Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 10:10 PM EDT

PDB ID	:	3D87
Title	:	Crystal structure of Interleukin-23
Authors	:	Beyer, B.M.; Ingram, R.; Ramanathan, L.; Reichert, P.; Le, H.; Madison, V.
Deposited on	:	2008-05-22
Resolution	:	2.90 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 (1)) were used in the production of this report:

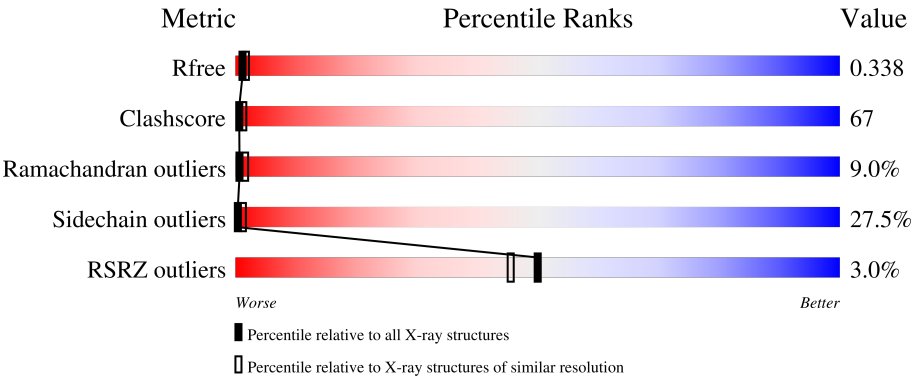
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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% 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	A	178	3% 24% 44% 20% • 10%
1	C	178	7% 20% 40% 25% • 11%
2	B	306	% 28% 50% 19% • •
2	D	306	2% 24% 50% 22% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	5001	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7104 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 Interleukin-23 subunit p19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1227	781	222	218	6			
1	C	159	Total	C	N	O	S	0	0	0
			1190	757	213	215	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q9NPF7
A	172	SER	-	expression tag	UNP Q9NPF7
A	173	HIS	-	expression tag	UNP Q9NPF7
A	174	HIS	-	expression tag	UNP Q9NPF7
A	175	HIS	-	expression tag	UNP Q9NPF7
A	176	HIS	-	expression tag	UNP Q9NPF7
A	177	HIS	-	expression tag	UNP Q9NPF7
A	178	HIS	-	expression tag	UNP Q9NPF7
C	171	GLY	-	expression tag	UNP Q9NPF7
C	172	SER	-	expression tag	UNP Q9NPF7
C	173	HIS	-	expression tag	UNP Q9NPF7
C	174	HIS	-	expression tag	UNP Q9NPF7
C	175	HIS	-	expression tag	UNP Q9NPF7
C	176	HIS	-	expression tag	UNP Q9NPF7
C	177	HIS	-	expression tag	UNP Q9NPF7
C	178	HIS	-	expression tag	UNP Q9NPF7

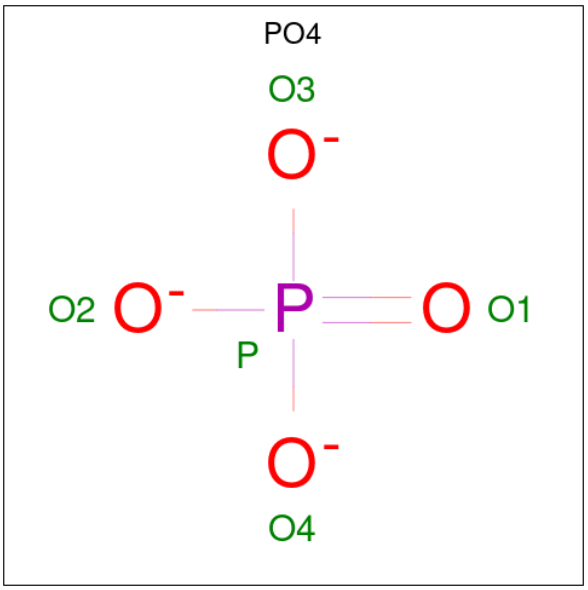
- Molecule 2 is a protein called Interleukin-12 subunit p40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2343	1481	382	468	12			
2	D	296	Total	C	N	O	S	0	0	0
			2321	1470	374	465	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	200	GLN	ASN	engineered mutation	UNP P29460
D	200	GLN	ASN	engineered mutation	UNP P29460

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

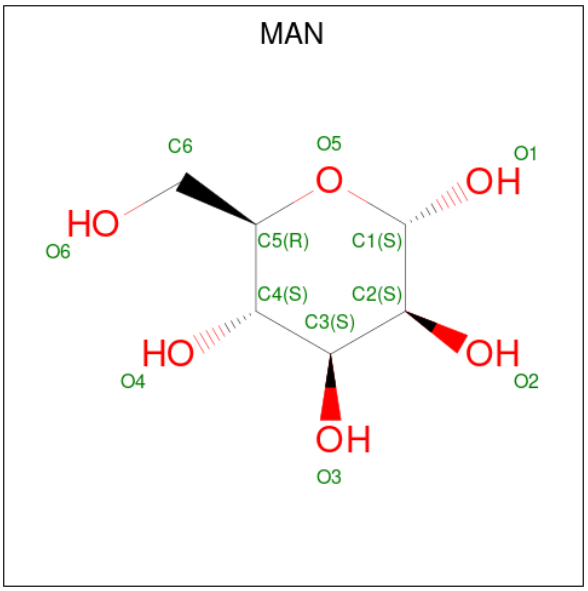


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



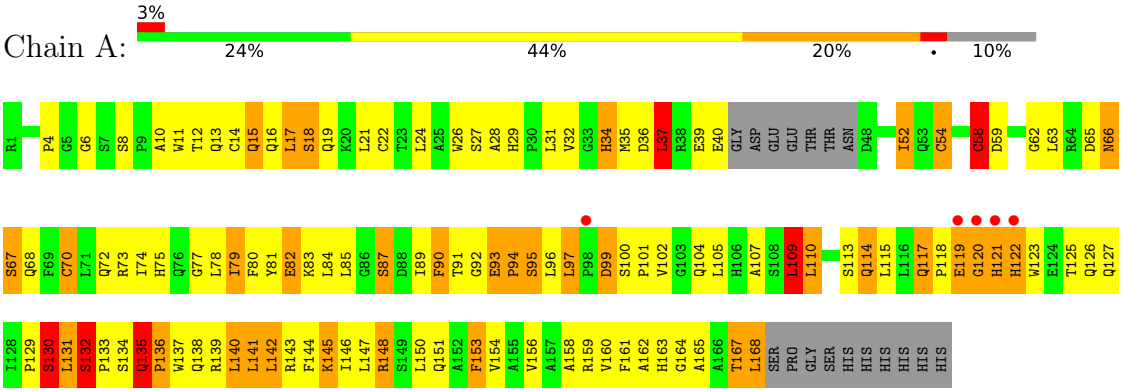
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 11 6 5	0	0

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 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.

