2:F:230:ALA:HB3	2.22	0.75
3:G:83:ALA:O	3:G:85:PRO:HD3	1.87	0.74
3:G:32:LEU:HD11	3:G:56:PHE:HD2	1.52	0.74
1:1:60:TYR:CD1	1:1:70:ARG:HD3	2.22	0.74
1:2:128:ARG:CG	1:2:128:ARG:O	2.35	0.74
1:2:137:ASP:HB3	1:2:140:GLU:C	2.07	0.74
2:F:215:TYR:CZ	2:F:219:ILE:HD13	2.22	0.74
1:2:99:GLU:HG3	1:2:117:ALA:H	1.52	0.74
2:F:364:LEU:HD12	2:F:364:LEU:H	1.53	0.74
1:2:108:ILE:O	1:2:111:VAL:HG22	1.87	0.74
3:G:32:LEU:O	3:G:33:GLN:HB2	1.86	0.74
3:G:26:ALA:H	3:G:55:GLY:H	1.35	0.74
4:B:114:VAL:O	4:B:118:GLY:HA2	1.88	0.74
3:G:60:ILE:HD13	3:G:161:LEU:CB	2.15	0.73
1:2:105:GLU:O	1:2:105:GLU:HG2	1.88	0.73
2:F:297:LYS:HB3	2:F:335:ARG:HB3	1.71	0.73
1:2:11:PHE:O	1:2:12:GLN:C	2.27	0.73
1:2:121:PHE:CE2	1:2:125:LEU:HD13	2.23	0.73
1:1:32:ASP:O	1:1:35:ASP:CB	2.36	0.73
1:4:27:LEU:N	1:4:27:LEU:HD23	2.04	0.73
1:1:105:GLU:HG2	1:2:126:ARG:HH12	1.53	0.73
2:F:74:ARG:NH1	2:F:279:GLU:OE2	2.22	0.72
1:2:7:GLN:O	1:2:9:VAL:N	2.22	0.72
2:F:208:ARG:HA	2:F:212:MET:CB	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:44:ILE:CG2	1:2:45:ALA:N	2.52	0.72
1:3:51:ALA:O	1:3:55:VAL:HG23	1.89	0.72
1:4:87:HIS:CE1	1:4:89:VAL:HB	2.24	0.72
3:G:62:MET:CG	3:G:131:VAL:HG12	2.13	0.72
1:1:20:LEU:HD11	1:2:91:ILE:HD12	1.71	0.72
3:G:62:MET:CE	3:G:73:VAL:CG2	2.68	0.72
1:4:36:PHE:CD2	1:4:36:PHE:C	2.63	0.72
1:4:50:ARG:HD2	1:4:53:ARG:HH21	1.54	0.72
2:F:88:GLY:O	2:F:90:ASN:N	2.22	0.71
1:2:18:ILE:HG13	1:2:62:THR:HG21	1.71	0.71
2:F:250:ASP:HA	2:F:260:PHE:HD2	1.54	0.71
1:2:17:SER:HB2	1:2:66:VAL:HG21	1.72	0.71
1:3:36:PHE:HZ	1:3:50:ARG:HB3	1.56	0.71
1:4:36:PHE:HD2	1:4:36:PHE:O	1.72	0.71
1:1:14:ALA:HB2	1:1:123:PHE:CE2	2.26	0.71
1:1:30:THR:HG23	1:1:33:ASP:HB2	1.73	0.71
3:G:164:VAL:HG12	3:G:164:VAL:O	1.90	0.71
1:4:59:VAL:CG1	1:4:60:TYR:N	2.53	0.71
2:F:319:LEU:O	2:F:323:LEU:HB2	1.91	0.71
1:4:62:THR:O	1:4:66:VAL:HG23	1.91	0.71
1:3:79:ALA:CA	1:3:124:THR:HG22	2.21	0.71
2:F:97:VAL:CG1	2:F:148:PRO:HD2	2.21	0.70
1:2:7:GLN:O	1:2:9:VAL:HG23	1.91	0.70
2:F:419:THR:O	2:F:423:ILE:HB	1.92	0.70
1:1:12:GLN:NE2	1:1:12:GLN:HA	2.07	0.70
3:G:72:VAL:HG22	3:G:128:THR:HG22	1.73	0.70
2:F:240:SER:OG	2:F:270:HIS:HD2	1.75	0.70
2:F:338:ASP:OD1	2:F:340:SER:HB3	1.91	0.70
3:G:57:LEU:HB3	3:G:145:MET:HB2	1.74	0.70
4:B:102:GLN:O	4:B:105:GLU:HB2	1.92	0.69
1:2:77:PHE:O	1:2:81:VAL:HG23	1.91	0.69
2:F:124:PHE:CZ	2:F:128:LEU:HD11	2.27	0.69
1:2:71:PHE:O	1:2:73:ALA:N	2.24	0.69
2:F:167:ASN:HB3	2:F:170:THR:CG2	2.22	0.69
2:F:322:ASN:HD22	2:F:322:ASN:H	1.40	0.69
1:2:111:VAL:HG23	1:2:111:VAL:O	1.93	0.69
1:3:104:THR:HG21	1:4:126:ARG:NH2	2.07	0.69
1:3:58:CYS:HB3	1:3:85:TYR:CE2	2.28	0.69
2:F:169:TRP:CZ3	2:F:375:PRO:HG2	2.28	0.69
1:2:18:ILE:HG13	1:2:62:THR:CG2	2.22	0.69
3:G:62:MET:HE1	3:G:73:VAL:CG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:137:ASP:O	1:3:140:GLU:HB2	1.92	0.69
1:2:73:ALA:HB3	1:2:103:PHE:CD2	2.27	0.69
1:4:87:HIS:CE1	1:4:88:PRO:HG2	2.27	0.69
1:2:99:GLU:HG3	1:2:117:ALA:N	2.07	0.69
3:G:91:LEU:HD22	3:G:143:GLY:O	1.92	0.69
2:F:328:ILE:HG22	2:F:329:SER:N	2.08	0.69
2:F:20:LEU:CD2	2:F:30:ILE:CG2	2.71	0.69
2:F:101:GLY:O	2:F:102:TYR:HD1	1.74	0.69
1:2:108:ILE:O	1:2:111:VAL:HG13	1.93	0.69
4:B:98:ASP:OD1	4:B:100:ARG:HD2	1.92	0.68
1:3:75:VAL:HG12	1:3:76:GLU:N	2.07	0.68
2:F:106:ALA:HB1	2:F:119:ILE:HD11	1.74	0.68
1:4:21:ILE:O	1:4:21:ILE:CG2	2.40	0.68
1:3:49:SER:O	1:3:52:ARG:HG3	1.93	0.68
4:B:3:GLN:NE2	4:B:104:ALA:HA	2.07	0.68
1:1:87:HIS:CE1	1:1:88:PRO:HG2	2.29	0.68
3:G:87:PHE:CB	3:G:148:SER:HB2	2.24	0.68
1:4:108:ILE:O	1:4:108:ILE:HG13	1.93	0.68
3:G:84:ASP:OD2	3:G:86:LYS:HE3	1.93	0.68
1:4:80:ALA:CB	1:4:135:LEU:HD11	2.21	0.68
1:1:92:GLN:HG3	1:1:121:PHE:CZ	2.27	0.68
3:G:169:ILE:CD1	3:G:169:ILE:H	2.05	0.68
2:F:24:ILE:HD11	2:F:291:PHE:HD1	1.58	0.68
1:1:94:ALA:HA	1:1:97:ILE:HD11	1.75	0.68
1:2:73:ALA:HB3	1:2:103:PHE:HD2	1.58	0.68
1:1:30:THR:HG23	1:1:33:ASP:CG	2.15	0.68
1:4:59:VAL:HG12	1:4:60:TYR:H	1.56	0.68
3:G:49:VAL:O	3:G:152:ALA:HA	1.94	0.68
1:4:123:PHE:HE2	1:4:134:VAL:HG12	1.59	0.67
4:B:3:GLN:HG2	4:B:87:SER:CB	2.24	0.67
1:3:30:THR:HG23	1:3:33:ASP:CG	2.14	0.67
4:B:3:GLN:HG2	4:B:87:SER:HA	1.76	0.67
1:1:75:VAL:HG11	1:1:103:PHE:HE2	1.59	0.67
1:3:26:VAL:HA	1:3:143:ARG:HG3	1.74	0.67
1:1:30:THR:HG23	1:1:33:ASP:CB	2.24	0.67
2:F:30:ILE:HD11	2:F:287:ALA:HB2	1.76	0.67
2:F:77:TYR:O	2:F:78:GLY:O	2.12	0.67
2:F:79:GLU:CA	2:F:82:ILE:HD13	2.25	0.67
1:2:73:ALA:CB	1:2:103:PHE:HD2	2.08	0.67
3:G:44:PHE:O	3:G:44:PHE:HD1	1.78	0.67
1:4:63:LEU:HD21	1:4:77:PHE:CE2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:81:PHE:CE1	3:G:155:CYS:HB3	2.30	0.67
4:B:76:ARG:NH2	4:B:77:ARG:HA	2.10	0.67
1:2:32:ASP:O	1:2:35:ASP:HB2	1.94	0.67
1:2:27:LEU:HD23	1:2:27:LEU:H	1.58	0.67
2:F:158:PHE:CZ	2:F:400:LEU:HD21	2.30	0.67
1:4:44:ILE:CG2	1:4:45:ALA:N	2.58	0.67
1:3:104:THR:HG22	1:4:126:ARG:NH2	2.10	0.67
1:2:71:PHE:CG	1:2:72:PRO:CD	2.75	0.66
3:G:57:LEU:HD23	3:G:57:LEU:C	2.13	0.66
2:F:70:TYR:HB3	2:F:235:LEU:CB	2.25	0.66
4:B:86:LYS:HA	4:B:89:GLN:OE1	1.95	0.66
2:F:174:PRO:HG2	2:F:177:THR:HG23	1.77	0.66
1:1:35:ASP:C	1:1:37:LEU:N	2.46	0.66
1:2:32:ASP:O	1:2:35:ASP:CB	2.43	0.66
2:F:153:GLN:CB	2:F:157:ARG:HH11	2.07	0.66
2:F:139:TRP:HZ2	2:F:383:VAL:HG21	1.60	0.66
2:F:153:GLN:HB2	2:F:157:ARG:NH1	2.11	0.66
1:4:36:PHE:HE1	1:4:50:ARG:CB	2.07	0.66
2:F:249:VAL:O	2:F:249:VAL:HG12	1.95	0.66
1:4:18:ILE:HG21	1:4:27:LEU:HD21	1.77	0.66
1:1:146:LEU:HD23	1:1:147:ARG:HG3	1.76	0.66
2:F:97:VAL:HG13	2:F:148:PRO:HD2	1.76	0.66
3:G:90:CYS:SG	3:G:109:VAL:CG2	2.84	0.66
1:2:116:LYS:O	1:2:119:GLU:HG2	1.96	0.66
2:F:63:THR:HG23	2:F:243:TRP:CE2	2.31	0.66
1:1:33:ASP:C	1:1:35:ASP:N	2.47	0.66
4:B:91:TYR:CD2	5:B:132:HOH:O	2.50	0.65
1:3:33:ASP:OD2	1:3:53:ARG:NH1	2.29	0.65
1:1:63:LEU:HD23	1:1:68:TYR:HB2	1.78	0.65
1:1:142:VAL:HG12	1:1:145:LYS:NZ	2.12	0.65
1:3:76:GLU:OE1	1:3:104:THR:HB	1.97	0.65
1:1:75:VAL:HG11	1:1:103:PHE:CE2	2.32	0.65
1:1:33:ASP:OD2	1:1:53:ARG:CZ	2.44	0.65
1:4:107:ILE:HG22	1:4:108:ILE:N	2.10	0.65
1:1:11:PHE:O	1:1:14:ALA:HB3	1.97	0.65
3:G:53:ASN:HB2	3:G:149:ASN:ND2	2.12	0.65
1:4:99:GLU:HG3	1:4:117:ALA:HB2	1.78	0.65
4:B:88:ALA:HA	4:B:91:TYR:CD1	2.32	0.65
1:4:151:VAL:O	1:4:152:MET:HB2	1.96	0.65
3:G:24:THR:O	3:G:24:THR:HG23	1.97	0.64
3:G:57:LEU:CB	3:G:145:MET:HB2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:87:HIS:CG	1:4:88:PRO:HD2	2.33	0.64
1:2:93:THR:O	1:2:97:ILE:HG13	1.96	0.64
2:F:421:ASP:HA	2:F:424:MET:O	1.97	0.64
2:F:392:GLN:O	2:F:392:GLN:HG2	1.95	0.64
3:G:73:VAL:HG11	3:G:142:VAL:HG11	1.80	0.64
1:1:135:LEU:O	1:1:138:ALA:N	2.24	0.64
1:1:43:TRP:CG	1:1:90:ASN:ND2	2.66	0.64
1:4:21:ILE:O	1:4:21:ILE:HG23	1.96	0.64
1:1:142:VAL:HG12	1:1:145:LYS:HZ3	1.62	0.64
2:F:320:TYR:HD2	2:F:347:GLU:HG3	1.63	0.64
1:1:44:ILE:HD12	1:1:47:ASP:OD2	1.97	0.64
1:4:76:GLU:HG3	1:4:123:PHE:CE2	2.33	0.64
1:3:44:ILE:HG23	1:3:45:ALA:N	2.12	0.64
2:F:169:TRP:CH2	2:F:375:PRO:CG	2.81	0.64
2:F:23:GLN:HG3	2:F:158:PHE:CD1	2.32	0.64
4:B:89:GLN:O	4:B:92:ALA:HB3	1.98	0.64
1:4:55:VAL:CG1	1:4:98:MET:SD	2.84	0.64
1:3:71:PHE:CZ	1:4:96:LEU:HB2	2.33	0.63
2:F:322:ASN:N	2:F:322:ASN:ND2	2.46	0.63
3:G:93:ARG:HG3	3:G:129:ILE:HG21	1.79	0.63
1:1:26:VAL:HG11	1:1:65:PHE:CG	2.33	0.63
2:F:169:TRP:CH2	2:F:375:PRO:HG3	2.33	0.63
1:1:9:VAL:O	1:1:12:GLN:HB2	1.99	0.63
2:F:328:ILE:HD11	2:F:345:ILE:HD12	1.78	0.63
1:4:111:VAL:O	1:4:113:ARG:HD2	1.97	0.63
4:B:101:ILE:HA	4:B:105:GLU:OE1	1.98	0.63
2:F:405:GLN:N	2:F:405:GLN:CD	2.49	0.63
2:F:24:ILE:HD11	2:F:291:PHE:CD1	2.34	0.63
3:G:62:MET:HB2	3:G:140:VAL:HG13	1.78	0.63
1:2:11:PHE:CG	1:2:127:VAL:HG22	2.34	0.63