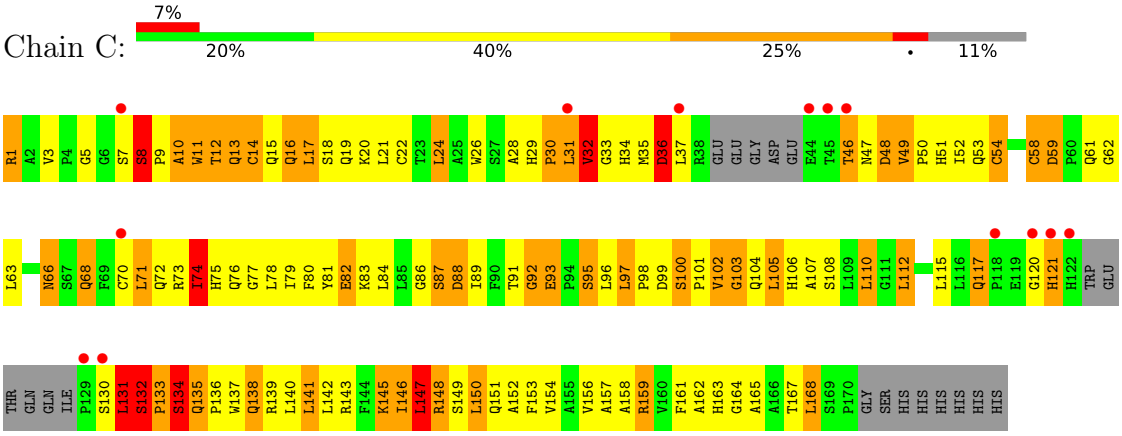
• Molecule 1: Interleukin-23 subunit p19

Chain A:



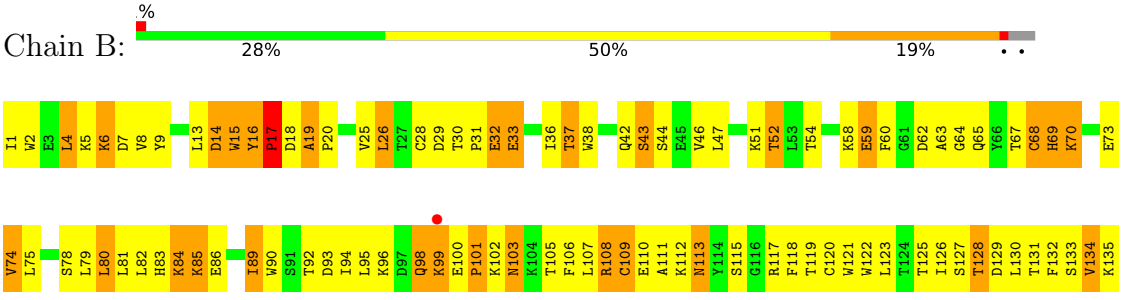
• Molecule 1: Interleukin-23 subunit p19

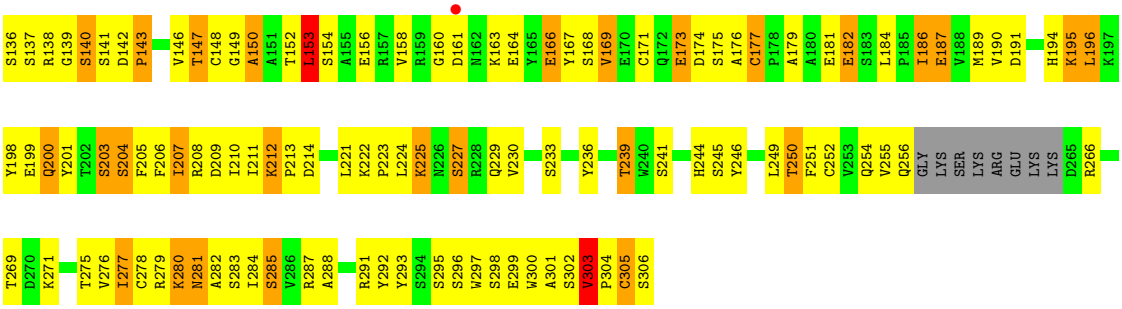
Chain C:



• Molecule 2: Interleukin-12 subunit p40

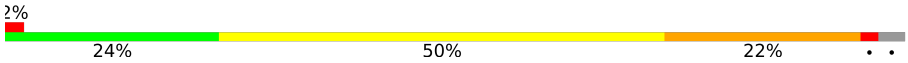
Chain B:

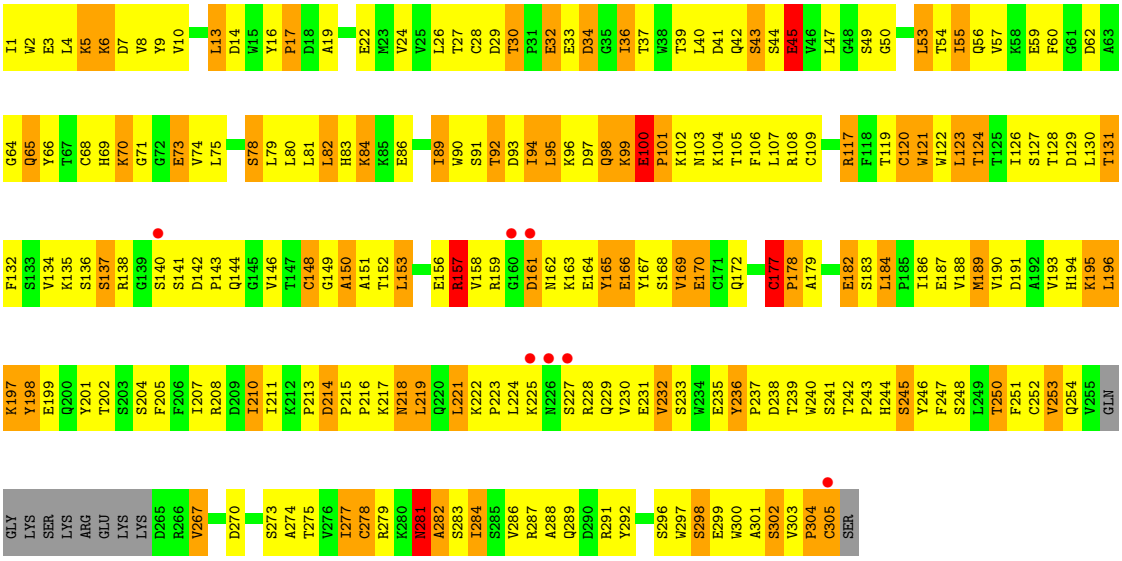




• Molecule 2: Interleukin-12 subunit p40

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.10Å 240.59Å 141.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.39 – 2.90 19.52 – 2.81	Depositor EDS
% Data completeness (in resolution range)	93.5 (20.39-2.90) 88.3 (19.52-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	7.34 (at 2.79Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.268 , 0.323 0.269 , 0.338	Depositor DCC
R_{free} test set	837 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å^2)	65.0	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7104	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, PO4, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.65	1/1260 (0.1%)	1.04	5/1716 (0.3%)
1	C	0.61	0/1220	0.96	4/1662 (0.2%)
2	B	0.77	0/2401	0.98	3/3270 (0.1%)
2	D	0.66	0/2379	0.94	8/3242 (0.2%)
All	All	0.69	1/7260 (0.0%)	0.98	20/9890 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	CYS	CB-SG	-5.63	1.72	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	177	CYS	C-N-CD	-14.77	88.10	120.60
1	A	135	GLN	C-N-CD	-13.91	90.01	120.60
1	A	93	GLU	C-N-CD	-9.36	100.01	120.60
1	C	8	SER	C-N-CD	-8.47	101.97	120.60
2	B	303	VAL	C-N-CD	-8.27	102.41	120.60
2	D	19	ALA	C-N-CD	-7.78	103.48	120.60
1	C	147	LEU	CA-CB-CG	-7.28	98.56	115.30
2	D	236	TYR	C-N-CD	6.99	143.09	128.40
2	B	14	ASP	N-CA-C	-6.82	92.59	111.00
2	D	100	GLU	C-N-CA	-6.39	95.14	122.00
2	B	153	LEU	N-CA-C	-6.14	94.41	111.00
1	A	132	SER	C-N-CD	-6.08	107.24	120.60
1	C	117	GLN	C-N-CD	-5.93	107.54	120.60
1	A	37	LEU	CA-CB-CG	5.77	128.57	115.30
1	C	134	SER	N-CA-C	-5.62	95.82	111.00
2	D	214	ASP	C-N-CD	-5.60	108.28	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	45	GLU	N-CA-C	-5.48	96.22	111.00
2	D	53	LEU	CA-CB-CG	-5.32	103.06	115.30
2	D	82	LEU	CA-CB-CG	-5.23	103.27	115.30
1	A	6	GLY	N-CA-C	5.22	126.14	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1227	0	1201	202	0
1	C	1190	0	1158	200	1
2	B	2343	0	2230	254	0
2	D	2321	0	2199	309	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	D	11	0	10	1	0
All	All	7104	0	6798	927	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 67.