1:2:87:HIS:CE1	1:2:89:VAL:H	2.16	0.63
2:F:252:THR:OG1	2:F:252:THR:O	2.14	0.63
1:3:37:LEU:CD2	1:3:85:TYR:HB3	2.28	0.63
1:4:79:ALA:CB	1:4:124:THR:HG22	2.28	0.63
2:F:421:ASP:HA	2:F:424:MET:C	2.18	0.63
1:4:121:PHE:CZ	1:4:125:LEU:HD22	2.32	0.63
1:2:34:PHE:CE2	1:2:38:THR:HG21	2.34	0.63
4:B:76:ARG:HE	4:B:76:ARG:C	2.01	0.63
2:F:418:THR:O	2:F:422:SER:CB	2.45	0.63
2:F:76:VAL:HG11	2:F:122:HIS:HA	1.81	0.63
2:F:60:ILE:HD11	2:F:370:PHE:HE2	1.61	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:ASP:OD1	2:F:414:ARG:HB2	1.99	0.62
1:2:44:ILE:HG22	1:2:45:ALA:N	2.13	0.62
1:2:68:TYR:CD2	1:3:96:LEU:HD13	2.34	0.62
4:B:3:GLN:CD	4:B:90:ILE:HB	2.19	0.62
2:F:212:MET:O	2:F:213:GLN:HG3	1.99	0.62
2:F:84:PHE:CD1	2:F:94:LEU:CD2	2.82	0.62
4:B:64:ARG:CA	4:B:67:ILE:HG22	2.28	0.62
1:4:18:ILE:HD11	1:4:26:VAL:HG11	1.80	0.62
2:F:16:HIS:O	2:F:408:PHE:HB2	2.00	0.62
1:1:14:ALA:HB2	1:1:123:PHE:HE2	1.65	0.62
3:G:62:MET:HE3	3:G:73:VAL:HG21	1.82	0.62
1:3:71:PHE:CE1	1:4:96:LEU:CG	2.81	0.62
1:2:59:VAL:HG12	1:2:63:LEU:CD1	2.29	0.62
1:3:113:ARG:O	1:3:113:ARG:HG2	1.98	0.62
3:G:39:SER:HA	3:G:60:ILE:HD11	1.81	0.62
3:G:57:LEU:O	3:G:57:LEU:HD23	1.98	0.62
1:3:21:ILE:O	1:3:22:GLN:C	2.38	0.62
1:2:11:PHE:CZ	1:2:127:VAL:HG23	2.35	0.62
1:2:68:TYR:OH	1:3:93:THR:CA	2.48	0.62
2:F:11:PRO:HB3	2:F:413:TYR:CE2	2.35	0.62
4:B:3:GLN:CG	4:B:90:ILE:HD12	2.29	0.62
2:F:297:LYS:CB	2:F:335:ARG:HB3	2.30	0.62
2:F:172:PRO:CG	2:F:379:LEU:CD1	2.72	0.62
2:F:153:GLN:HB2	2:F:157:ARG:HH11	1.62	0.62
3:G:9:HIS:C	3:G:9:HIS:CD2	2.73	0.62
1:3:72:PRO:HD2	1:4:118:ALA:HB2	1.81	0.61
3:G:62:MET:HE2	3:G:142:VAL:CG2	2.30	0.61
2:F:368:PHE:HB3	2:F:370:PHE:CD1	2.35	0.61
3:G:62:MET:HE1	3:G:73:VAL:HG21	1.80	0.61
4:B:3:GLN:HG2	4:B:87:SER:CA	2.31	0.61
1:1:92:GLN:CA	1:1:121:PHE:HE1	2.13	0.61
1:2:66:VAL:O	1:2:66:VAL:HG12	2.01	0.61
1:4:40:ASN:HD22	1:4:40:ASN:H	1.48	0.61
3:G:114:GLY:C	3:G:115:ARG:HD2	2.20	0.61
1:4:63:LEU:HD21	1:4:77:PHE:HE2	1.64	0.61
1:4:19:LYS:HB2	1:4:85:TYR:CE2	2.35	0.61
1:2:128:ARG:HG2	1:2:128:ARG:O	2.00	0.61
2:F:257:LEU:O	2:F:259:GLN:N	2.32	0.61
1:3:92:GLN:CB	1:3:121:PHE:HE2	2.12	0.61
1:1:25:ALA:HB3	1:1:62:THR:CG2	2.29	0.61
3:G:85:PRO:O	3:G:87:PHE:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:168:ILE:HD11	2:F:345:ILE:HD11	1.83	0.61
2:F:163:CYS:HB3	2:F:383:VAL:HG12	1.83	0.61
1:2:92:GLN:HG3	1:2:121:PHE:CE1	2.35	0.61
1:2:43:TRP:CG	1:2:90:ASN:OD1	2.54	0.61
1:2:88:PRO:HA	1:2:91:ILE:HD12	1.83	0.61
3:G:83:ALA:O	3:G:85:PRO:CD	2.47	0.61
1:3:98:MET:HA	1:3:98:MET:CE	2.31	0.61
2:F:1:SER:OG	2:F:3:ILE:HG12	2.00	0.61
1:1:134:VAL:HG11	1:1:136:THR:HG23	1.82	0.61
1:2:9:VAL:HG13	1:3:88:PRO:HB3	1.83	0.61
1:1:11:PHE:HE2	1:1:15:LEU:HD11	1.66	0.61
2:F:405:GLN:N	2:F:405:GLN:NE2	2.48	0.61
1:2:36:PHE:CE1	1:2:50:ARG:HB3	2.35	0.61
3:G:29:ALA:HB3	3:G:103:LEU:HB3	1.81	0.60
3:G:71:GLN:HG3	3:G:131:VAL:CG2	2.30	0.60
1:3:98:MET:HA	1:3:98:MET:HE2	1.83	0.60
2:F:15:SER:HB2	2:F:410:VAL:H	1.65	0.60
2:F:152:ASN:O	2:F:153:GLN:C	2.40	0.60
3:G:77:ALA:CB	3:G:159:VAL:HA	2.31	0.60
1:2:71:PHE:HD2	1:2:72:PRO:CD	1.97	0.60
1:3:26:VAL:O	1:3:26:VAL:HG12	2.02	0.60
3:G:77:ALA:HB2	3:G:159:VAL:HA	1.82	0.60
3:G:75:VAL:HB	3:G:161:LEU:CD1	2.32	0.60
2:F:66:ILE:CD1	2:F:268:TYR:CE1	2.83	0.60
3:G:87:PHE:HB3	3:G:148:SER:HB2	1.83	0.60
3:G:85:PRO:O	3:G:87:PHE:N	2.34	0.60
2:F:108:PHE:CE1	2:F:109:LEU:HD21	2.36	0.60
1:1:138:ALA:O	1:1:141:ASN:N	2.23	0.60
1:4:67:GLY:O	1:4:68:TYR:C	2.40	0.60
2:F:49:LEU:HA	2:F:404:SER:HB2	1.84	0.60
2:F:82:ILE:HD12	2:F:82:ILE:N	2.17	0.60
2:F:75:HIS:HD2	2:F:232:ASN:HA	1.64	0.60
1:4:109:ASN:HA	1:4:112:GLU:CG	2.31	0.60
2:F:66:ILE:CD1	2:F:268:TYR:HE1	2.14	0.60
1:4:48:ARG:O	1:4:51:ALA:HB3	2.01	0.60
2:F:55:ARG:HH11	2:F:366:GLU:HG2	1.67	0.60
1:3:120:LEU:O	1:3:124:THR:HG23	2.02	0.60
2:F:70:TYR:HB3	2:F:235:LEU:HB3	1.83	0.60
2:F:101:GLY:HA2	2:F:117:ASN:OD1	2.01	0.60
3:G:30:PRO:HD2	3:G:56:PHE:HA	1.84	0.60
2:F:368:PHE:HB3	2:F:370:PHE:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:87:HIS:CE1	1:1:89:VAL:H	2.18	0.60
1:4:21:ILE:O	1:4:22:GLN:C	2.40	0.60
2:F:43:MET:CE	2:F:45:ALA:HB2	2.31	0.60
2:F:49:LEU:O	2:F:50:ARG:HG2	2.01	0.60
2:F:286:LEU:CD1	2:F:286:LEU:N	2.64	0.60
3:G:103:LEU:HD21	3:G:107:TYR:CD1	2.37	0.59
1:3:108:ILE:HD13	1:4:123:PHE:CE1	2.36	0.59
1:4:47:ASP:O	1:4:48:ARG:C	2.40	0.59
1:1:34:PHE:CE2	1:1:38:THR:HG21	2.36	0.59
3:G:4:THR:HG22	3:G:5:PHE:N	2.16	0.59
1:4:111:VAL:HG12	1:4:113:ARG:NE	2.17	0.59
2:F:306:GLY:O	2:F:307:ALA:C	2.40	0.59
1:3:37:LEU:HD21	1:3:85:TYR:CB	2.32	0.59
2:F:67:PHE:O	2:F:285:THR:HA	2.01	0.59
1:1:79:ALA:HA	1:1:124:THR:HG22	1.84	0.59
2:F:138:PRO:HD3	4:B:119:TYR:CD2	2.37	0.59
1:1:11:PHE:CE2	1:1:15:LEU:HD11	2.38	0.59
2:F:312:ASP:O	2:F:350:TRP:CZ3	2.55	0.59
1:4:19:LYS:HB2	1:4:85:TYR:HE2	1.66	0.59
1:2:65:PHE:CZ	1:3:44:ILE:HD11	2.37	0.59
4:B:98:ASP:CG	4:B:100:ARG:HD2	2.23	0.59
2:F:165:LEU:HD23	2:F:165:LEU:N	2.17	0.59
1:2:68:TYR:OH	1:3:93:THR:HA	2.02	0.59
3:G:70:ASN:N	3:G:70:ASN:HD22	2.01	0.59
1:2:26:VAL:HG13	5:2:158:HOH:O	2.02	0.59
1:2:56:GLU:HG3	1:2:103:PHE:CE1	2.37	0.59
4:B:75:SER:O	4:B:79:GLY:N	2.29	0.59
3:G:13:PHE:HD2	3:G:13:PHE:H	1.50	0.59
1:2:30:THR:O	1:2:31:GLU:C	2.40	0.59
2:F:176:GLU:N	2:F:176:GLU:OE1	2.36	0.59
1:2:73:ALA:CB	1:2:103:PHE:CD2	2.86	0.58
3:G:40:SER:H	3:G:60:ILE:HD11	1.68	0.58
1:3:58:CYS:SG	1:3:85:TYR:HD2	2.26	0.58
1:4:68:TYR:C	1:4:69:PRO:O	2.41	0.58
4:B:3:GLN:HE22	4:B:104:ALA:CA	2.16	0.58
1:4:36:PHE:HD2	1:4:36:PHE:C	2.03	0.58
1:3:104:THR:HG22	1:3:105:GLU:N	2.17	0.58
2:F:52:SER:O	2:F:53:PRO:C	2.39	0.58
2:F:241:ASN:OD1	2:F:242:LEU:N	2.35	0.58
1:2:78:ILE:HD11	1:2:103:PHE:CE2	2.38	0.58
1:1:87:HIS:ND1	1:1:88:PRO:N	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:ILE:CG2	2:F:329:SER:N	2.67	0.58
1:3:121:PHE:CE1	1:3:125:LEU:HG	2.37	0.58
4:B:85:ASP:O	4:B:89:GLN:HG3	2.04	0.58
1:1:14:ALA:CB	1:1:123:PHE:HE2	2.16	0.58
1:2:21:ILE:CD1	1:2:62:THR:HA	2.33	0.58
2:F:78:GLY:O	2:F:79:GLU:HB2	2.03	0.58
3:G:64:THR:O	3:G:64:THR:OG1	2.18	0.58
2:F:185:THR:HG21	2:F:190:ILE:HG23	1.84	0.58
3:G:19:VAL:HG13	3:G:20:LEU:N	2.17	0.58
4:B:76:ARG:HH21	4:B:77:ARG:HA	1.67	0.58
1:4:99:GLU:CG	1:4:117:ALA:HB2	2.33	0.58
1:3:60:TYR:O	1:3:63:LEU:HB2	2.03	0.58
2:F:297:LYS:HG2	2:F:335:ARG:CG	2.34	0.58
1:2:104:THR:HB	1:2:115:VAL:CG2	2.33	0.58
1:1:30:THR:O	1:1:31:GLU:C	2.41	0.58
2:F:313:ILE:HD13	2:F:351:TYR:OH	2.03	0.58
2:F:315:GLY:CA	2:F:320:TYR:HE1	2.14	0.58
2:F:84:PHE:CD1	2:F:94:LEU:HD21	2.39	0.58
2:F:362:TYR:O	2:F:363:HIS:C	2.40	0.58
1:4:78:ILE:CG2	1:4:120:LEU:HD11	2.33	0.58
4:B:3:GLN:HG3	4:B:90:ILE:HD12	1.84	0.58
1:4:96:LEU:HD23	1:4:96:LEU:O	2.03	0.58
2:F:241:ASN:OD1	2:F:241:ASN:C	2.42	0.58
1:4:128:ARG:CG	1:4:128:ARG:NH1	2.57	0.58
1:3:47:ASP:O	1:3:48:ARG:C	2.42	0.58
2:F:139:TRP:CZ2	2:F:383:VAL:HG21	2.39	0.57
1:3:96:LEU:HD23	1:3:96:LEU:C	2.25	0.57
2:F:70:TYR:HB3	2:F:235:LEU:HB2	1.86	0.57
1:1:20:LEU:HD11	1:2:91:ILE:CD1	2.33	0.57
2:F:418:THR:C	2:F:420:ARG:H	2.05	0.57
2:F:158:PHE:CE2	2:F:400:LEU:HD21	2.38	0.57
3:G:18:LEU:HD12	3:G:44:PHE:HD2	1.68	0.57
3:G:66:VAL:CG2	3:G:165:ILE:HD11	2.34	0.57
1:3:14:ALA:O	1:3:17:SER:HB2	2.04	0.57
2:F:286:LEU:CD1	2:F:286:LEU:H	2.14	0.57
1:2:43:TRP:HZ3	1:2:94:ALA:HB2	1.69	0.57
2:F:87:ASP:HB2	2:F:91:ALA:HB2	1.86	0.57
2:F:250:ASP:HA	2:F:260:PHE:CD2	2.37	0.57
2:F:113:ASN:OD1	2:F:114:PRO:HD2	2.04	0.57
3:G:18:LEU:HD11	3:G:32:LEU:HD23	1.86	0.57
1:4:99:GLU:HG3	1:4:117:ALA:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:13:PHE:CD2	3:G:13:PHE:N	2.71	0.57
1:3:58:CYS:SG	1:3:85:TYR:CD2	2.98	0.57