All (927) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLN:NE2	1:C:137:TRP:HE1	1.43	1.15
2:D:126:ILE:HG21	2:D:130:LEU:HD21	1.29	1.14
1:A:35:MET:HE3	1:A:145:LYS:HE3	1.32	1.11
2:B:173:GLU:HG2	2:B:176:ALA:HB2	1.22	1.11
2:D:123:LEU:HD13	2:D:164:GLU:HG2	1.30	1.11
1:A:15:GLN:HG2	1:A:162:ALA:HA	1.35	1.09
2:D:92:THR:HG22	2:D:201:TYR:HE2	1.21	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ASP:HB3	1:C:37:LEU:HA	1.03	1.02
2:D:100:GLU:HB3	2:D:101:PRO:HD3	1.35	1.02
2:B:19:ALA:HB1	2:B:20:PRO:HD2	1.42	1.02
1:C:88:ASP:HA	1:C:91:THR:HB	1.39	1.02
1:A:132:SER:HB3	1:A:133:PRO:HA	1.43	1.00
1:C:36:ASP:HB3	1:C:37:LEU:CA	1.93	0.98
2:D:283:SER:HB3	2:D:304:PRO:HA	1.44	0.98
1:C:8:SER:HB2	1:C:9:PRO:HA	1.45	0.97
2:D:207:ILE:HA	2:D:210:ILE:HD13	1.46	0.97
2:B:16:TYR:CD1	2:B:17:PRO:HD2	2.00	0.96
2:B:16:TYR:CG	2:B:17:PRO:HD2	1.99	0.96
1:C:36:ASP:CB	1:C:37:LEU:HA	1.96	0.96
1:C:12:THR:HG22	1:C:16:GLN:HE22	1.30	0.95
2:B:208:ARG:HD2	2:B:293:TYR:CZ	2.02	0.95
1:A:36:ASP:HB3	1:A:37:LEU:HB2	1.47	0.94
1:C:164:GLY:HA2	1:C:168:LEU:HG	1.47	0.93
1:C:52:ILE:HG21	1:C:156:VAL:HG11	1.50	0.93
2:D:95:LEU:HD11	2:D:122:TRP:HB2	1.46	0.93
2:D:92:THR:HG22	2:D:201:TYR:CE2	2.03	0.93
2:D:187:GLU:HB3	2:D:189:MET:CE	1.99	0.92
2:D:282:ALA:HB2	5:D:1281:MAN:C1	2.00	0.91
2:D:100:GLU:HB3	2:D:101:PRO:CD	2.00	0.91
1:A:85:LEU:HD21	1:A:105:LEU:HD23	1.53	0.91
2:D:253:VAL:HA	2:D:286:VAL:HG22	1.50	0.90
1:C:8:SER:HB2	1:C:9:PRO:CA	2.01	0.90
2:B:100:GLU:C	2:B:102:LYS:HA	1.91	0.89
1:A:136:PRO:HA	1:A:139:ARG:HB3	1.54	0.89
2:D:36:ILE:H	2:D:36:ILE:HD12	1.37	0.89
1:C:19:GLN:HE22	2:D:291:ARG:HD3	1.35	0.89
2:D:219:LEU:HB2	2:D:303:VAL:CG2	2.03	0.89
1:A:66:ASN:HD22	1:A:67:SER:H	1.18	0.88
1:A:96:LEU:HD11	1:C:32:VAL:HG11	1.55	0.88
2:B:255:VAL:HG23	2:B:256:GLN:H	1.37	0.88
2:B:283:SER:HB3	2:B:304:PRO:HA	1.56	0.88
2:D:70:LYS:HB3	2:D:75:LEU:HD11	1.55	0.88
1:A:66:ASN:HD22	1:A:68:GLN:H	1.21	0.88
1:A:93:GLU:HA	1:A:95:SER:N	1.88	0.87
1:C:84:LEU:HD13	1:C:146:ILE:HG12	1.58	0.86
1:A:117:GLN:HA	1:A:117:GLN:NE2	1.90	0.85
2:D:117:ARG:NH1	2:D:170:GLU:HG3	1.91	0.85
2:B:134:VAL:CG2	2:B:190:VAL:HG22	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HD21	1:C:32:VAL:HG12	1.58	0.85
1:A:138:GLN:HG2	1:C:137:TRP:CD1	2.12	0.85
2:D:126:ILE:HG21	2:D:130:LEU:CD2	2.07	0.84
1:A:163:HIS:O	1:A:167:THR:HG23	1.77	0.84
1:A:135:GLN:NE2	1:A:138:GLN:HG3	1.93	0.84
2:D:219:LEU:HB2	2:D:303:VAL:HG21	1.59	0.83
1:A:85:LEU:HD21	1:A:105:LEU:CD2	2.06	0.83
1:A:97:LEU:HD13	1:A:97:LEU:H	1.41	0.83
1:C:1:ARG:HG3	1:C:1:ARG:HH11	1.43	0.83
2:D:13:LEU:CD2	2:D:82:LEU:HD22	2.08	0.83
2:D:284:ILE:HD12	2:D:284:ILE:H	1.43	0.83
1:A:24:LEU:HD21	1:A:104:GLN:HB2	1.58	0.82
2:B:282:ALA:O	2:B:305:CYS:HB2	1.79	0.82
2:B:108:ARG:HG2	2:B:108:ARG:HH11	1.45	0.82
2:D:53:LEU:HD12	2:D:54:THR:N	1.94	0.82
2:D:32:GLU:HG2	2:D:70:LYS:HZ1	1.43	0.81
2:D:53:LEU:HD12	2:D:54:THR:H	1.45	0.81
1:A:11:TRP:HB3	1:A:165:ALA:HA	1.61	0.81
1:A:93:GLU:HA	1:A:95:SER:H	1.46	0.81
1:A:150:LEU:O	1:A:154:VAL:HG22	1.80	0.81
2:B:138:ARG:CZ	2:B:186:ILE:HD11	2.11	0.80
1:A:138:GLN:HG2	1:C:137:TRP:HD1	1.43	0.80
1:C:1:ARG:HD2	1:C:1:ARG:N	1.97	0.80
1:C:82:GLU:OE2	1:C:110:LEU:HG	1.82	0.80
1:A:63:LEU:HD11	1:A:160:VAL:HG13	1.62	0.79
2:D:253:VAL:HB	2:D:267:VAL:HG13	1.64	0.79
1:A:36:ASP:CB	1:A:37:LEU:HB2	2.12	0.79
1:C:163:HIS:ND1	2:D:245:SER:HB2	1.97	0.79
2:B:98:GLN:O	2:B:101:PRO:HD3	1.83	0.78
1:C:88:ASP:O	1:C:92:GLY:N	2.16	0.78
2:B:107:LEU:HD11	2:B:201:TYR:HB3	1.65	0.78
2:D:250:THR:HG22	2:D:291:ARG:HA	1.65	0.78
1:C:12:THR:HG22	1:C:16:GLN:NE2	1.98	0.78
2:D:250:THR:CG2	2:D:291:ARG:HA	2.14	0.78
2:D:24:VAL:HG11	2:D:80:LEU:HD11	1.66	0.78
2:D:221:LEU:HB2	2:D:230:VAL:HG11	1.63	0.78
2:B:137:SER:HA	2:B:146:VAL:HG23	1.65	0.78