1:4:70:ARG:HD2	1:4:107:ILE:CD1	2.35	0.57
1:4:59:VAL:HG12	1:4:60:TYR:CD1	2.40	0.57
2:F:414:ARG:HG3	2:F:415:ASN:N	2.19	0.57
3:G:28:SER:O	3:G:29:ALA:C	2.43	0.57
3:G:23:VAL:HG11	3:G:56:PHE:CG	2.39	0.57
2:F:349:GLN:OE1	2:F:349:GLN:HA	2.04	0.57
1:4:18:ILE:HD11	1:4:65:PHE:CE1	2.39	0.57
1:3:51:ALA:O	1:3:52:ARG:C	2.43	0.57
1:2:7:GLN:O	1:2:8:SER:C	2.42	0.57
1:3:63:LEU:CD1	1:3:69:PRO:O	2.50	0.57
1:2:10:ARG:HG2	1:2:76:GLU:HG2	1.85	0.57
3:G:62:MET:HE3	3:G:73:VAL:CG2	2.32	0.57
1:2:29:LEU:HD21	1:2:57:ALA:HB3	1.85	0.57
1:3:11:PHE:O	1:3:14:ALA:HB3	2.05	0.57
1:1:139:GLU:O	1:1:142:VAL:CG2	2.52	0.57
1:3:79:ALA:CB	1:3:124:THR:HG22	2.35	0.57
1:4:123:PHE:CE2	1:4:134:VAL:HG12	2.38	0.56
1:2:75:VAL:HG11	1:2:123:PHE:CD1	2.40	0.56
2:F:58:LEU:HD13	2:F:262:GLY:HA3	1.87	0.56
2:F:212:MET:O	2:F:213:GLN:CG	2.53	0.56
2:F:104:ASP:O	2:F:157:ARG:HG2	2.05	0.56
3:G:3:GLN:HG3	3:G:4:THR:O	2.05	0.56
1:4:133:ASP:O	1:4:135:LEU:N	2.39	0.56
1:2:68:TYR:CE2	1:3:93:THR:HB	2.40	0.56
1:1:94:ALA:O	1:1:97:ILE:HG13	2.05	0.56
1:1:82:ILE:HA	1:1:86:VAL:HG23	1.87	0.56
3:G:15:SER:HB3	3:G:41:THR:CG2	2.35	0.56
2:F:82:ILE:HD12	2:F:82:ILE:H	1.70	0.56
3:G:113:ASN:O	3:G:113:ASN:ND2	2.37	0.56
4:B:64:ARG:HA	4:B:67:ILE:CG2	2.35	0.56
1:1:86:VAL:HB	1:1:91:ILE:CD1	2.36	0.56
1:2:82:ILE:HA	1:2:86:VAL:HG23	1.87	0.56
1:2:27:LEU:HD12	1:2:29:LEU:HD12	1.88	0.56
1:3:30:THR:O	1:3:31:GLU:C	2.41	0.56
3:G:80:ALA:O	3:G:155:CYS:HA	2.06	0.56
1:4:79:ALA:HA	1:4:124:THR:HG22	1.87	0.56
2:F:61:ASP:OD2	2:F:245:SER:HB2	2.06	0.56
1:1:86:VAL:O	1:1:91:ILE:HD11	2.05	0.56
2:F:27:LEU:HD11	2:F:286:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:TYR:CG	2:F:94:LEU:HD13	2.40	0.56
2:F:338:ASP:OD1	2:F:340:SER:N	2.38	0.56
3:G:93:ARG:NH1	3:G:134:ARG:CZ	2.69	0.56
1:1:29:LEU:HD22	1:1:33:ASP:CB	2.24	0.56
2:F:84:PHE:CD1	2:F:94:LEU:HD23	2.41	0.56
1:3:131:ASN:HA	1:3:134:VAL:CG2	2.36	0.56
1:3:54:CYS:O	1:3:57:ALA:HB3	2.06	0.56
1:4:79:ALA:HB1	1:4:124:THR:HG22	1.88	0.56
1:4:27:LEU:CD2	1:4:27:LEU:N	2.68	0.56
1:1:105:GLU:HG2	1:2:126:ARG:NH1	2.18	0.56
4:B:86:LYS:O	4:B:90:ILE:HG13	2.06	0.56
1:4:33:ASP:OD2	1:4:53:ARG:NH1	2.39	0.56
1:2:111:VAL:O	1:2:111:VAL:CG2	2.54	0.56
1:4:9:VAL:O	1:4:66:VAL:HG11	2.06	0.56
4:B:86:LYS:HE2	4:B:89:GLN:HE22	1.69	0.56
1:1:86:VAL:HB	1:1:91:ILE:HD13	1.87	0.56
1:3:105:GLU:O	1:3:107:ILE:N	2.39	0.56
1:2:21:ILE:HD13	1:2:62:THR:HA	1.85	0.56
1:2:43:TRP:H	1:2:90:ASN:HD21	1.54	0.55
2:F:97:VAL:HG13	2:F:147:ASN:HB3	1.88	0.55
2:F:52:SER:HB2	2:F:394:PHE:HD2	1.70	0.55
1:4:138:ALA:O	1:4:142:VAL:HG23	2.06	0.55
3:G:91:LEU:HD13	3:G:142:VAL:HG13	1.87	0.55
3:G:39:SER:CA	3:G:60:ILE:HD11	2.35	0.55
1:1:134:VAL:HG12	1:1:136:THR:HG23	1.88	0.55
1:1:134:VAL:HG12	1:1:136:THR:N	2.21	0.55
1:2:68:TYR:HE2	1:3:93:THR:HB	1.72	0.55
1:1:92:GLN:CA	1:1:121:PHE:CE1	2.87	0.55
1:4:93:THR:O	1:4:97:ILE:HG13	2.06	0.55
1:4:43:TRP:CZ3	1:4:51:ALA:HB1	2.40	0.55
2:F:159:GLY:O	2:F:160:PHE:O	2.24	0.55
3:G:25:PRO:HD2	3:G:50:ASN:O	2.06	0.55
1:3:95:CYS:O	1:3:98:MET:N	2.38	0.55
1:4:35:ASP:O	1:4:39:SER:N	2.38	0.55
2:F:148:PRO:O	2:F:149:ASN:C	2.44	0.55
2:F:164:HIS:HA	2:F:385:ILE:HD11	1.88	0.55
1:3:47:ASP:O	1:3:49:SER:N	2.39	0.55
1:4:30:THR:O	1:4:31:GLU:C	2.44	0.55
1:3:34:PHE:CE2	1:3:38:THR:CG2	2.88	0.55
2:F:70:TYR:CZ	2:F:72:PRO:HG3	2.41	0.55
2:F:28:ILE:HD11	2:F:159:GLY:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:57:LEU:H	3:G:57:LEU:HD22	1.71	0.55
1:4:151:VAL:O	1:4:152:MET:CB	2.55	0.55
1:1:109:ASN:O	1:1:111:VAL:HG23	2.07	0.55
2:F:49:LEU:HD13	2:F:64:VAL:HG11	1.89	0.55
1:2:128:ARG:HH11	1:2:128:ARG:CB	2.17	0.55
1:3:84:TYR:CD2	1:3:85:TYR:CE1	2.94	0.55
2:F:168:ILE:HG12	2:F:168:ILE:O	2.06	0.55
1:3:88:PRO:HA	1:3:91:ILE:HD12	1.89	0.55
2:F:257:LEU:C	2:F:259:GLN:H	2.10	0.55
1:3:99:GLU:HG3	1:3:117:ALA:N	2.22	0.55
1:2:17:SER:OG	1:2:62:THR:HG22	2.07	0.55
2:F:297:LYS:HG2	2:F:335:ARG:HB3	1.88	0.55
4:B:76:ARG:HE	4:B:77:ARG:N	2.05	0.55
1:4:74:PRO:HG2	1:4:77:PHE:CD1	2.42	0.55
1:1:75:VAL:HB	1:1:103:PHE:HD2	1.72	0.55
1:3:26:VAL:CG1	1:3:65:PHE:CD2	2.73	0.54
1:2:128:ARG:O	1:2:128:ARG:HG3	2.07	0.54
1:4:109:ASN:H	1:4:109:ASN:ND2	2.04	0.54
1:1:59:VAL:HG21	1:1:78:ILE:HD13	1.89	0.54
2:F:17:LEU:CD1	2:F:19:PHE:CE1	2.91	0.54
1:3:63:LEU:HD23	1:4:93:THR:HG22	1.90	0.54
3:G:12:ASN:OD1	3:G:13:PHE:N	2.41	0.54
2:F:394:PHE:N	2:F:394:PHE:CD1	2.75	0.54
1:3:20:LEU:HD23	1:4:128:ARG:HD2	1.89	0.54
1:1:146:LEU:CD2	1:1:147:ARG:HG2	2.35	0.54
1:3:79:ALA:HA	1:3:124:THR:CG2	2.33	0.54
2:F:1:SER:HB3	2:F:3:ILE:HD11	1.88	0.54
1:2:39:SER:OG	1:2:40:ASN:N	2.35	0.54
4:B:64:ARG:HA	4:B:67:ILE:HG22	1.90	0.54
1:4:68:TYR:OH	1:4:139:GLU:OE1	2.24	0.54
1:2:43:TRP:CZ3	1:2:94:ALA:HB2	2.40	0.54
1:4:87:HIS:ND1	1:4:89:VAL:N	2.45	0.54
1:3:48:ARG:O	1:3:51:ALA:HB3	2.07	0.54
1:1:48:ARG:O	1:1:51:ALA:HB3	2.07	0.54
2:F:316:ASP:OD1	2:F:316:ASP:C	2.46	0.54
3:G:25:PRO:O	3:G:26:ALA:HB2	2.08	0.54
4:B:6:LYS:HG2	4:B:83:CYS:CA	2.38	0.54
1:4:70:ARG:HD2	1:4:107:ILE:HD12	1.90	0.54
2:F:421:ASP:H	2:F:424:MET:CB	2.20	0.54
2:F:102:TYR:HD2	2:F:105:HIS:CE1	2.26	0.54
2:F:172:PRO:CD	2:F:379:LEU:HD11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:92:GLN:HB2	1:3:121:PHE:CE2	2.34	0.54
1:1:14:ALA:CB	1:1:123:PHE:CE2	2.89	0.54
1:2:15:LEU:O	1:2:18:ILE:HB	2.08	0.54
3:G:164:VAL:CG1	3:G:164:VAL:O	2.55	0.54
2:F:45:ALA:O	2:F:269:LYS:HA	2.08	0.54
2:F:164:HIS:CD2	2:F:385:ILE:HD11	2.43	0.54
3:G:44:PHE:O	3:G:44:PHE:CD1	2.60	0.54
2:F:268:TYR:OH	2:F:406:VAL:CG1	2.54	0.54
2:F:237:VAL:O	4:B:109:PHE:HB2	2.08	0.54
1:2:100:GLY:O	1:2:101:ALA:C	2.46	0.54
3:G:103:LEU:HD21	3:G:107:TYR:CG	2.44	0.53
3:G:47:LEU:HB3	3:G:155:CYS:SG	2.48	0.53
3:G:62:MET:HE2	3:G:142:VAL:HB	1.90	0.53
1:1:63:LEU:HD22	1:1:69:PRO:O	2.09	0.53
1:4:32:ASP:O	1:4:33:ASP:C	2.47	0.53
2:F:2:ASN:O	2:F:5:THR:HG23	2.07	0.53
3:G:71:GLN:HG3	3:G:131:VAL:HG21	1.90	0.53
1:3:71:PHE:CE1	1:4:96:LEU:HB2	2.43	0.53
1:4:79:ALA:O	1:4:80:ALA:C	2.45	0.53
1:1:60:TYR:CG	1:1:70:ARG:HD3	2.43	0.53
1:2:104:THR:HB	1:2:115:VAL:HG21	1.88	0.53
1:3:49:SER:HA	1:3:52:ARG:HE	1.72	0.53
1:4:59:VAL:C	1:4:61:GLY:H	2.11	0.53
1:3:104:THR:O	1:3:107:ILE:HB	2.09	0.53
2:F:378:ASP:O	2:F:382:ARG:HB2	2.08	0.53
1:3:71:PHE:CE1	1:4:96:LEU:CB	2.92	0.53
1:3:36:PHE:CZ	1:3:50:ARG:HB3	2.42	0.53
1:1:33:ASP:O	1:1:35:ASP:N	2.41	0.53
1:2:98:MET:HB2	1:2:120:LEU:CD1	2.39	0.53
1:1:87:HIS:ND1	1:1:87:HIS:C	2.61	0.53
2:F:207:GLU:O	2:F:209:ASP:N	2.42	0.53
1:1:134:VAL:HG12	1:1:135:LEU:N	2.23	0.53
1:1:60:TYR:CD2	1:1:70:ARG:HG2	2.44	0.53
1:1:93:THR:O	1:1:97:ILE:CG1	2.51	0.53
1:3:44:ILE:CG2	1:3:45:ALA:N	2.71	0.53
2:F:78:GLY:O	2:F:80:GLN:N	2.42	0.53
2:F:24:ILE:CD1	2:F:291:PHE:CD1	2.91	0.53
1:4:59:VAL:HG21	1:4:78:ILE:HG13	1.89	0.53
1:2:8:SER:O	1:2:9:VAL:C	2.47	0.53
1:1:10:ARG:O	1:1:11:PHE:C	2.47	0.53
1:3:59:VAL:HG12	1:3:60:TYR:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:103:PHE:O	1:4:104:THR:HG23	2.09	0.53
1:2:27:LEU:HD12	1:2:29:LEU:CD1	2.39	0.53
2:F:77:TYR:CD2	2:F:94:LEU:HD13	2.43	0.53
2:F:219:ILE:HG22	2:F:220:SER:N	2.23	0.52
3:G:93:ARG:NH1	3:G:134:ARG:NH1	2.56	0.52
3:G:19:VAL:CG1	3:G:20:LEU:N	2.71	0.52
1:2:87:HIS:ND1	1:2:89:VAL:N	2.54	0.52
2:F:79:GLU:O	2:F:82:ILE:N	2.42	0.52
3:G:67:ASN:O	3:G:68:ALA:HB2	2.09	0.52
1:2:68:TYR:OH	1:3:93:THR:N	2.43	0.52
3:G:15:SER:CA	3:G:41:THR:HG22	2.34	0.52
1:2:22:GLN:O	1:2:23:ALA:C	2.47	0.52
4:B:112:ALA:O	4:B:116:THR:HG23	2.08	0.52
1:3:15:LEU:O	1:3:18:ILE:HB	2.09	0.52
1:4:115:VAL:HG11	1:4:120:LEU:HD22	1.90	0.52
1:2:121:PHE:CE2	1:2:125:LEU:CD1	2.93	0.52
2:F:230:ALA:O	2:F:232:ASN:N	2.42	0.52
1:2:47:ASP:O	1:2:48:ARG:C	2.48	0.52