1:C:168:LEU:HD23	1:C:168:LEU:N	1.98	0.78
2:D:73:GLU:HA	2:D:73:GLU:OE1	1.82	0.78
2:D:95:LEU:HD11	2:D:122:TRP:CB	2.14	0.78
2:D:219:LEU:CD2	2:D:303:VAL:HG23	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:GLU:HG2	2:B:176:ALA:CB	2.09	0.77
1:C:52:ILE:CG2	1:C:156:VAL:HG11	2.14	0.77
2:D:231:GLU:CG	2:D:275:THR:HG22	2.13	0.77
1:C:49:VAL:HB	1:C:80:PHE:CE2	2.20	0.77
1:A:19:GLN:HE22	2:B:291:ARG:HD3	1.49	0.77
1:A:117:GLN:HA	1:A:117:GLN:HE21	1.49	0.77
2:D:214:ASP:OD2	2:D:239:THR:HG21	1.85	0.76
1:A:163:HIS:CE1	1:A:167:THR:HG21	2.21	0.76
1:C:93:GLU:H	1:C:139:ARG:NH1	1.84	0.76
2:B:19:ALA:HB1	2:B:20:PRO:CD	2.16	0.76
1:C:132:SER:CB	1:C:133:PRO:HA	2.15	0.76
2:D:187:GLU:HB3	2:D:189:MET:HE1	1.65	0.76
2:D:283:SER:CB	2:D:304:PRO:HA	2.15	0.76
1:A:134:SER:O	1:A:135:GLN:HG3	1.86	0.76
1:C:49:VAL:HG21	1:C:81:TYR:OH	1.84	0.76
2:B:70:LYS:HB2	2:B:75:LEU:HD11	1.68	0.75
2:D:60:PHE:CE1	2:D:84:LYS:HE2	2.20	0.75
2:D:134:VAL:O	2:D:135:LYS:HD3	1.87	0.75
1:A:142:LEU:HD13	1:A:146:ILE:HD11	1.69	0.75
2:D:120:CYS:O	2:D:168:SER:HA	1.86	0.75
1:A:75:HIS:CE1	1:A:117:GLN:HB2	2.22	0.74
2:B:223:PRO:HA	2:B:230:VAL:HG12	1.69	0.74
2:D:64:GLY:O	2:D:79:LEU:HD12	1.88	0.74
1:A:15:GLN:NE2	1:A:162:ALA:HB2	2.01	0.74
2:D:41:ASP:HB3	2:D:42:GLN:OE1	1.85	0.74
1:A:52:ILE:HG22	1:A:58:CYS:SG	2.28	0.74
1:A:150:LEU:CD1	1:A:154:VAL:HG13	2.18	0.73
1:C:139:ARG:O	1:C:143:ARG:HG3	1.88	0.73
2:D:95:LEU:HD21	2:D:122:TRP:HB2	1.70	0.73
1:A:93:GLU:HG2	1:C:34:HIS:CE1	2.23	0.73
2:B:153:LEU:HB2	2:B:167:TYR:CE2	2.23	0.73
2:B:101:PRO:N	2:B:102:LYS:HA	2.00	0.73
2:D:286:VAL:HA	2:D:300:TRP:HZ3	1.53	0.73
1:C:1:ARG:HG3	1:C:1:ARG:NH1	2.02	0.73
1:A:89:ILE:HG22	1:A:90:PHE:CD1	2.23	0.73
2:B:101:PRO:HD2	2:B:105:THR:OG1	1.87	0.73
1:C:112:LEU:O	1:C:112:LEU:HD12	1.88	0.73
1:A:79:ILE:HD11	1:A:113:SER:HB3	1.71	0.73
2:B:63:ALA:HB1	2:B:80:LEU:O	1.89	0.73
2:D:117:ARG:HH12	2:D:170:GLU:HG3	1.53	0.73
2:B:100:GLU:CA	2:B:103:ASN:H	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:ILE:HA	2:D:69:HIS:O	1.88	0.72
2:B:158:VAL:HG12	2:B:160:GLY:H	1.53	0.72
2:D:3:GLU:HG3	2:D:9:TYR:CE2	2.24	0.72
2:D:32:GLU:HG2	2:D:70:LYS:NZ	2.04	0.72
1:A:66:ASN:ND2	1:A:68:GLN:H	1.87	0.72
2:D:70:LYS:CB	2:D:75:LEU:HD11	2.19	0.72
1:A:93:GLU:HG3	1:A:94:PRO:HA	1.71	0.72
1:C:96:LEU:HD13	1:C:102:VAL:HG21	1.70	0.72
2:D:253:VAL:HG22	2:D:286:VAL:HG21	1.72	0.72
1:A:28:ALA:HB2	1:A:34:HIS:CE1	2.25	0.71
2:B:152:THR:HG22	2:B:153:LEU:H	1.55	0.71
2:D:28:CYS:SG	2:D:68:CYS:HB3	2.30	0.71
2:D:253:VAL:HG22	2:D:286:VAL:CG2	2.20	0.71
1:A:66:ASN:ND2	1:A:67:SER:H	1.86	0.71
2:D:117:ARG:HH21	2:D:172:GLN:HB2	1.56	0.71
2:B:134:VAL:HG22	2:B:190:VAL:HG22	1.72	0.71
1:A:37:LEU:HD22	2:B:206:PHE:HE1	1.55	0.71
2:B:134:VAL:HG12	2:B:148:CYS:HB3	1.70	0.71
1:C:5:GLY:HA2	1:C:68:GLN:HG2	1.73	0.70
2:B:16:TYR:CE2	2:B:17:PRO:HG2	2.26	0.70
2:D:250:THR:HG22	2:D:291:ARG:CA	2.20	0.70
1:A:96:LEU:CD2	1:C:32:VAL:HG12	2.20	0.70
2:D:60:PHE:HE1	2:D:84:LYS:HE2	1.56	0.70
2:D:126:ILE:CG2	2:D:130:LEU:HD11	2.20	0.70
1:C:163:HIS:CE1	2:D:245:SER:HB2	2.25	0.70
2:B:108:ARG:HG2	2:B:108:ARG:NH1	2.05	0.70
1:C:74:ILE:HG22	1:C:75:HIS:N	2.05	0.70
1:A:120:GLY:C	1:A:122:HIS:H	1.94	0.70
2:D:41:ASP:N	2:D:65:GLN:O	2.25	0.70
1:A:97:LEU:HD13	1:A:97:LEU:N	2.07	0.70
1:C:91:THR:O	1:C:95:SER:HB3	1.92	0.70
1:A:35:MET:CE	1:A:145:LYS:HE3	2.18	0.70
1:A:132:SER:HB3	1:A:133:PRO:CA	2.22	0.69
1:C:12:THR:O	1:C:16:GLN:NE2	2.24	0.69
1:C:52:ILE:HG21	1:C:156:VAL:CG1	2.23	0.69
2:D:136:SER:HA	2:D:187:GLU:O	1.92	0.69
2:B:83:HIS:HD2	2:B:90:TRP:CE3	2.10	0.69
2:B:125:THR:OG1	2:B:126:ILE:HD12	1.91	0.69
1:C:1:ARG:HH11	1:C:1:ARG:CG	2.05	0.69
1:C:104:GLN:O	1:C:107:ALA:HB3	1.93	0.69