1:2:48:ARG:HG2	1:2:49:SER:N	2.25	0.52
1:1:106:ASN:ND2	1:1:113:ARG:HE	2.04	0.52
2:F:188:THR:O	2:F:189:SER:HB3	2.10	0.52
2:F:26:ARG:HD3	2:F:159:GLY:O	2.10	0.52
3:G:163:GLN:HG2	3:G:163:GLN:O	2.10	0.52
1:1:63:LEU:HD23	1:1:68:TYR:CB	2.39	0.52
2:F:35:VAL:HG11	2:F:277:VAL:HG21	1.91	0.52
2:F:63:THR:HG23	2:F:243:TRP:CD2	2.45	0.52
2:F:49:LEU:C	2:F:50:ARG:HG2	2.30	0.52
1:2:18:ILE:O	1:2:21:ILE:HB	2.10	0.52
2:F:335:ARG:HG3	2:F:336:SER:OG	2.09	0.52
4:B:3:GLN:CG	4:B:87:SER:HB2	2.38	0.52
2:F:215:TYR:O	2:F:216:ARG:C	2.48	0.52
2:F:364:LEU:C	2:F:365:LEU:HD23	2.30	0.52
3:G:158:LEU:H	3:G:158:LEU:HD23	1.74	0.52
1:3:32:ASP:HA	1:3:35:ASP:HB2	1.91	0.52
2:F:305:LYS:HZ1	2:F:312:ASP:CG	2.14	0.52
1:2:87:HIS:CG	1:2:88:PRO:HD2	2.45	0.52
2:F:104:ASP:CG	2:F:104:ASP:O	2.49	0.52
2:F:153:GLN:HB3	2:F:157:ARG:HD3	1.92	0.52
2:F:171:ALA:N	2:F:172:PRO:HD3	2.25	0.52
2:F:67:PHE:CD1	2:F:67:PHE:N	2.78	0.52
1:1:138:ALA:O	1:1:139:GLU:C	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:87:SER:O	4:B:90:ILE:N	2.43	0.52
1:1:43:TRP:CZ3	1:1:94:ALA:HB2	2.45	0.52
1:4:93:THR:O	1:4:97:ILE:CG1	2.57	0.52
3:G:95:GLU:HB2	3:G:138:ASN:HB3	1.92	0.52
1:2:92:GLN:O	1:2:95:CYS:N	2.42	0.51
2:F:326:ARG:NE	2:F:347:GLU:OE2	2.42	0.51
1:2:21:ILE:HG22	1:2:22:GLN:N	2.23	0.51
3:G:83:ALA:C	3:G:85:PRO:HD3	2.30	0.51
3:G:91:LEU:HD13	3:G:142:VAL:CG1	2.41	0.51
1:3:52:ARG:O	1:3:53:ARG:C	2.48	0.51
1:4:62:THR:O	1:4:65:PHE:HB3	2.10	0.51
1:3:98:MET:O	1:3:99:GLU:C	2.45	0.51
4:B:4:LEU:N	4:B:91:TYR:OH	2.43	0.51
1:3:74:PRO:HG3	1:4:125:LEU:HD23	1.91	0.51
3:G:37:ALA:O	3:G:61:GLN:O	2.28	0.51
1:2:79:ALA:O	1:2:80:ALA:C	2.49	0.51
1:3:71:PHE:CE1	1:4:96:LEU:HG	2.45	0.51
1:2:33:ASP:C	1:2:35:ASP:H	2.14	0.51
1:3:77:PHE:CD1	1:4:125:LEU:HD21	2.44	0.51
3:G:39:SER:HB2	3:G:162:ASN:OD1	2.10	0.51
1:3:18:ILE:HA	1:3:21:ILE:HD12	1.92	0.51
1:1:135:LEU:O	1:1:136:THR:C	2.49	0.51
1:2:11:PHE:CD2	1:2:127:VAL:HG22	2.44	0.51
2:F:419:THR:HB	2:F:423:ILE:CD1	2.39	0.51
1:2:36:PHE:CZ	5:2:160:HOH:O	2.42	0.51
3:G:32:LEU:HD21	3:G:47:LEU:CD2	2.41	0.51
1:3:58:CYS:HB3	1:3:85:TYR:HE2	1.73	0.51
2:F:68:THR:OG1	2:F:270:HIS:CE1	2.63	0.51
2:F:331:LYS:O	2:F:331:LYS:HG3	2.10	0.51
1:4:123:PHE:HE2	1:4:134:VAL:CG1	2.21	0.51
1:2:98:MET:HB2	1:2:120:LEU:HD11	1.93	0.51
1:2:131:ASN:HA	1:2:134:VAL:HG21	1.92	0.51
1:2:92:GLN:O	1:2:95:CYS:HB2	2.11	0.51
2:F:14:LEU:HD11	2:F:414:ARG:NH2	2.24	0.51
1:2:20:LEU:HB3	1:2:65:PHE:CZ	2.45	0.51
1:2:34:PHE:O	1:2:38:THR:OG1	2.22	0.51
3:G:32:LEU:HD21	3:G:47:LEU:HD22	1.92	0.51
2:F:172:PRO:HG2	2:F:379:LEU:HD13	1.85	0.51
2:F:227:SER:O	2:F:228:TYR:C	2.48	0.51
2:F:137:ALA:CB	2:F:140:MET:CE	2.88	0.51
2:F:166:LYS:HE2	4:B:117:PHE:CG	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:117:ASP:O	3:G:120:TYR:HB2	2.11	0.51
3:G:153:THR:OG1	3:G:154:LYS:N	2.42	0.51
3:G:84:ASP:OD1	3:G:86:LYS:HE3	2.10	0.51
1:2:135:LEU:O	1:2:137:ASP:OD1	2.29	0.51
3:G:57:LEU:CD1	3:G:103:LEU:HB2	2.41	0.51
2:F:26:ARG:HB3	2:F:159:GLY:CA	2.41	0.51
3:G:62:MET:CB	3:G:140:VAL:HG13	2.40	0.51
3:G:75:VAL:HB	3:G:161:LEU:HD11	1.93	0.51
3:G:75:VAL:HG11	3:G:112:LEU:HD11	1.93	0.51
2:F:67:PHE:HE2	4:B:120:PHE:CG	2.29	0.51
1:4:127:VAL:O	1:4:129:ALA:O	2.29	0.51
3:G:74:SER:CB	3:G:126:CYS:HB3	2.40	0.51
2:F:299:ILE:HG22	2:F:300:GLN:N	2.25	0.51
1:1:29:LEU:CD2	1:1:33:ASP:HB3	2.26	0.51
2:F:137:ALA:CB	2:F:140:MET:SD	2.97	0.51
2:F:297:LYS:HG2	2:F:335:ARG:CB	2.41	0.51
2:F:82:ILE:CD1	2:F:82:ILE:H	2.24	0.50
3:G:130:ASP:N	3:G:130:ASP:OD1	2.44	0.50
1:3:28:ASP:OD2	1:3:28:ASP:O	2.29	0.50
1:3:121:PHE:CD1	1:3:125:LEU:HG	2.45	0.50
2:F:338:ASP:OD1	2:F:338:ASP:C	2.49	0.50
2:F:28:ILE:CD1	2:F:159:GLY:N	2.75	0.50
2:F:28:ILE:HD11	2:F:159:GLY:N	2.26	0.50
1:2:71:PHE:CG	1:2:72:PRO:N	2.72	0.50
2:F:20:LEU:HD22	2:F:30:ILE:HG23	1.90	0.50
4:B:98:ASP:OD2	4:B:100:ARG:HD2	2.11	0.50
3:G:158:LEU:CD2	3:G:158:LEU:N	2.74	0.50
2:F:299:ILE:HG21	2:F:304:ALA:HB2	1.92	0.50
1:3:108:ILE:HD13	1:4:123:PHE:CZ	2.46	0.50
2:F:5:THR:O	2:F:7:ALA:N	2.44	0.50
1:2:130:GLY:O	1:2:134:VAL:HG23	2.11	0.50
4:B:71:LYS:HE2	4:B:92:ALA:O	2.12	0.50
1:3:75:VAL:CG1	1:3:76:GLU:N	2.73	0.50
1:3:81:VAL:O	1:3:82:ILE:C	2.50	0.50
2:F:218:VAL:O	2:F:219:ILE:C	2.49	0.50
1:1:88:PRO:HA	1:1:91:ILE:CG1	2.36	0.50
1:2:14:ALA:HB2	1:2:77:PHE:CD1	2.47	0.50
2:F:82:ILE:CG2	2:F:86:LYS:HE3	2.41	0.50
1:2:71:PHE:CD2	1:2:72:PRO:N	2.79	0.50
3:G:112:LEU:O	3:G:114:GLY:N	2.44	0.50
2:F:169:TRP:HH2	2:F:375:PRO:HG3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:12:GLN:CB	1:3:89:VAL:HA	2.42	0.50
1:2:86:VAL:HG11	1:2:94:ALA:HB2	1.94	0.50
3:G:2:PHE:CD2	3:G:2:PHE:N	2.80	0.50
2:F:20:LEU:HD13	2:F:30:ILE:CG2	2.36	0.50
2:F:72:PRO:HD2	2:F:75:HIS:ND1	2.26	0.50
1:2:126:ARG:O	1:2:127:VAL:C	2.50	0.49
4:B:103:PRO:HD2	4:B:104:ALA:H	1.76	0.49
1:4:50:ARG:CD	1:4:53:ARG:HH21	2.23	0.49
3:G:92:VAL:O	3:G:142:VAL:HA	2.12	0.49
1:2:107:ILE:CG1	1:2:112:GLU:HG3	2.42	0.49
2:F:26:ARG:NH2	2:F:161:ARG:HD3	2.26	0.49
2:F:169:TRP:CH2	2:F:375:PRO:HG2	2.47	0.49
1:2:95:CYS:SG	1:2:121:PHE:HA	2.52	0.49
1:3:71:PHE:HZ	1:4:96:LEU:HB2	1.77	0.49
2:F:195:LEU:O	2:F:198:ALA:HB3	2.12	0.49
1:4:87:HIS:CD2	1:4:88:PRO:HD2	2.47	0.49
1:3:65:PHE:C	1:3:65:PHE:HD1	2.16	0.49
1:1:14:ALA:HB2	1:1:123:PHE:CZ	2.46	0.49
2:F:256:SER:HB2	2:F:259:GLN:HB2	1.94	0.49
1:1:39:SER:OG	1:1:40:ASN:N	2.45	0.49
3:G:39:SER:C	3:G:60:ILE:HD11	2.33	0.49
1:3:18:ILE:HG22	1:3:19:LYS:N	2.26	0.49
1:3:19:LYS:O	1:3:20:LEU:C	2.49	0.49
1:3:58:CYS:HG	1:3:85:TYR:HD2	1.55	0.49
1:2:9:VAL:O	1:2:12:GLN:HG2	2.13	0.49
1:2:69:PRO:CD	1:3:96:LEU:HD11	2.38	0.49
1:4:36:PHE:CD2	1:4:36:PHE:O	2.59	0.49
1:1:21:ILE:O	1:1:24:SER:N	2.46	0.49
1:2:30:THR:HG23	1:2:33:ASP:HB2	1.95	0.49
1:2:82:ILE:O	1:2:86:VAL:HG23	2.13	0.49
2:F:102:TYR:O	2:F:103:ILE:C	2.50	0.49
1:2:27:LEU:CD2	1:2:27:LEU:N	2.67	0.49
2:F:137:ALA:HB3	2:F:140:MET:CE	2.42	0.49
2:F:169:TRP:CE2	2:F:170:THR:HG22	2.48	0.49
1:1:63:LEU:HD12	1:2:92:GLN:OE1	2.12	0.49
1:3:92:GLN:HA	1:3:121:PHE:CE2	2.47	0.49
1:1:43:TRP:HZ3	1:1:94:ALA:HA	1.77	0.49
1:3:9:VAL:HG11	1:4:126:ARG:NH1	2.27	0.49
1:1:11:PHE:HZ	1:1:130:GLY:HA3	1.77	0.49
3:G:69:ALA:HB2	3:G:132:LEU:HD12	1.93	0.49
3:G:70:ASN:ND2	3:G:70:ASN:N	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:16:ALA:HB1	1:3:42:VAL:HG21	1.95	0.49
1:1:68:TYR:HB3	1:1:69:PRO:HD2	1.95	0.49
1:2:131:ASN:O	1:2:134:VAL:N	2.36	0.49
1:1:75:VAL:HG13	1:1:120:LEU:CD2	2.43	0.49
1:4:13:THR:O	1:4:17:SER:HB2	2.12	0.49
1:2:121:PHE:CZ	1:2:125:LEU:CD1	2.96	0.49
1:3:87:HIS:CE1	1:3:89:VAL:H	2.28	0.49
2:F:208:ARG:HG3	2:F:212:MET:HG2	1.94	0.49
1:2:71:PHE:HB3	1:2:72:PRO:HD2	1.88	0.48
1:3:90:ASN:O	1:3:94:ALA:HB2	2.12	0.48
2:F:31:SER:O	2:F:285:THR:HG23	2.13	0.48
1:4:54:CYS:O	1:4:57:ALA:HB3	2.13	0.48
1:4:87:HIS:ND1	1:4:89:VAL:HB	2.28	0.48
1:2:7:GLN:C	1:2:9:VAL:HG23	2.33	0.48
1:4:39:SER:HB2	1:4:41:LYS:HE3	1.95	0.48
1:1:15:LEU:O	1:1:18:ILE:N	2.46	0.48
2:F:26:ARG:CG	2:F:160:PHE:O	2.59	0.48
2:F:68:THR:HA	2:F:285:THR:HA	1.95	0.48
1:4:99:GLU:O	1:4:115:VAL:HB	2.14	0.48
1:4:27:LEU:HB2	1:4:29:LEU:HD12	1.95	0.48
1:3:91:ILE:HG22	1:3:92:GLN:N	2.28	0.48
1:2:29:LEU:HD21	1:2:57:ALA:CB	2.43	0.48
2:F:338:ASP:OD1	2:F:340:SER:CB	2.59	0.48
3:G:4:THR:CG2	3:G:5:PHE:N	2.76	0.48
3:G:24:THR:O	3:G:24:THR:CG2	2.62	0.48
4:B:6:LYS:HG2	4:B:83:CYS:HA	1.95	0.48
1:4:99:GLU:HG3	1:4:117:ALA:CB	2.44	0.48
3:G:7:SER:OG	3:G:8:ARG:N	2.45	0.48
1:2:108:ILE:O	1:2:111:VAL:CG1	2.61	0.48
2:F:73:HIS:CD2	2:F:281:GLY:HA2	2.48	0.48
3:G:18:LEU:HD12	3:G:44:PHE:CD2	2.48	0.48
3:G:29:ALA:O	3:G:102:THR:HA	2.14	0.48
2:F:230:ALA:O	2:F:231:ASP:C	2.52	0.48
1:2:43:TRP:HZ3	1:2:94:ALA:CB	2.26	0.48
2:F:319:LEU:HA	2:F:319:LEU:HD23	1.60	0.48
2:F:4:GLN:O	2:F:6:GLY:N	2.47	0.48
2:F:357:TYR:CD1	2:F:357:TYR:C	2.85	0.48
1:2:21:ILE:HD11	1:2:65:PHE:HB3	1.96	0.48
2:F:425:THR:OG1	2:F:426:SER:N	2.45	0.48
3:G:163:GLN:O	3:G:163:GLN:CG	2.62	0.48
1:4:71:PHE:O	1:4:72:PRO:C	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:65:PHE:CE2	1:3:44:ILE:HD11	2.49	0.48
2:F:175:PRO:HG2	2:F:176:GLU:OE1	2.14	0.48
2:F:316:ASP:HA	2:F:317:PRO:HD2	1.72	0.48
1:4:7:GLN:CD	1:4:7:GLN:N	2.68	0.48
2:F:374:PRO:O	2:F:375:PRO:O	2.31	0.48
1:4:18:ILE:CG1	1:4:26:VAL:HG11	2.43	0.48
2:F:294:THR:OG1	2:F:370:PHE:HD2	1.97	0.48
2:F:102:TYR:CD2	2:F:105:HIS:CE1	3.02	0.48
3:G:102:THR:O	3:G:104:PRO:HD3	2.14	0.47
1:3:65:PHE:C	1:3:65:PHE:CD1	2.87	0.47
1:4:99:GLU:HG3	1:4:117:ALA:H	1.78	0.47
1:2:131:ASN:HA	1:2:134:VAL:CB	2.44	0.47
1:2:108:ILE:O	1:2:111:VAL:CG2	2.57	0.47
2:F:43:MET:HE3	2:F:45:ALA:HB2	1.94	0.47
2:F:58:LEU:N	2:F:248:ASP:OD1	2.43	0.47
2:F:302:LEU:HD23	2:F:308:LEU:CD2	2.44	0.47
3:G:29:ALA:CA	3:G:55:GLY:O	2.55	0.47
2:F:329:SER:O	2:F:331:LYS:N	2.47	0.47
1:4:79:ALA:CA	1:4:124:THR:HG22	2.44	0.47
1:2:12:GLN:HB3	1:3:89:VAL:HA	1.96	0.47
1:1:43:TRP:CD2	1:1:90:ASN:ND2	2.81	0.47
1:2:107:ILE:HG13	1:2:112:GLU:HG3	1.96	0.47
3:G:20:LEU:HD12	3:G:21:THR:H	1.78	0.47
2:F:380:GLN:HG3	2:F:384:LEU:HD12	1.95	0.47
4:B:4:LEU:HD22	4:B:108:ARG:NH2	2.30	0.47
4:B:71:LYS:HD3	4:B:92:ALA:HB1	1.95	0.47
1:2:48:ARG:O	1:2:51:ALA:HB3	2.14	0.47
2:F:297:LYS:CG	2:F:335:ARG:HB3	2.43	0.47
2:F:106:ALA:CB	2:F:119:ILE:HD11	2.41	0.47
2:F:402:TRP:CD2	2:F:402:TRP:O	2.68	0.47
1:1:136:THR:OG1	1:1:137:ASP:N	2.47	0.47
1:1:72:PRO:HG2	1:2:118:ALA:HB2	1.97	0.47
1:1:94:ALA:HA	1:1:97:ILE:CD1	2.42	0.47
2:F:420:ARG:C	2:F:422:SER:H	2.17	0.47
1:3:79:ALA:O	1:3:80:ALA:C	2.52	0.47
2:F:35:VAL:CG1	2:F:277:VAL:HG21	2.44	0.47
1:2:126:ARG:O	1:2:129:ALA:N	2.41	0.47
2:F:326:ARG:HG3	2:F:347:GLU:OE1	2.15	0.47
2:F:120:PRO:O	2:F:121:LYS:C	2.52	0.47
2:F:58:LEU:HA	2:F:58:LEU:HD12	1.71	0.47
3:G:100:PRO:HD3	3:G:141:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:21:ILE:O	1:3:23:ALA:N	2.47	0.47
1:3:54:CYS:O	1:3:55:VAL:C	2.53	0.47
2:F:168:ILE:HD11	2:F:345:ILE:CD1	2.44	0.47
1:1:35:ASP:C	1:1:37:LEU:H	2.16	0.47
2:F:61:ASP:O	2:F:243:TRP:HZ3	1.98	0.47
2:F:318:VAL:O	2:F:322:ASN:ND2	2.48	0.47
3:G:69:ALA:HB2	3:G:132:LEU:CD1	2.44	0.47
4:B:116:THR:OG1	4:B:117:PHE:N	2.46	0.47
3:G:94:PHE:CD1	3:G:103:LEU:HD12	2.50	0.47
3:G:26:ALA:H	3:G:55:GLY:N	2.08	0.47
1:1:36:PHE:CE1	1:1:50:ARG:HD3	2.48	0.47
1:4:18:ILE:CG2	1:4:27:LEU:HD21	2.45	0.47
1:3:121:PHE:O	1:3:122:ALA:C	2.53	0.47
1:3:95:CYS:O	1:3:96:LEU:C	2.53	0.47
1:3:93:THR:O	1:3:97:ILE:CD1	2.51	0.47
1:4:146:LEU:HB3	1:4:151:VAL:HB	1.96	0.47
2:F:419:THR:CA	2:F:422:SER:OG	2.57	0.47
2:F:228:TYR:CZ	2:F:230:ALA:CB	2.96	0.47
2:F:102:TYR:HB2	2:F:105:HIS:ND1	2.29	0.47
1:3:77:PHE:CE1	1:4:121:PHE:HZ	2.33	0.47
2:F:302:LEU:HD23	2:F:308:LEU:HD21	1.96	0.47
2:F:178:GLU:OE2	2:F:181:ARG:NH2	2.48	0.47
1:1:51:ALA:O	1:1:52:ARG:C	2.52	0.47
1:4:59:VAL:C	1:4:61:GLY:N	2.67	0.47
1:1:60:TYR:CG	1:1:70:ARG:HG2	2.49	0.47
1:2:131:ASN:O	1:2:132:THR:C	2.51	0.47
1:2:43:TRP:CH2	1:2:86:VAL:HG13	2.50	0.47
2:F:364:LEU:HD12	2:F:364:LEU:N	2.19	0.47
2:F:114:PRO:HG2	2:F:118:LYS:O	2.14	0.47
1:2:68:TYR:CG	1:3:96:LEU:CD1	2.98	0.47
2:F:421:ASP:N	2:F:424:MET:H	2.13	0.47
2:F:79:GLU:C	2:F:81:TRP:N	2.66	0.47
3:G:87:PHE:HB2	3:G:148:SER:HB2	1.97	0.47
2:F:153:GLN:HB3	2:F:157:ARG:HH11	1.77	0.47
1:3:50:ARG:O	1:3:51:ALA:C	2.54	0.47
1:4:85:TYR:CD2	1:4:85:TYR:N	2.81	0.47
4:B:103:PRO:C	4:B:105:GLU:N	2.68	0.47
2:F:418:THR:C	2:F:420:ARG:N	2.69	0.47
2:F:421:ASP:H	2:F:424:MET:HB2	1.78	0.47
2:F:309:THR:HG23	2:F:312:ASP:OD1	2.14	0.47
1:2:33:ASP:C	1:2:35:ASP:N	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:43:TRP:CD2	1:2:90:ASN:OD1	2.68	0.47
1:2:20:LEU:HB3	1:2:65:PHE:CE2	2.50	0.47
2:F:138:PRO:CD	4:B:119:TYR:CD2	2.98	0.47
2:F:378:ASP:C	2:F:380:GLN:H	2.19	0.46
3:G:84:ASP:OD2	3:G:84:ASP:C	2.53	0.46
1:1:92:GLN:HG3	1:1:121:PHE:CE1	2.50	0.46
1:2:108:ILE:O	1:2:109:ASN:ND2	2.48	0.46
1:4:99:GLU:CD	1:4:117:ALA:HB2	2.34	0.46
1:1:43:TRP:HZ3	1:1:94:ALA:CA	2.28	0.46
2:F:420:ARG:HA	2:F:424:MET:CG	2.36	0.46
3:G:169:ILE:HD13	3:G:169:ILE:N	2.20	0.46
2:F:11:PRO:HB3	2:F:413:TYR:CD2	2.50	0.46
1:1:34:PHE:CD2	1:1:34:PHE:O	2.69	0.46
3:G:69:ALA:C	3:G:70:ASN:HD22	2.19	0.46
1:3:19:LYS:O	1:3:21:ILE:N	2.49	0.46
1:1:69:PRO:HG2	1:2:96:LEU:HD11	1.96	0.46
2:F:320:TYR:CD2	2:F:347:GLU:HG3	2.44	0.46
2:F:101:GLY:O	2:F:102:TYR:CD1	2.62	0.46
3:G:30:PRO:HD2	3:G:55:GLY:O	2.15	0.46
3:G:59:CYS:SG	3:G:94:PHE:CZ	3.08	0.46
3:G:94:PHE:CD2	3:G:94:PHE:O	2.68	0.46
2:F:328:ILE:HB	2:F:343:PHE:CE1	2.50	0.46
1:1:71:PHE:HB2	1:1:72:PRO:HD2	1.96	0.46
1:1:121:PHE:O	1:1:122:ALA:C	2.52	0.46
2:F:79:GLU:N	2:F:82:ILE:HD13	2.31	0.46
4:B:100:ARG:HG3	4:B:100:ARG:H	1.46	0.46
2:F:248:ASP:HA	2:F:262:GLY:HA2	1.97	0.46
1:4:27:LEU:HD12	1:4:58:CYS:SG	2.56	0.46
1:3:87:HIS:CE1	1:3:89:VAL:HB	2.50	0.46
1:1:14:ALA:HB1	1:1:127:VAL:CG2	2.45	0.46
2:F:208:ARG:CA	2:F:212:MET:HB3	2.40	0.46
2:F:137:ALA:O	2:F:140:MET:HB2	2.15	0.46
4:B:111:ASP:O	4:B:114:VAL:HG13	2.15	0.46
1:2:71:PHE:CD2	1:2:72:PRO:CG	2.98	0.46
4:B:76:ARG:CZ	4:B:77:ARG:HA	2.45	0.46
1:1:146:LEU:HD23	1:1:147:ARG:CD	2.44	0.46
1:3:63:LEU:HD12	1:3:70:ARG:HA	1.98	0.46
2:F:365:LEU:HD23	2:F:365:LEU:N	2.31	0.46
2:F:353:TYR:OH	2:F:355:PRO:HA	2.15	0.46
3:G:58:HIS:CD2	3:G:59:CYS:H	2.33	0.46
1:4:132:THR:O	1:4:134:VAL:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:121:PHE:CD2	1:2:125:LEU:HD13	2.49	0.46
2:F:220:SER:C	2:F:222:PHE:N	2.69	0.46
1:2:50:ARG:O	1:2:51:ALA:C	2.55	0.46
3:G:29:ALA:HB3	3:G:103:LEU:CB	2.46	0.46
1:1:107:ILE:HG21	1:2:119:GLU:HA	1.98	0.46
1:2:131:ASN:HA	1:2:134:VAL:HB	1.97	0.46
1:2:7:GLN:C	1:2:9:VAL:N	2.69	0.46
1:4:81:VAL:HG12	1:4:82:ILE:N	2.30	0.46
1:3:139:GLU:HA	1:3:142:VAL:CG2	2.46	0.46
3:G:42:LEU:HB2	3:G:58:HIS:CE1	2.51	0.46
1:3:20:LEU:HD21	1:4:91:ILE:CD1	2.43	0.46
2:F:68:THR:CG2	2:F:285:THR:HB	2.26	0.46
1:4:30:THR:O	1:4:33:ASP:N	2.49	0.46
1:2:66:VAL:O	1:2:66:VAL:CG1	2.64	0.46
1:2:80:ALA:HA	1:2:127:VAL:HG11	1.98	0.45
1:1:18:ILE:O	1:1:22:GLN:HG3	2.16	0.45
2:F:295:ALA:HB2	2:F:371:ILE:HB	1.97	0.45
3:G:143:GLY:HA2	3:G:161:LEU:CD2	2.35	0.45
2:F:274:ARG:HD3	4:B:105:GLU:OE2	2.16	0.45
2:F:21:ALA:HA	2:F:403:ASN:HA	1.98	0.45
2:F:155:ASP:O	2:F:158:PHE:O	2.33	0.45
3:G:24:THR:O	3:G:25:PRO:O	2.35	0.45
2:F:274:ARG:CD	4:B:105:GLU:OE2	2.65	0.45
2:F:104:ASP:OD2	2:F:104:ASP:O	2.34	0.45
2:F:357:TYR:CD1	2:F:358:VAL:N	2.84	0.45
1:2:87:HIS:ND1	1:2:88:PRO:N	2.65	0.45
1:1:120:LEU:HD23	1:1:120:LEU:HA	1.72	0.45
2:F:340:SER:OG	2:F:341:LYS:HE2	2.16	0.45
2:F:179:LEU:HD21	2:F:325:PRO:HB2	1.98	0.45
3:G:110:TYR:HA	3:G:111:PRO:HD3	1.86	0.45
1:1:27:LEU:HA	1:1:27:LEU:HD23	1.67	0.45
1:3:29:LEU:HD22	1:3:33:ASP:HB3	1.99	0.45
1:3:49:SER:OG	1:3:50:ARG:N	2.49	0.45
1:1:140:GLU:O	1:1:143:ARG:HB3	2.15	0.45
1:1:48:ARG:HG2	1:1:48:ARG:H	1.57	0.45
1:2:116:LYS:O	1:2:119:GLU:CG	2.64	0.45
1:1:14:ALA:HB1	1:1:127:VAL:HG22	1.98	0.45
1:2:87:HIS:CE1	1:2:89:VAL:HB	2.51	0.45
3:G:28:SER:O	3:G:102:THR:CG2	2.60	0.45
2:F:60:ILE:HG22	2:F:61:ASP:N	2.31	0.45
2:F:393:CYS:C	2:F:394:PHE:CD1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:108:ILE:HD12	1:4:110:GLY:HA3	1.99	0.45
1:2:116:LYS:HB2	1:2:119:GLU:OE1	2.16	0.45
2:F:421:ASP:C	2:F:423:ILE:N	2.70	0.45
1:1:23:ALA:O	1:1:24:SER:C	2.55	0.45
1:1:134:VAL:CG1	1:1:135:LEU:N	2.80	0.45
1:3:87:HIS:CG	1:3:88:PRO:HD2	2.52	0.45