2:B:236:TYR:CD2	2:B:249:LEU:HD12	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:HA	1:A:40:GLU:CB	2.23	0.69
1:A:52:ILE:HD11	1:A:153:PHE:CE1	2.28	0.69
1:A:156:VAL:O	1:A:160:VAL:HG23	1.91	0.69
2:B:207:ILE:O	2:B:211:ILE:HG12	1.92	0.69
2:D:95:LEU:CD1	2:D:122:TRP:HB2	2.20	0.69
2:D:289:GLN:HB2	2:D:297:TRP:CD2	2.29	0.69
2:D:126:ILE:HG22	2:D:130:LEU:HD11	1.76	0.68
1:A:150:LEU:HD12	1:A:154:VAL:HG13	1.74	0.68
2:B:112:LYS:HE3	2:B:214:ASP:OD1	1.93	0.68
1:A:26:TRP:HZ2	2:B:293:TYR:CD2	2.11	0.68
1:A:18:SER:O	1:A:21:LEU:HB2	1.93	0.68
1:C:132:SER:HB3	1:C:133:PRO:HA	1.75	0.68
2:D:98:GLN:O	2:D:100:GLU:N	2.27	0.68
1:A:132:SER:CB	1:A:133:PRO:HA	2.22	0.68
1:C:52:ILE:HG23	1:C:58:CYS:SG	2.32	0.68
2:D:221:LEU:HB3	2:D:232:VAL:HG13	1.76	0.68
2:D:223:PRO:HB3	2:D:230:VAL:HG22	1.76	0.68
1:A:78:LEU:O	1:A:82:GLU:HB3	1.94	0.68
2:B:98:GLN:O	2:B:100:GLU:N	2.27	0.68
1:C:102:VAL:O	1:C:105:LEU:N	2.27	0.68
2:B:37:THR:O	2:B:68:CYS:HA	1.94	0.67
2:D:283:SER:HB3	2:D:304:PRO:CA	2.23	0.67
2:D:187:GLU:HB3	2:D:189:MET:HE3	1.76	0.67
2:B:100:GLU:CB	2:B:103:ASN:H	2.07	0.67
2:B:134:VAL:HG12	2:B:148:CYS:CB	2.23	0.67
1:C:79:ILE:O	1:C:83:LYS:HG3	1.94	0.67
2:D:219:LEU:HB2	2:D:303:VAL:HG23	1.77	0.67
2:D:86:GLU:O	2:D:89:ILE:HD13	1.94	0.67
2:B:80:LEU:N	2:B:80:LEU:HD23	2.10	0.67
2:B:236:TYR:CE2	2:B:249:LEU:HD12	2.29	0.67
2:D:288:ALA:H	2:D:298:SER:HB3	1.58	0.67
1:A:137:TRP:CH2	1:C:141:LEU:HA	2.30	0.67
1:C:89:ILE:HD13	1:C:142:LEU:HD13	1.76	0.67
2:B:187:GLU:HA	2:B:203:SER:O	1.95	0.67
1:C:52:ILE:HD12	1:C:153:PHE:CE1	2.30	0.67
2:D:207:ILE:HA	2:D:210:ILE:CD1	2.25	0.67
2:B:186:ILE:HD13	2:B:186:ILE:N	2.10	0.66
2:B:256:GLN:O	2:B:282:ALA:HB1	1.95	0.66
2:D:34:ASP:N	2:D:34:ASP:OD2	2.27	0.66
2:B:280:LYS:O	2:B:281:ASN:HB2	1.94	0.66
1:C:58:CYS:HB3	1:C:70:CYS:SG	2.34	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LYS:N	2:B:62:ASP:OD1	2.19	0.66
2:B:134:VAL:HG23	2:B:190:VAL:HG22	1.77	0.66
1:C:102:VAL:O	1:C:104:GLN:N	2.28	0.66
2:B:96:LYS:NZ	2:B:164:GLU:HG3	2.10	0.66
2:D:138:ARG:HB3	2:D:144:GLN:HB2	1.77	0.66
2:B:85:LYS:HD2	2:B:90:TRP:CE2	2.31	0.66
2:D:70:LYS:O	2:D:73:GLU:HB2	1.95	0.66
2:B:205:PHE:CE1	2:B:210:ILE:HD13	2.31	0.65
2:D:37:THR:OG1	2:D:69:HIS:HB2	1.95	0.65
1:A:115:LEU:HD23	1:A:115:LEU:O	1.97	0.65
2:D:3:GLU:HG3	2:D:9:TYR:CD2	2.31	0.65
1:C:15:GLN:HG3	1:C:162:ALA:HA	1.76	0.65
2:D:36:ILE:H	2:D:36:ILE:CD1	1.97	0.65
1:A:77:GLY:HA3	1:A:153:PHE:CZ	2.32	0.65
2:B:256:GLN:O	2:B:256:GLN:HG2	1.95	0.65
2:D:248:SER:HB2	2:D:292:TYR:CE1	2.32	0.65
1:A:93:GLU:HG3	1:A:95:SER:H	1.62	0.65
2:B:152:THR:HG22	2:B:153:LEU:N	2.10	0.65
2:D:142:ASP:N	2:D:143:PRO:HD3	2.11	0.65
2:D:219:LEU:HD22	2:D:303:VAL:HG23	1.79	0.65
2:D:243:PRO:HB2	2:D:245:SER:OG	1.97	0.65
2:D:219:LEU:HD13	2:D:219:LEU:H	1.62	0.65
2:D:289:GLN:HB2	2:D:297:TRP:CE3	2.32	0.64
1:A:36:ASP:CA	1:A:37:LEU:HB2	2.27	0.64
1:C:93:GLU:N	1:C:139:ARG:NH1	2.44	0.64
1:C:117:GLN:HE21	1:C:120:GLY:CA	2.10	0.64
1:A:75:HIS:ND1	1:A:117:GLN:HB2	2.13	0.64
2:D:32:GLU:OE1	2:D:32:GLU:HA	1.97	0.64
2:B:283:SER:CB	2:B:304:PRO:HA	2.26	0.64
2:D:123:LEU:CD1	2:D:164:GLU:HG2	2.18	0.64
2:B:152:THR:O	2:B:167:TYR:HD2	1.80	0.64
2:B:191:ASP:OD1	2:B:200:GLN:NE2	2.30	0.64
2:D:241:SER:HB3	2:D:247:PHE:CD1	2.32	0.64
2:B:137:SER:CA	2:B:146:VAL:HG23	2.28	0.64
2:D:26:LEU:HG	2:D:55:ILE:HD13	1.79	0.64
2:D:13:LEU:HD21	2:D:82:LEU:HD22	1.79	0.64
1:A:10:ALA:CB	1:A:13:GLN:HB2	2.27	0.64
1:A:119:GLU:O	1:A:121:HIS:N	2.28	0.64
2:B:221:LEU:HD21	2:B:284:ILE:HD13	1.79	0.64
2:D:30:THR:HG21	2:D:75:LEU:HD22	1.78	0.64
2:B:138:ARG:HB2	2:B:186:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:PRO:HD2	1:C:80:PHE:CD2	2.33	0.64
2:D:124:THR:HG21	2:D:167:TYR:HE1	1.63	0.64
2:D:170:GLU:HA	2:D:170:GLU:OE2	1.98	0.64
1:A:11:TRP:HB3	1:A:165:ALA:CA	2.27	0.64