1:3:94:ALA:O	1:3:97:ILE:HB	2.17	0.45
2:F:418:THR:HB	2:F:420:ARG:HD2	1.97	0.45
1:1:7:GLN:O	1:1:10:ARG:HB2	2.16	0.45
2:F:74:ARG:NH2	2:F:229:ASP:OD2	2.42	0.45
3:G:79:ILE:CG1	3:G:121:TYR:HB3	2.46	0.45
2:F:92:THR:HA	2:F:93:PRO:HD2	1.75	0.45
2:F:191:ASP:O	2:F:192:ILE:C	2.54	0.45
3:G:35:PRO:HB3	3:G:59:CYS:HB3	1.99	0.45
1:3:109:ASN:O	1:3:111:VAL:HG23	2.17	0.45
2:F:277:VAL:O	2:F:277:VAL:HG12	2.17	0.45
2:F:211:PHE:O	2:F:212:MET:CB	2.61	0.45
2:F:257:LEU:HD23	2:F:257:LEU:HA	1.63	0.45
2:F:300:GLN:O	2:F:301:TYR:C	2.54	0.45
2:F:376:SER:O	2:F:377:GLY:O	2.35	0.45
2:F:67:PHE:HE2	4:B:120:PHE:CD2	2.34	0.45
2:F:168:ILE:CD1	2:F:345:ILE:HD11	2.46	0.45
2:F:215:TYR:C	2:F:215:TYR:CD2	2.90	0.45
4:B:114:VAL:O	4:B:118:GLY:CA	2.59	0.45
3:G:3:GLN:NE2	3:G:4:THR:H	2.15	0.45
3:G:62:MET:HE2	3:G:142:VAL:CB	2.47	0.44
1:1:71:PHE:CD2	1:2:96:LEU:HD21	2.52	0.44
2:F:47:GLY:HA3	2:F:406:VAL:HG12	1.99	0.44
3:G:9:HIS:CD2	3:G:10:ASN:N	2.84	0.44
1:4:75:VAL:O	1:4:76:GLU:C	2.56	0.44
1:4:78:ILE:HG22	1:4:79:ALA:N	2.33	0.44
1:1:87:HIS:ND1	1:1:88:PRO:CD	2.80	0.44
2:F:305:LYS:O	2:F:305:LYS:HG3	2.16	0.44
2:F:88:GLY:C	2:F:90:ASN:H	2.20	0.44
1:3:142:VAL:O	1:3:142:VAL:HG12	2.18	0.44
1:3:17:SER:O	1:3:18:ILE:C	2.56	0.44
2:F:169:TRP:CZ3	2:F:375:PRO:CG	2.97	0.44
1:1:44:ILE:CD1	1:1:47:ASP:OD2	2.64	0.44
2:F:305:LYS:HZ1	2:F:309:THR:HG23	1.83	0.44
1:3:72:PRO:O	1:4:118:ALA:HB1	2.16	0.44
1:1:109:ASN:O	1:1:110:GLY:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:125:ASP:OD1	3:G:126:CYS:N	2.43	0.44
2:F:9:ARG:NH2	2:F:40:SER:HB2	2.32	0.44
3:G:57:LEU:HB2	3:G:145:MET:HB2	2.00	0.44
4:B:76:ARG:HB2	4:B:82:THR:N	2.32	0.44
1:3:34:PHE:CD2	1:3:34:PHE:O	2.71	0.44
2:F:140:MET:HB3	2:F:141:PRO:HD2	1.99	0.44
2:F:77:TYR:O	2:F:78:GLY:C	2.55	0.44
1:3:143:ARG:HD3	1:3:143:ARG:HA	1.60	0.44
1:1:138:ALA:C	1:1:140:GLU:N	2.68	0.44
1:1:33:ASP:O	1:1:37:LEU:HB2	2.18	0.44
2:F:266:GLN:OE1	2:F:266:GLN:HA	2.16	0.44
4:B:71:LYS:O	4:B:74:CYS:HB3	2.18	0.44
1:1:11:PHE:O	1:1:12:GLN:C	2.56	0.44
1:3:71:PHE:HE1	1:4:96:LEU:HG	1.71	0.44
2:F:116:THR:OG1	2:F:118:LYS:HB2	2.17	0.44
2:F:132:ASN:OD1	2:F:143:ARG:N	2.41	0.44
2:F:143:ARG:NH2	2:F:155:ASP:OD2	2.39	0.44
2:F:334:PHE:CD2	2:F:374:PRO:HB3	2.53	0.44
1:1:37:LEU:HG	1:1:54:CYS:HB3	2.00	0.44
4:B:103:PRO:C	4:B:105:GLU:H	2.21	0.44
1:2:36:PHE:HB2	1:2:43:TRP:HE1	1.82	0.44
1:2:15:LEU:HA	1:2:15:LEU:HD23	1.81	0.44
3:G:62:MET:HE1	3:G:73:VAL:HG22	1.99	0.44
1:3:98:MET:C	1:3:99:GLU:O	2.54	0.44
1:1:88:PRO:CA	1:1:91:ILE:HG12	2.36	0.44
1:1:119:GLU:O	1:1:120:LEU:C	2.56	0.44
2:F:153:GLN:O	2:F:154:ASP:C	2.56	0.44
3:G:5:PHE:C	3:G:6:ILE:HG13	2.37	0.44
3:G:31:VAL:O	3:G:33:GLN:N	2.51	0.44
1:1:49:SER:O	1:1:50:ARG:C	2.54	0.44
1:4:99:GLU:HG3	1:4:117:ALA:CA	2.47	0.44
4:B:103:PRO:HA	4:B:106:PHE:CD1	2.53	0.44
2:F:70:TYR:OH	2:F:278:PRO:HD2	2.17	0.44
2:F:79:GLU:H	2:F:82:ILE:HD13	1.83	0.44
1:3:74:PRO:CG	1:4:125:LEU:HD23	2.47	0.44
1:3:66:VAL:HG12	1:3:67:GLY:H	1.81	0.44
1:1:97:ILE:H	1:1:97:ILE:HG12	1.30	0.44
3:G:74:SER:HA	3:G:126:CYS:HA	1.98	0.44
3:G:58:HIS:CD2	3:G:59:CYS:N	2.85	0.43
1:4:87:HIS:CG	1:4:88:PRO:CD	3.00	0.43
1:4:123:PHE:CE2	1:4:134:VAL:CG1	3.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:95:CYS:SG	1:1:121:PHE:HA	2.58	0.43
2:F:37:ALA:HB2	2:F:279:GLU:HA	2.00	0.43
1:1:78:ILE:HD12	1:1:98:MET:HE3	2.00	0.43
3:G:158:LEU:CD2	3:G:158:LEU:H	2.30	0.43
1:1:52:ARG:O	1:1:53:ARG:C	2.56	0.43
1:1:54:CYS:O	1:1:55:VAL:C	2.53	0.43
2:F:230:ALA:C	2:F:232:ASN:N	2.70	0.43
2:F:195:LEU:HD23	2:F:195:LEU:HA	1.76	0.43
3:G:33:GLN:O	3:G:34:THR:C	2.56	0.43
1:3:36:PHE:O	1:3:37:LEU:C	2.54	0.43
2:F:345:ILE:HG23	2:F:346:ALA:N	2.31	0.43
1:4:18:ILE:CD1	1:4:26:VAL:HG11	2.45	0.43
1:3:34:PHE:HE2	1:3:38:THR:HG21	1.73	0.43
1:1:22:GLN:NE2	1:1:133:ASP:HB3	2.33	0.43
2:F:268:TYR:CZ	2:F:406:VAL:HG11	2.53	0.43
1:2:9:VAL:O	1:2:11:PHE:N	2.51	0.43
1:1:11:PHE:CE2	1:1:15:LEU:CD1	3.01	0.43
1:3:68:TYR:HA	1:3:69:PRO:HD3	1.74	0.43
1:4:140:GLU:O	1:4:144:GLN:HG3	2.19	0.43
1:3:65:PHE:HD1	1:3:65:PHE:O	2.02	0.43
2:F:170:THR:O	2:F:383:VAL:HG13	2.18	0.43
1:1:30:THR:CG2	1:1:33:ASP:CG	2.84	0.43
1:4:133:ASP:O	1:4:136:THR:N	2.50	0.43
1:4:27:LEU:H	1:4:27:LEU:HD23	1.79	0.43
1:2:126:ARG:HG2	1:2:126:ARG:H	1.66	0.43
1:4:52:ARG:O	1:4:53:ARG:C	2.57	0.43
1:4:40:ASN:H	1:4:40:ASN:ND2	2.16	0.43
1:1:98:MET:O	1:1:99:GLU:C	2.56	0.43
1:3:49:SER:O	1:3:50:ARG:C	2.56	0.43
1:1:60:TYR:O	1:1:61:GLY:O	2.36	0.43
2:F:159:GLY:C	2:F:160:PHE:O	2.56	0.43
3:G:57:LEU:CD2	3:G:57:LEU:H	2.31	0.43
1:4:116:LYS:O	1:4:117:ALA:C	2.57	0.43
4:B:3:GLN:CB	4:B:87:SER:HB2	2.49	0.43
1:1:21:ILE:O	1:1:22:GLN:C	2.57	0.43
3:G:85:PRO:O	3:G:87:PHE:CD2	2.69	0.43
2:F:36:ILE:O	2:F:37:ALA:C	2.56	0.43
2:F:143:ARG:NH1	2:F:160:PHE:CD2	2.87	0.43
2:F:167:ASN:OD1	2:F:168:ILE:N	2.52	0.43
1:4:68:TYR:OH	1:4:139:GLU:HG2	2.18	0.43
1:3:82:ILE:HD13	1:3:94:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:95:ASP:OD2	4:B:98:ASP:N	2.52	0.43
2:F:191:ASP:C	2:F:191:ASP:OD1	2.56	0.43
3:G:43:TYR:CG	3:G:43:TYR:O	2.72	0.43
3:G:23:VAL:HG11	3:G:56:PHE:CD2	2.54	0.43
1:3:15:LEU:HA	1:3:15:LEU:HD22	1.76	0.43
1:1:50:ARG:O	1:1:51:ALA:C	2.56	0.43
4:B:6:LYS:HZ2	4:B:84:ASP:HA	1.84	0.43
1:4:18:ILE:HD11	1:4:65:PHE:CD1	2.53	0.43
1:3:99:GLU:HG3	1:3:117:ALA:CA	2.49	0.43
4:B:4:LEU:HD13	4:B:110:HIS:CE1	2.54	0.43
2:F:27:LEU:HD11	2:F:286:LEU:CB	2.49	0.43
2:F:319:LEU:C	2:F:321:GLY:N	2.69	0.43
2:F:249:VAL:O	2:F:249:VAL:CG1	2.56	0.43
3:G:5:PHE:C	3:G:6:ILE:CG1	2.87	0.43
2:F:397:VAL:O	2:F:397:VAL:HG12	2.19	0.43
1:4:41:LYS:HG3	1:4:41:LYS:H	1.62	0.43
1:2:35:ASP:O	1:2:36:PHE:C	2.54	0.43
2:F:66:ILE:HD11	2:F:268:TYR:CE1	2.54	0.43
3:G:90:CYS:SG	3:G:109:VAL:HG21	2.58	0.43
2:F:17:LEU:HD11	2:F:19:PHE:CE1	2.54	0.43
1:2:24:SER:O	1:2:25:ALA:O	2.36	0.43
3:G:163:GLN:O	3:G:165:ILE:N	2.51	0.42
1:4:18:ILE:HG12	1:4:27:LEU:HD21	2.01	0.42
2:F:44:ASP:OD1	2:F:271:SER:CB	2.53	0.42
1:2:32:ASP:O	1:2:35:ASP:N	2.46	0.42
1:2:17:SER:CB	1:2:66:VAL:HG21	2.45	0.42
2:F:299:ILE:CG2	2:F:300:GLN:N	2.81	0.42
2:F:136:LYS:HG2	2:F:136:LYS:O	2.12	0.42
2:F:196:GLN:O	2:F:199:TYR:N	2.51	0.42
4:B:64:ARG:O	4:B:67:ILE:HG23	2.05	0.42
2:F:161:ARG:NH2	2:F:381:GLU:OE2	2.52	0.42
3:G:32:LEU:CD1	3:G:56:PHE:HD2	2.27	0.42
2:F:240:SER:OG	2:F:270:HIS:CD2	2.63	0.42
1:1:47:ASP:O	1:1:48:ARG:C	2.57	0.42
4:B:76:ARG:NE	4:B:77:ARG:N	2.67	0.42
1:4:72:PRO:HG3	1:4:111:VAL:HB	2.00	0.42
1:4:76:GLU:CG	1:4:123:PHE:CZ	2.96	0.42
1:3:125:LEU:HD22	1:3:125:LEU:HA	1.58	0.42
1:3:70:ARG:H	1:3:70:ARG:HG3	1.58	0.42
2:F:323:LEU:HD23	2:F:323:LEU:HA	1.78	0.42
3:G:8:ARG:HB3	3:G:126:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:99:TRP:HA	4:B:99:TRP:CE3	2.54	0.42
1:3:49:SER:HA	1:3:52:ARG:CG	2.49	0.42
1:2:92:GLN:HG3	1:2:121:PHE:HE1	1.84	0.42
2:F:245:SER:H	2:F:266:GLN:HE21	1.66	0.42
2:F:60:ILE:HD11	2:F:370:PHE:CD2	2.50	0.42
2:F:305:LYS:NZ	2:F:312:ASP:CG	2.72	0.42
1:2:30:THR:O	1:2:33:ASP:N	2.53	0.42
1:2:82:ILE:HA	1:2:86:VAL:CG2	2.49	0.42
3:G:79:ILE:HG13	3:G:121:TYR:HB3	2.01	0.42
4:B:99:TRP:HA	4:B:99:TRP:HE3	1.84	0.42
2:F:205:ASP:O	2:F:206:GLN:C	2.57	0.42
3:G:58:HIS:O	3:G:143:GLY:HA3	2.19	0.42
2:F:220:SER:C	2:F:222:PHE:H	2.23	0.42
2:F:335:ARG:O	2:F:335:ARG:HD2	2.19	0.42
1:2:108:ILE:H	1:2:111:VAL:HG22	1.85	0.42
1:2:44:ILE:HG22	1:2:46:THR:H	1.84	0.42
1:4:21:ILE:O	1:4:22:GLN:O	2.37	0.42
2:F:143:ARG:HG2	2:F:160:PHE:CE2	2.54	0.42
2:F:235:LEU:HD22	2:F:235:LEU:HA	1.80	0.42
2:F:70:TYR:HB2	2:F:283:MET:CE	2.48	0.42
2:F:208:ARG:HA	2:F:212:MET:HB2	2.01	0.42
2:F:405:GLN:NE2	2:F:405:GLN:CA	2.80	0.42
3:G:20:LEU:CD1	3:G:22:SER:H	2.33	0.42