2:D:207:ILE:HD12	2:D:210:ILE:HD11	1.80	0.64
2:D:40:LEU:HD13	2:D:66:TYR:CE1	2.32	0.63
2:D:183:SER:O	2:D:184:LEU:HD23	1.98	0.63
1:A:13:GLN:O	1:A:16:GLN:HG2	1.99	0.63
2:B:123:LEU:HD13	2:B:164:GLU:OE2	1.98	0.63
2:D:32:GLU:C	2:D:33:GLU:HG3	2.18	0.63
2:D:221:LEU:HD12	2:D:221:LEU:H	1.63	0.63
1:C:137:TRP:HE3	1:C:138:GLN:HG2	1.64	0.63
2:D:130:LEU:O	2:D:131:THR:HG23	1.99	0.63
1:A:85:LEU:CD2	1:A:105:LEU:HD23	2.28	0.62
2:B:303:VAL:HG22	2:B:304:PRO:HD2	1.79	0.62
2:D:97:ASP:O	2:D:99:LYS:N	2.32	0.62
1:C:100:SER:C	1:C:104:GLN:HE21	2.02	0.62
2:D:236:TYR:CE2	2:D:244:HIS:HB3	2.35	0.62
2:D:122:TRP:CE2	2:D:167:TYR:HB2	2.34	0.62
1:A:164:GLY:HA2	1:A:168:LEU:HD11	1.79	0.62
1:A:13:GLN:O	1:A:17:LEU:HB2	2.00	0.62
2:B:108:ARG:HH11	2:B:108:ARG:CG	2.12	0.62
2:B:28:CYS:SG	2:B:30:THR:HG22	2.40	0.61
1:C:24:LEU:HD22	1:C:105:LEU:HA	1.81	0.61
2:D:60:PHE:HD2	2:D:196:LEU:HB3	1.65	0.61
2:D:30:THR:HG21	2:D:75:LEU:CD2	2.30	0.61
2:B:32:GLU:HG3	2:B:70:LYS:HZ2	1.65	0.61
1:A:164:GLY:HA2	1:A:168:LEU:CD1	2.30	0.61
2:B:100:GLU:O	2:B:102:LYS:HA	2.00	0.61
2:D:96:LYS:N	2:D:123:LEU:O	2.33	0.61
2:B:79:LEU:C	2:B:80:LEU:HD23	2.21	0.61
2:B:129:ASP:O	2:B:194:HIS:HA	2.00	0.61
2:D:121:TRP:HA	2:D:167:TYR:O	2.00	0.61
2:B:156:GLU:OE1	2:B:163:LYS:NZ	2.27	0.61
1:C:59:ASP:OD2	1:C:59:ASP:N	2.28	0.61
2:D:221:LEU:CB	2:D:232:VAL:HG13	2.31	0.61
2:B:140:SER:O	2:B:143:PRO:HD3	2.01	0.60
1:C:9:PRO:O	1:C:11:TRP:N	2.32	0.60
2:D:132:PHE:HB2	2:D:151:ALA:CB	2.30	0.60
1:A:136:PRO:CA	1:A:139:ARG:HB3	2.29	0.60
2:B:83:HIS:HD1	2:B:198:TYR:HE2	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ARG:HD2	2:B:293:TYR:CE2	2.36	0.60
2:D:286:VAL:HA	2:D:300:TRP:CZ3	2.34	0.60
1:C:117:GLN:HE21	1:C:120:GLY:HA2	1.65	0.60
2:D:252:CYS:O	2:D:286:VAL:HG13	2.02	0.60
1:C:137:TRP:HE3	1:C:138:GLN:N	1.99	0.60
2:B:79:LEU:HD21	2:B:81:LEU:HD21	1.82	0.60
1:A:137:TRP:CZ3	1:C:141:LEU:HA	2.36	0.60
1:C:12:THR:O	1:C:16:GLN:N	2.29	0.60
2:D:100:GLU:OE1	2:D:101:PRO:HD3	2.00	0.60
2:D:221:LEU:HB2	2:D:230:VAL:CG1	2.30	0.60
1:A:93:GLU:HG3	1:A:94:PRO:CA	2.31	0.60
1:C:49:VAL:HG23	1:C:50:PRO:O	2.01	0.60
1:C:93:GLU:O	1:C:136:PRO:HB3	2.00	0.60
2:B:255:VAL:HG23	2:B:256:GLN:N	2.13	0.60
1:C:134:SER:O	1:C:135:GLN:O	2.20	0.59
1:C:137:TRP:CE3	1:C:138:GLN:N	2.70	0.59
1:C:17:LEU:HD12	1:C:17:LEU:O	2.01	0.59
1:C:134:SER:O	1:C:138:GLN:HG3	2.02	0.59
1:A:94:PRO:O	1:A:96:LEU:HD23	2.03	0.59
2:D:93:ASP:OD2	2:D:197:LYS:NZ	2.32	0.59
1:C:101:PRO:HA	1:C:104:GLN:NE2	2.17	0.59
2:D:284:ILE:O	2:D:302:SER:HA	2.02	0.59
1:A:117:GLN:O	1:A:119:GLU:N	2.33	0.59
2:B:83:HIS:CD2	2:B:90:TRP:CE3	2.90	0.59
2:D:161:ASP:OD1	2:D:162:ASN:N	2.32	0.59
2:D:252:CYS:O	2:D:286:VAL:HG22	2.03	0.59
2:B:186:ILE:O	2:B:204:SER:HA	2.02	0.59
2:D:26:LEU:HB2	2:D:53:LEU:HB3	1.85	0.59
2:D:197:LYS:HG3	2:D:198:TYR:N	2.17	0.59
2:D:219:LEU:HD23	2:D:303:VAL:HG23	1.84	0.59
1:A:37:LEU:HD22	2:B:206:PHE:CE1	2.36	0.59
1:A:54:CYS:SG	2:B:177:CYS:HB2	2.43	0.59
1:A:79:ILE:CD1	1:A:113:SER:HB3	2.33	0.59
1:A:89:ILE:HD13	1:A:142:LEU:CD1	2.32	0.59
2:D:2:TRP:N	2:D:2:TRP:CD1	2.71	0.59
2:B:283:SER:HB3	2:B:304:PRO:CA	2.31	0.59
2:D:60:PHE:CD2	2:D:196:LEU:HB3	2.38	0.59
1:A:18:SER:O	1:A:21:LEU:N	2.36	0.58
2:B:32:GLU:HG3	2:B:70:LYS:NZ	2.18	0.58
1:C:1:ARG:HD2	1:C:1:ARG:H1	1.67	0.58
1:A:81:TYR:HA	1:A:84:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LYS:HD2	2:B:90:TRP:CZ2	2.39	0.58
2:B:149:GLY:O	2:B:150:ALA:HB3	2.02	0.58
1:C:49:VAL:HB	1:C:80:PHE:HE2	1.64	0.58
1:C:11:TRP:CE3	1:C:164:GLY:HA3	2.38	0.58
1:C:150:LEU:HD13	1:C:154:VAL:HG13	1.83	0.58
2:D:128:THR:O	2:D:129:ASP:HB2	2.03	0.58
1:C:28:ALA:HB3	1:C:105:LEU:HD21	1.86	0.58
1:A:133:PRO:O	1:A:134:SER:HB3	2.02	0.58
1:C:19:GLN:HE22	2:D:291:ARG:CD	2.13	0.58
2:D:284:ILE:HD11	2:D:303:VAL:O	2.04	0.58
2:D:117:ARG:HH12	2:D:170:GLU:HB3	1.68	0.58
1:A:119:GLU:C	1:A:121:HIS:H	2.06	0.58
1:C:19:GLN:NE2	2:D:291:ARG:HD3	2.14	0.58
1:A:135:GLN:HE22	1:C:137:TRP:HE1	0.66	0.57
2:B:285:SER:HA	2:B:301:ALA:O	2.04	0.57
2:D:16:TYR:CZ	2:D:84:LYS:HD2	2.39	0.57
1:A:120:GLY:C	1:A:122:HIS:N	2.57	0.57
2:D:94:ILE:CD1	2:D:194:HIS:HB2	2.34	0.57
2:B:110:GLU:HA	2:B:210:ILE:HB	1.86	0.57
1:C:150:LEU:HD12	1:C:150:LEU:C	2.25	0.57
2:D:165:TYR:N	2:D:165:TYR:CD1	2.72	0.57
2:B:81:LEU:HD23	2:B:196:LEU:HA	1.86	0.57
2:D:219:LEU:HA	2:D:233:SER:O	2.04	0.57
2:D:2:TRP:CE2	2:D:10:VAL:HB	2.39	0.57
1:A:35:MET:HE2	1:A:141:LEU:O	2.04	0.57
1:A:35:MET:CE	1:A:145:LYS:HB2	2.34	0.57
1:A:97:LEU:HD22	1:A:100:SER:HB3	1.85	0.57
1:A:150:LEU:HD11	1:A:154:VAL:HG13	1.86	0.57
2:B:83:HIS:HD2	2:B:90:TRP:CZ3	2.23	0.57
1:A:59:ASP:HA	2:B:179:ALA:CB	2.35	0.57
2:B:173:GLU:CG	2:B:176:ALA:HB2	2.15	0.57
2:D:219:LEU:HD21	2:D:301:ALA:C	2.25	0.57
2:B:221:LEU:HD11	2:B:284:ILE:HD13	1.87	0.56
1:C:154:VAL:HA	1:C:157:ALA:HB3	1.87	0.56
2:D:136:SER:OG	2:D:146:VAL:HG11	2.05	0.56
2:D:253:VAL:O	2:D:253:VAL:HG12	2.05	0.56
2:B:108:ARG:HG2	2:B:108:ARG:O	2.04	0.56
2:B:221:LEU:HD11	2:B:284:ILE:CD1	2.35	0.56
2:D:57:VAL:HG11	2:D:82:LEU:HD21	1.87	0.56
1:C:29:HIS:N	1:C:30:PRO:HD3	2.21	0.56
2:D:123:LEU:HD13	2:D:164:GLU:CG	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:HIS:CE1	1:A:117:GLN:CB	2.89	0.56
1:A:94:PRO:HD2	1:A:143:ARG:CZ	2.36	0.56
2:B:236:TYR:CZ	2:B:249:LEU:HB2	2.41	0.56
2:D:95:LEU:HD21	2:D:122:TRP:CB	2.35	0.56
1:A:100:SER:HB2	1:A:101:PRO:CD	2.36	0.56
2:B:287:ARG:HD2	2:B:297:TRP:HB3	1.88	0.56
2:D:44:SER:O	2:D:45:GLU:HB2	2.05	0.56
2:D:98:GLN:O	2:D:98:GLN:HG2	2.06	0.56
1:A:29:HIS:CE1	1:A:31:LEU:HB2	2.40	0.56
2:B:277:ILE:O	2:B:277:ILE:HG22	2.06	0.56
1:C:24:LEU:HD21	1:C:104:GLN:HB2	1.88	0.56
1:A:125:THR:O	1:A:125:THR:HG22	2.06	0.56
2:D:250:THR:HB	2:D:270:ASP:OD2	2.06	0.56
1:A:15:GLN:HG2	1:A:162:ALA:CA	2.23	0.56
1:C:130:SER:O	1:C:131:LEU:HB2	2.06	0.56
1:A:90:PHE:CD1	1:A:90:PHE:N	2.74	0.55
2:B:102:LYS:CB	1:C:98:PRO:HD3	2.36	0.55
2:B:230:VAL:HG23	2:B:276:VAL:CG2	2.35	0.55
2:D:36:ILE:HD12	2:D:36:ILE:N	2.15	0.55
2:D:40:LEU:HD13	2:D:66:TYR:CZ	2.41	0.55
2:D:198:TYR:C	2:D:198:TYR:CD2	2.78	0.55
1:A:100:SER:HB2	1:A:101:PRO:HD2	1.87	0.55
1:A:110:LEU:HD12	1:A:110:LEU:C	2.26	0.55
2:D:287:ARG:HD2	2:D:297:TRP:HB3	1.88	0.55
2:B:283:SER:HB2	2:B:303:VAL:O	2.06	0.55
1:C:79:ILE:HG22	1:C:83:LYS:HE3	1.88	0.55
1:C:150:LEU:C	1:C:150:LEU:CD1	2.75	0.55
2:D:117:ARG:HH12	2:D:170:GLU:CG	2.18	0.55
2:D:215:PRO:HG3	2:D:299:GLU:HB2	1.88	0.55
1:C:52:ILE:O	1:C:52:ILE:HG22	2.05	0.55
1:A:119:GLU:HA	1:A:119:GLU:OE2	2.07	0.55
1:C:14:CYS:O	1:C:18:SER:HB3	2.06	0.55
1:C:79:ILE:HD13	1:C:79:ILE:N	2.22	0.55
2:D:287:ARG:HG2	2:D:300:TRP:CZ3	2.41	0.55
1:A:26:TRP:HZ2	2:B:293:TYR:CE2	2.25	0.55
1:A:82:GLU:HA	1:A:109:LEU:HD12	1.87	0.55
1:A:140:LEU:HD22	1:A:144:PHE:HE1	1.72	0.55
1:C:59:ASP:O	1:C:63:LEU:HD12	2.07	0.55
2:D:169:VAL:HG23	2:D:170:GLU:O	2.06	0.55
2:B:126:ILE:HD12	2:B:126:ILE:N	2.22	0.55
2:D:182:GLU:HG3	2:D:208:ARG:HH11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:PHE:HZ	2:B:84:LYS:HD3	1.72	0.54
2:D:177:CYS:N	2:D:178:PRO:CD	2.70	0.54
1:A:10:ALA:HB1	1:A:13:GLN:HB2	1.89	0.54
2:B:32:GLU:CD	2:B:70:LYS:HZ1	2.09	0.54
1:C:73:ARG:O	1:C:76:GLN:HB3	2.07	0.54
1:C:137:TRP:HE3	1:C:138:GLN:CG	2.20	0.54
2:D:1:ILE:HG23	2:D:1:ILE:O	2.07	0.54
2:B:117:ARG:HA	2:B:171:CYS:O	2.07	0.54
1:C:93:GLU:N	1:C:93:GLU:OE2	2.40	0.54
2:D:219:LEU:HD13	2:D:219:LEU:N	2.22	0.54
2:D:219:LEU:N	2:D:219:LEU:CD1	2.71	0.54
2:B:126:ILE:H	2:B:126:ILE:CD1	2.20	0.54
1:A:14:CYS:O	1:A:18:SER:OG	2.25	0.54
2:B:28:CYS:SG	2:B:30:THR:CG2	2.96	0.54
2:B:67:THR:CG2	2:B:74:VAL:HG22	2.38	0.54