2:F:68:THR:OG1	2:F:270:HIS:HE1	2.02	0.42
4:B:6:LYS:NZ	4:B:84:ASP:HA	2.34	0.42
1:1:76:GLU:CD	1:1:104:THR:HG23	2.39	0.42
1:4:32:ASP:O	1:4:35:ASP:N	2.53	0.42
3:G:41:THR:OG1	3:G:160:SER:HB2	2.20	0.42
2:F:102:TYR:O	2:F:105:HIS:HB2	2.19	0.42
3:G:32:LEU:O	3:G:33:GLN:CB	2.60	0.42
1:1:60:TYR:HE2	1:1:71:PHE:O	2.03	0.42
1:3:93:THR:C	1:3:97:ILE:HD12	2.37	0.42
4:B:4:LEU:HD12	4:B:4:LEU:O	2.20	0.42
1:1:123:PHE:CE2	1:1:127:VAL:CG2	3.03	0.42
1:1:18:ILE:HA	1:1:21:ILE:HD12	2.01	0.42
1:1:7:GLN:OE1	1:1:126:ARG:NE	2.52	0.42
3:G:93:ARG:HD2	3:G:129:ILE:CG2	2.49	0.42
1:3:28:ASP:CG	1:3:28:ASP:O	2.57	0.42
2:F:345:ILE:CG2	2:F:346:ALA:N	2.83	0.42
1:4:133:ASP:O	1:4:134:VAL:C	2.57	0.42
1:4:26:VAL:HG12	1:4:27:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:218:VAL:O	2:F:221:SER:N	2.53	0.42
2:F:27:LEU:HD22	2:F:135:PHE:CD2	2.55	0.42
2:F:10:MET:HE3	2:F:11:PRO:HD3	2.02	0.42
1:2:84:TYR:CZ	1:2:136:THR:HG23	2.54	0.42
2:F:8:GLU:HG2	2:F:8:GLU:O	2.20	0.42
3:G:131:VAL:O	3:G:140:VAL:HG11	2.19	0.42
3:G:162:ASN:OD1	3:G:163:GLN:N	2.53	0.42
1:4:75:VAL:HG13	1:4:120:LEU:HD13	2.01	0.42
1:2:124:THR:O	1:2:125:LEU:C	2.57	0.42
1:2:129:ALA:C	1:2:131:ASN:H	2.23	0.42
1:1:32:ASP:O	1:1:35:ASP:CA	2.67	0.42
1:2:80:ALA:O	1:2:83:ALA:HB3	2.19	0.42
1:3:56:GLU:O	1:3:59:VAL:N	2.52	0.42
2:F:99:THR:HG23	2:F:148:PRO:HG2	2.02	0.42
1:2:14:ALA:O	1:2:15:LEU:C	2.58	0.42
2:F:76:VAL:HG13	2:F:121:LYS:HG2	2.01	0.42
1:3:139:GLU:HA	1:3:142:VAL:HG21	2.02	0.42
3:G:161:LEU:HA	3:G:161:LEU:HD12	1.61	0.41
1:3:35:ASP:O	1:3:39:SER:HB3	2.20	0.41
1:4:59:VAL:HG21	1:4:78:ILE:CG1	2.50	0.41
1:4:146:LEU:O	1:4:147:ARG:C	2.57	0.41
2:F:298:GLU:OE2	2:F:353:TYR:OH	2.34	0.41
1:3:49:SER:HA	1:3:52:ARG:HG3	2.02	0.41
2:F:346:ALA:O	2:F:348:GLY:N	2.53	0.41
3:G:84:ASP:O	3:G:86:LYS:HD2	2.20	0.41
1:1:43:TRP:CD1	1:1:90:ASN:ND2	2.88	0.41
2:F:362:TYR:HA	2:F:365:LEU:HG	2.02	0.41
1:4:63:LEU:HD21	1:4:77:PHE:CD2	2.55	0.41
1:2:12:GLN:O	1:2:13:THR:C	2.59	0.41
1:1:113:ARG:O	1:1:113:ARG:HD2	2.20	0.41
1:2:17:SER:C	1:2:21:ILE:HD12	2.38	0.41
3:G:90:CYS:HB2	3:G:109:VAL:HG22	2.01	0.41
2:F:204:THR:O	2:F:205:ASP:C	2.57	0.41
1:4:92:GLN:O	1:4:95:CYS:HB2	2.20	0.41
1:2:73:ALA:HA	1:2:74:PRO:HD3	1.84	0.41
3:G:20:LEU:HD12	3:G:21:THR:N	2.35	0.41
2:F:345:ILE:HG23	2:F:349:GLN:HB2	2.03	0.41
1:2:92:GLN:O	1:2:93:THR:C	2.58	0.41
1:1:121:PHE:CD2	1:1:125:LEU:HD23	2.55	0.41
1:1:12:GLN:NE2	1:1:12:GLN:CA	2.78	0.41
1:1:21:ILE:O	1:1:23:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:VAL:CG2	2:F:283:MET:HG3	2.50	0.41
1:4:121:PHE:CE1	1:4:125:LEU:HD22	2.55	0.41
2:F:371:ILE:O	2:F:371:ILE:HG22	2.19	0.41
2:F:71:VAL:HG22	2:F:234:PRO:HB3	2.02	0.41
2:F:310:TYR:CD1	2:F:314:ALA:HB2	2.56	0.41
2:F:310:TYR:O	2:F:314:ALA:HB3	2.19	0.41
3:G:18:LEU:HD11	3:G:32:LEU:CD2	2.49	0.41
1:3:32:ASP:O	1:3:35:ASP:N	2.54	0.41
1:2:121:PHE:CZ	1:2:125:LEU:HD13	2.55	0.41
4:B:3:GLN:OE1	4:B:91:TYR:CD2	2.74	0.41
4:B:89:GLN:H	4:B:89:GLN:HG3	1.44	0.41
1:1:43:TRP:HZ3	1:1:94:ALA:CB	2.33	0.41
1:4:36:PHE:CE1	1:4:50:ARG:CB	2.89	0.41
1:3:34:PHE:CD2	1:3:34:PHE:C	2.94	0.41
2:F:315:GLY:HA2	2:F:320:TYR:CZ	2.51	0.41
2:F:121:LYS:O	2:F:122:HIS:C	2.59	0.41
4:B:95:ASP:O	4:B:97:ASN:N	2.53	0.41
2:F:43:MET:HE2	2:F:45:ALA:HB2	2.01	0.41
4:B:119:TYR:O	4:B:119:TYR:CD1	2.74	0.41
1:1:32:ASP:O	1:1:33:ASP:C	2.58	0.41
1:2:30:THR:HG23	1:2:33:ASP:CG	2.40	0.41
2:F:212:MET:O	2:F:213:GLN:CB	2.68	0.41
1:2:105:GLU:OE1	1:2:107:ILE:HD11	2.20	0.41
2:F:43:MET:HE3	2:F:408:PHE:HD1	1.85	0.41
1:3:132:THR:C	1:3:134:VAL:H	2.24	0.41
2:F:253:ASP:O	2:F:254:GLN:C	2.58	0.41
1:2:96:LEU:HA	1:2:96:LEU:HD22	1.79	0.41
1:1:125:LEU:HD13	1:1:125:LEU:HA	1.69	0.41
2:F:97:VAL:HG11	2:F:148:PRO:HD2	1.98	0.41
1:4:71:PHE:HE1	1:4:74:PRO:HD3	1.85	0.41
1:1:104:THR:O	1:1:105:GLU:C	2.58	0.41
1:4:126:ARG:O	1:4:127:VAL:C	2.59	0.41
2:F:353:TYR:CZ	2:F:355:PRO:HA	2.55	0.41
3:G:91:LEU:HD22	3:G:91:LEU:HA	1.93	0.41
2:F:345:ILE:HD13	2:F:349:GLN:HB3	2.01	0.41
2:F:374:PRO:C	2:F:375:PRO:O	2.58	0.41
1:4:66:VAL:O	1:4:66:VAL:HG12	2.21	0.41
1:3:87:HIS:ND1	1:3:89:VAL:N	2.60	0.41
4:B:68:GLU:O	4:B:71:LYS:HB3	2.21	0.41
1:1:43:TRP:HZ3	1:1:94:ALA:HB2	1.84	0.41
1:4:30:THR:HG23	1:4:33:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:33:ASP:O	1:4:36:PHE:HB3	2.20	0.41
1:1:22:GLN:HE22	1:1:133:ASP:HB3	1.85	0.41
1:1:11:PHE:HE2	1:1:15:LEU:CD1	2.31	0.41
2:F:72:PRO:HG2	2:F:75:HIS:HE1	1.86	0.41
1:2:52:ARG:O	1:2:53:ARG:C	2.58	0.41
1:2:27:LEU:H	1:2:27:LEU:CD2	2.25	0.41
1:2:20:LEU:CB	1:2:65:PHE:CE2	3.03	0.41
3:G:53:ASN:HA	3:G:149:ASN:HA	2.03	0.41
2:F:108:PHE:H	2:F:108:PHE:HD2	1.68	0.41
1:3:134:VAL:O	1:3:135:LEU:HD23	2.20	0.41
1:2:64:ASP:OD2	1:2:70:ARG:NH1	2.53	0.41
2:F:56:ARG:HG2	2:F:57:GLY:H	1.86	0.41
1:1:70:ARG:O	1:1:71:PHE:HB3	2.21	0.41
1:2:121:PHE:CZ	1:2:125:LEU:HD11	2.56	0.41
1:2:68:TYR:CZ	1:3:93:THR:HA	2.56	0.41
2:F:137:ALA:HB2	2:F:140:MET:CE	2.50	0.41
1:2:21:ILE:HD11	1:2:62:THR:HA	2.03	0.41
1:2:107:ILE:HA	1:2:111:VAL:O	2.20	0.41
3:G:93:ARG:HH11	3:G:134:ARG:NH1	2.19	0.41
1:3:123:PHE:O	1:3:127:VAL:HG23	2.20	0.41
2:F:210:TYR:N	2:F:210:TYR:CD1	2.89	0.41
2:F:26:ARG:HB3	2:F:159:GLY:C	2.42	0.40
1:2:73:ALA:O	1:2:104:THR:HG22	2.21	0.40
1:3:84:TYR:CD2	1:3:85:TYR:HE1	2.39	0.40
1:2:79:ALA:HA	1:2:124:THR:HG22	2.03	0.40
2:F:310:TYR:O	2:F:314:ALA:CB	2.70	0.40
3:G:18:LEU:HD23	3:G:19:VAL:N	2.35	0.40
1:1:86:VAL:HG11	1:1:94:ALA:HB2	2.03	0.40
2:F:230:ALA:O	2:F:232:ASN:CG	2.59	0.40
2:F:55:ARG:HH11	2:F:366:GLU:CG	2.32	0.40
1:3:42:VAL:CG1	1:3:43:TRP:N	2.81	0.40
2:F:9:ARG:NH2	2:F:40:SER:CB	2.84	0.40
1:4:140:GLU:O	1:4:141:ASN:C	2.58	0.40
1:4:20:LEU:O	1:4:20:LEU:HG	2.21	0.40
1:4:10:ARG:O	1:4:11:PHE:C	2.60	0.40
1:4:23:ALA:O	1:4:24:SER:C	2.58	0.40
4:B:67:ILE:HD13	4:B:67:ILE:HG21	1.85	0.40
2:F:67:PHE:HD1	2:F:67:PHE:H	1.67	0.40
4:B:71:LYS:NZ	4:B:92:ALA:O	2.49	0.40
2:F:420:ARG:C	2:F:422:SER:N	2.74	0.40
2:F:216:ARG:O	2:F:217:ASP:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:315:GLY:HA2	2:F:320:TYR:OH	2.22	0.40
2:F:280:HIS:N	2:F:280:HIS:ND1	2.69	0.40
3:G:30:PRO:O	3:G:57:LEU:HD22	2.22	0.40
1:4:74:PRO:O	1:4:77:PHE:HB2	2.22	0.40
1:1:104:THR:O	1:1:107:ILE:HB	2.22	0.40
1:1:71:PHE:CD2	1:2:96:LEU:CD2	3.04	0.40
2:F:70:TYR:CD1	2:F:283:MET:HE3	2.57	0.40
1:2:32:ASP:N	1:2:32:ASP:OD1	2.52	0.40
2:F:128:LEU:HD23	2:F:128:LEU:HA	1.90	0.40
1:3:115:VAL:HG13	1:3:116:LYS:O	2.21	0.40
2:F:123:LEU:HG	2:F:123:LEU:O	2.22	0.40
1:2:104:THR:HB	1:2:115:VAL:HG23	2.03	0.40
3:G:107:TYR:N	3:G:107:TYR:CD2	2.90	0.40
3:G:56:PHE:CE1	3:G:146:VAL:CG2	3.05	0.40
1:3:48:ARG:CG	1:3:48:ARG:NH1	2.63	0.40
1:1:145:LYS:CG	1:1:145:LYS:O	2.70	0.40
1:2:50:ARG:HG3	1:2:53:ARG:NH2	2.37	0.40
2:F:207:GLU:C	2:F:209:ASP:N	2.75	0.40
2:F:12:HIS:ND1	2:F:12:HIS:N	2.69	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	141/152 (93%)	96 (68%)	33 (23%)	12 (8%)	1 13
1	2	133/152 (88%)	81 (61%)	39 (29%)	13 (10%)	1 10
1	3	138/152 (91%)	97 (70%)	28 (20%)	13 (9%)	1 10
1	4	144/152 (95%)	89 (62%)	44 (31%)	11 (8%)	1 15
2	F	424/426 (100%)	314 (74%)	71 (17%)	39 (9%)	1 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	G	173/175 (99%)	143 (83%)	19 (11%)	11 (6%)	2 20
4	B	64/120 (53%)	48 (75%)	12 (19%)	4 (6%)	2 21
All	All	1217/1329 (92%)	868 (71%)	246 (20%)	103 (8%)	1 13

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	GLU
1	2	8	SER
1	2	9	VAL
1	2	12	GLN
1	2	23	ALA
1	2	24	SER
1	2	25	ALA
1	2	39	SER
1	2	48	ARG
1	2	71	PHE
1	3	39	SER
1	3	99	GLU
1	4	48	ARG
1	4	69	PRO
1	4	100	GLY
1	4	133	ASP
1	4	134	VAL
2	F	5	THR
2	F	7	ALA
2	F	78	GLY
2	F	89	VAL
2	F	160	PHE
2	F	189	SER
2	F	208	ARG
2	F	212	MET
2	F	213	GLN
2	F	254	GLN
2	F	330	MET
2	F	347	GLU
2	F	377	GLY
3	G	33	GLN
3	G	37	ALA
3	G	86	LYS
3	G	113	ASN

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Mol	Chain	Res	Type
4	B	7	ASN
1	1	10	ARG
1	1	24	SER
1	1	36	PHE
1	1	39	SER
1	1	48	ARG
1	1	61	GLY
1	1	117	ALA
1	2	10	ARG
1	3	26	VAL
1	3	48	ARG
1	3	66	VAL
1	3	100	GLY
1	3	105	GLU
1	3	106	ASN
1	3	136	THR
1	3	142	VAL
1	4	22	GLN
2	F	3	ILE
2	F	103	ILE
2	F	206	GLN
2	F	231	ASP
2	F	258	GLY
2	F	363	HIS
2	F	372	GLN
3	G	32	LEU
3	G	164	VAL
4	B	83	CYS
4	B	85	ASP
1	1	12	GLN
1	1	34	PHE
1	2	22	GLN
1	4	117	ALA
2	F	307	ALA
2	F	375	PRO
2	F	379	LEU
3	G	25	PRO
3	G	34	THR
3	G	68	ALA
4	B	96	LYS
1	1	22	GLN
1	1	136	THR

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Mol	Chain	Res	Type
1	2	13	THR
1	4	15	LEU
2	F	6	GLY
2	F	153	GLN
2	F	274	ARG
1	4	99	GLU
1	4	107	ILE
2	F	8	GLU
2	F	105	HIS
2	F	175	PRO
2	F	207	GLU
2	F	325	PRO
2	F	349	GLN
2	F	425	THR
1	2	117	ALA
1	3	20	LEU
1	3	22	GLN
1	4	59	VAL
2	F	11	PRO
2	F	148	PRO
3	G	46	SER
2	F	293	PRO
2	F	328	ILE
2	F	360	PRO
3	G	136	PRO
2	F	369	PRO
1	3	81	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	119/127 (94%)	83 (70%)	36 (30%)	0 3
1	2	112/127 (88%)	77 (69%)	35 (31%)	0 3
1	3	117/127 (92%)	75 (64%)	42 (36%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	4	121/127 (95%)	85 (70%)	36 (30%)	0 3
2	F	372/372 (100%)	252 (68%)	120 (32%)	0 2
3	G	153/153 (100%)	106 (69%)	47 (31%)	0 3
4	B	58/101 (57%)	43 (74%)	15 (26%)	0 4
All	All	1052/1134 (93%)	721 (68%)	331 (32%)	0 3

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	6	GLU
1	1	7	GLN
1	1	9	VAL
1	1	11	PHE
1	1	13	THR
1	1	19	LYS
1	1	26	VAL
1	1	27	LEU
1	1	30	THR
1	1	32	ASP
1	1	35	ASP
1	1	37	LEU
1	1	39	SER
1	1	44	ILE
1	1	50	ARG
1	1	62	THR
1	1	63	LEU
1	1	70	ARG
1	1	87	HIS
1	1	89	VAL
1	1	92	GLN
1	1	93	THR
1	1	97	ILE
1	1	108	ILE
1	1	115	VAL
1	1	116	LYS
1	1	120	LEU
1	1	125	LEU
1	1	132	THR
1	1	135	LEU
1	1	139	GLU
1	1	143	ARG

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Mol	Chain	Res	Type
1	1	144	GLN
1	1	145	LYS
1	1	146	LEU
1	1	147	ARG
1	2	6	GLU
1	2	7	GLN
1	2	17	SER
1	2	19	LYS
1	2	20	LEU
1	2	21	ILE
1	2	22	GLN
1	2	26	VAL
1	2	27	LEU
1	2	30	THR
1	2	32	ASP
1	2	36	PHE
1	2	49	SER
1	2	50	ARG
1	2	62	THR
1	2	77	PHE
1	2	86	VAL
1	2	93	THR
1	2	96	LEU
1	2	102	GLU
1	2	104	THR
1	2	105	GLU
1	2	108	ILE
1	2	109	ASN
1	2	113	ARG
1	2	116	LYS
1	2	124	THR
1	2	125	LEU
1	2	126	ARG
1	2	128	ARG
1	2	133	ASP
1	2	135	LEU
1	2	136	THR
1	2	137	ASP
1	2	139	GLU
1	3	5	THR
1	3	6	GLU
1	3	7	GLN

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Mol	Chain	Res	Type
1	3	8	SER
1	3	15	LEU
1	3	20	LEU
1	3	28	ASP
1	3	30	THR
1	3	31	GLU
1	3	32	ASP
1	3	36	PHE
1	3	37	LEU
1	3	39	SER
1	3	40	ASN
1	3	44	ILE
1	3	48	ARG
1	3	59	VAL
1	3	62	THR
1	3	63	LEU
1	3	65	PHE
1	3	70	ARG
1	3	71	PHE
1	3	82	ILE
1	3	89	VAL
1	3	91	ILE
1	3	93	THR
1	3	98	MET
1	3	102	GLU
1	3	104	THR
1	3	105	GLU
1	3	106	ASN
1	3	107	ILE
1	3	108	ILE
1	3	113	ARG
1	3	125	LEU
1	3	126	ARG
1	3	133	ASP
1	3	135	LEU
1	3	136	THR
1	3	139	GLU
1	3	143	ARG
1	3	144	GLN
1	4	7	GLN
1	4	9	VAL
1	4	17	SER

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Mol	Chain	Res	Type
1	4	18	ILE
1	4	21	ILE
1	4	24	SER
1	4	27	LEU
1	4	30	THR
1	4	35	ASP
1	4	36	PHE
1	4	37	LEU
1	4	38	THR
1	4	39	SER
1	4	40	ASN
1	4	48	ARG
1	4	52	ARG
1	4	55	VAL
1	4	59	VAL
1	4	78	ILE
1	4	82	ILE
1	4	89	VAL
1	4	97	ILE
1	4	105	GLU
1	4	109	ASN
1	4	111	VAL
1	4	119	GLU
1	4	120	LEU
1	4	123	PHE
1	4	124	THR
1	4	126	ARG
1	4	128	ARG
1	4	133	ASP
1	4	134	VAL
1	4	136	THR
1	4	143	ARG
1	4	152	MET
2	F	2	ASN
2	F	3	ILE
2	F	4	GLN
2	F	9	ARG
2	F	10	MET
2	F	15	SER
2	F	20	LEU
2	F	23	GLN
2	F	24	ILE

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Mol	Chain	Res	Type
2	F	28	ILE
2	F	35	VAL
2	F	40	SER
2	F	50	ARG
2	F	54	LEU
2	F	55	ARG
2	F	58	LEU
2	F	62	SER
2	F	63	THR
2	F	74	ARG
2	F	86	LYS
2	F	89	VAL
2	F	94	LEU
2	F	96	THR
2	F	97	VAL
2	F	98	ASN
2	F	100	THR
2	F	105	HIS
2	F	108	PHE
2	F	111	THR
2	F	118	LYS
2	F	136	LYS
2	F	144	THR
2	F	145	GLU
2	F	147	ASN
2	F	153	GLN
2	F	163	CYS
2	F	166	LYS
2	F	170	THR
2	F	176	GLU
2	F	177	THR
2	F	179	LEU
2	F	181	ARG
2	F	182	GLN
2	F	183	MET
2	F	184	THR
2	F	185	THR
2	F	186	SER
2	F	187	THR
2	F	190	ILE
2	F	195	LEU
2	F	202	LEU

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Mol	Chain	Res	Type
2	F	204	THR
2	F	206	GLN
2	F	212	MET
2	F	215	TYR
2	F	216	ARG
2	F	219	ILE
2	F	220	SER
2	F	225	LYS
2	F	233	ARG
2	F	235	LEU
2	F	236	LEU
2	F	238	MET
2	F	241	ASN
2	F	247	TYR
2	F	249	VAL
2	F	252	THR
2	F	253	ASP
2	F	257	LEU
2	F	259	GLN
2	F	261	SER
2	F	263	ARG
2	F	267	THR
2	F	268	TYR
2	F	275	PHE
2	F	277	VAL
2	F	280	HIS
2	F	283	MET
2	F	285	THR
2	F	286	LEU
2	F	294	THR
2	F	296	THR
2	F	302	LEU
2	F	309	THR
2	F	312	ASP
2	F	313	ILE
2	F	322	ASN
2	F	323	LEU
2	F	326	ARG
2	F	327	GLU
2	F	331	LYS
2	F	333	VAL
2	F	336	SER

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Mol	Chain	Res	Type
2	F	339	SER
2	F	340	SER
2	F	341	LYS
2	F	342	LYS
2	F	345	ILE
2	F	350	TRP
2	F	356	SER
2	F	364	LEU
2	F	366	GLU
2	F	385	ILE
2	F	386	ARG
2	F	392	GLN
2	F	393	CYS
2	F	394	PHE
2	F	395	GLN
2	F	399	LEU
2	F	403	ASN
2	F	404	SER
2	F	405	GLN
2	F	406	VAL
2	F	411	THR
2	F	414	ARG
2	F	418	THR
2	F	419	THR
2	F	420	ARG
2	F	422	SER
2	F	425	THR
3	G	1	MET
3	G	2	PHE
3	G	6	ILE
3	G	10	ASN
3	G	13	PHE
3	G	18	LEU
3	G	20	LEU
3	G	22	SER
3	G	27	SER
3	G	32	LEU
3	G	36	LYS
3	G	38	THR
3	G	41	THR
3	G	44	PHE
3	G	45	ASP

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Mol	Chain	Res	Type
3	G	46	SER
3	G	49	VAL
3	G	57	LEU
3	G	60	ILE
3	G	62	MET
3	G	64	THR
3	G	75	VAL
3	G	86	LYS
3	G	91	LEU
3	G	92	VAL
3	G	95	GLU
3	G	98	SER
3	G	102	THR
3	G	105	THR
3	G	109	VAL
3	G	113	ASN
3	G	115	ARG
3	G	122	THR
3	G	127	VAL
3	G	135	THR
3	G	149	ASN
3	G	151	THR
3	G	158	LEU
3	G	159	VAL
3	G	161	LEU
3	G	163	GLN
3	G	164	VAL
3	G	165	ILE
3	G	166	LYS
3	G	169	ILE
3	G	171	LEU
3	G	175	LYS
4	B	7	ASN
4	B	8	GLN
4	B	64	ARG
4	B	76	ARG
4	B	82	THR
4	B	83	CYS
4	B	84	ASP
4	B	89	GLN
4	B	93	ARG
4	B	96	LYS

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Mol	Chain	Res	Type
4	B	99	TRP
4	B	100	ARG
4	B	102	GLN
4	B	114	VAL
4	B	116	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	12	GLN
1	1	22	GLN
1	1	106	ASN
1	1	141	ASN
1	2	7	GLN
1	2	22	GLN
1	2	90	ASN
1	2	109	ASN
1	4	40	ASN
1	4	106	ASN
1	4	109	ASN
2	F	23	GLN
2	F	73	HIS
2	F	75	HIS
2	F	80	GLN
2	F	270	HIS
2	F	322	ASN
2	F	372	GLN
2	F	387	HIS
2	F	395	GLN
2	F	401	GLN
2	F	403	ASN
2	F	405	GLN
3	G	3	GLN
3	G	10	ASN
3	G	70	ASN
3	G	149	ASN
4	B	3	GLN
4	B	89	GLN
4	B	102	GLN
4	B	110	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	143/152 (94%)	-0.18	4 (2%) 56 46	3, 23, 72, 90	0
1	2	135/152 (88%)	-0.15	2 (1%) 76 67	5, 24, 86, 100	0
1	3	140/152 (92%)	-0.18	4 (2%) 55 45	4, 24, 87, 96	0
1	4	146/152 (96%)	-0.07	3 (2%) 67 58	4, 26, 82, 100	0
2	F	426/426 (100%)	-0.25	2 (0%) 91 88	2, 8, 61, 92	0
3	G	175/175 (100%)	-0.13	0 100 100	2, 15, 32, 44	0
4	B	68/120 (56%)	0.37	4 (5%) 26 20	7, 44, 79, 98	0
All	All	1233/1329 (92%)	-0.15	19 (1%) 76 67	2, 18, 76, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	3	144	GLN	6.7
1	1	6	GLU	3.7
1	4	106	ASN	3.7
4	B	2	GLU	3.5
1	4	108	ILE	3.3
1	1	148	ALA	3.3
1	3	143	ARG	3.0
1	4	101	ALA	2.8
1	1	146	LEU	2.5
4	B	8	GLN	2.5
1	2	6	GLU	2.5
1	3	141	ASN	2.4
4	B	80	GLY	2.3
4	B	1	MET	2.2
1	3	140	GLU	2.2
2	F	1	SER	2.2
2	F	420	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	1	144	GLN	2.1
1	2	28	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.