2:D:156:GLU:O	2:D:157:ARG:O	2.25	0.54
1:A:35:MET:HE3	1:A:145:LYS:HB2	1.89	0.54
2:B:67:THR:HG21	2:B:74:VAL:CG2	2.38	0.54
1:C:5:GLY:CA	1:C:68:GLN:HG2	2.37	0.54
1:A:167:THR:C	1:A:168:LEU:HG	2.26	0.54
1:C:28:ALA:O	1:C:29:HIS:HB2	2.08	0.54
1:A:15:GLN:HE21	1:A:162:ALA:N	2.05	0.54
2:B:140:SER:O	2:B:142:ASP:N	2.41	0.54
2:B:113:ASN:HB2	2:B:241:SER:OG	2.08	0.54
2:D:122:TRP:NE1	2:D:167:TYR:HB2	2.23	0.53
2:D:124:THR:CG2	2:D:167:TYR:HE1	2.22	0.53
1:A:15:GLN:CG	1:A:162:ALA:HA	2.24	0.53
2:B:47:LEU:N	2:B:47:LEU:HD23	2.23	0.53
2:B:223:PRO:CA	2:B:230:VAL:HG12	2.37	0.53
2:D:117:ARG:NH2	2:D:172:GLN:HB2	2.20	0.53
2:B:59:GLU:O	2:B:62:ASP:HB2	2.08	0.53
1:C:52:ILE:HD12	1:C:153:PHE:CD1	2.44	0.53
2:D:97:ASP:O	2:D:97:ASP:OD1	2.26	0.53
2:D:95:LEU:HB2	2:D:201:TYR:CZ	2.44	0.53
2:D:108:ARG:O	2:D:120:CYS:HB3	2.08	0.53
2:B:16:TYR:CD1	2:B:84:LYS:HB3	2.43	0.53
2:D:65:GLN:HB2	2:D:79:LEU:CD1	2.38	0.53
2:D:91:SER:O	2:D:199:GLU:HG2	2.08	0.53
2:D:109:CYS:HA	2:D:119:THR:O	2.09	0.53
2:D:156:GLU:O	2:D:156:GLU:HG2	2.08	0.53
2:B:122:TRP:NE1	2:B:167:TYR:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:THR:O	2:B:129:ASP:HB2	2.09	0.53
2:D:70:LYS:N	2:D:75:LEU:CD1	2.72	0.53
2:D:124:THR:HG23	2:D:165:TYR:HB2	1.90	0.53
1:A:10:ALA:HB3	1:A:13:GLN:HB2	1.91	0.53
2:B:138:ARG:NH1	2:B:184:LEU:O	2.33	0.53
1:C:1:ARG:HD2	1:C:1:ARG:H3	1.71	0.53
2:D:70:LYS:N	2:D:75:LEU:HD11	2.24	0.53
2:D:89:ILE:HG12	2:D:90:TRP:O	2.09	0.53
2:D:283:SER:OG	2:D:304:PRO:HB3	2.08	0.53
1:C:10:ALA:O	1:C:12:THR:N	2.42	0.53
1:C:29:HIS:HB3	1:C:147:LEU:HD22	1.91	0.53
2:B:95:LEU:HD21	2:B:122:TRP:CD1	2.45	0.52
1:C:137:TRP:CE3	1:C:138:GLN:CA	2.91	0.52
2:D:8:VAL:HG22	2:D:79:LEU:HD23	1.92	0.52
1:A:59:ASP:HB3	2:B:179:ALA:HB3	1.91	0.52
1:C:34:HIS:O	1:C:36:ASP:N	2.30	0.52
1:C:87:SER:OG	1:C:89:ILE:HB	2.10	0.52
2:D:32:GLU:O	2:D:33:GLU:HG3	2.09	0.52
1:A:22:CYS:O	1:A:26:TRP:HD1	1.91	0.52
1:A:52:ILE:CG2	1:A:58:CYS:SG	2.97	0.52
1:A:58:CYS:HB3	1:A:70:CYS:SG	2.49	0.52
1:A:96:LEU:CD1	1:C:32:VAL:HG11	2.31	0.52
1:C:117:GLN:NE2	1:C:120:GLY:HA2	2.25	0.52
2:D:303:VAL:O	2:D:303:VAL:HG12	2.09	0.52
2:B:33:GLU:HB3	2:B:51:LYS:NZ	2.24	0.52
1:C:58:CYS:CB	1:C:70:CYS:HG	2.21	0.52
2:D:95:LEU:CD2	2:D:122:TRP:HB2	2.37	0.52
1:A:92:GLY:O	1:A:143:ARG:NH2	2.42	0.52
1:A:110:LEU:HD12	1:A:110:LEU:O	2.09	0.52
1:A:137:TRP:CE2	1:C:141:LEU:HB2	2.44	0.52
1:A:140:LEU:HD22	1:A:144:PHE:CE1	2.44	0.52
1:A:140:LEU:CD2	1:A:144:PHE:HE1	2.23	0.52
1:C:99:ASP:OD1	1:C:99:ASP:N	2.43	0.52
2:D:57:VAL:HA	2:D:62:ASP:CB	2.40	0.52
2:B:134:VAL:CG1	2:B:148:CYS:HB3	2.39	0.52
1:C:12:THR:O	1:C:16:GLN:HB2	2.10	0.52
1:C:87:SER:OG	1:C:89:ILE:HG13	2.10	0.52
2:D:251:PHE:N	2:D:251:PHE:CD1	2.78	0.52
1:A:164:GLY:CA	1:A:168:LEU:CD1	2.87	0.52
1:C:33:GLY:HA3	1:C:148:ARG:NH1	2.24	0.52
2:B:283:SER:HB3	2:B:305:CYS:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:VAL:HA	2:D:286:VAL:CG2	2.31	0.51
1:C:49:VAL:HA	1:C:80:PHE:CE2	2.45	0.51
2:D:40:LEU:HB2	2:D:47:LEU:HD11	1.92	0.51
2:D:140:SER:O	2:D:143:PRO:HD3	2.10	0.51
2:D:177:CYS:N	2:D:178:PRO:HD3	2.24	0.51
2:B:139:GLY:O	2:B:143:PRO:HA	2.10	0.51
2:B:60:PHE:CZ	2:B:84:LYS:HD3	2.46	0.51
1:C:61:GLN:HG3	1:C:62:GLY:N	2.25	0.51
2:B:123:LEU:HD13	2:B:164:GLU:CD	2.31	0.51
2:D:57:VAL:CG1	2:D:82:LEU:HD21	2.41	0.51
2:D:232:VAL:HG12	2:D:233:SER:H	1.74	0.51
1:A:93:GLU:CA	1:A:95:SER:H	2.19	0.51
1:A:110:LEU:O	1:A:113:SER:HB2	2.10	0.51
2:D:3:GLU:HG2	2:D:5:LYS:O	2.10	0.51
2:D:100:GLU:O	2:D:102:LYS:HA	2.11	0.51
1:C:24:LEU:HD23	1:C:105:LEU:HD22	1.93	0.50
1:C:52:ILE:CD1	1:C:153:PHE:CE1	2.94	0.50
1:C:168:LEU:N	1:C:168:LEU:CD2	2.69	0.50
2:D:121:TRP:N	2:D:121:TRP:CE3	2.78	0.50
1:A:68:GLN:O	1:A:72:GLN:HB2	2.11	0.50
2:B:136:SER:HB3	2:B:148:CYS:SG	2.50	0.50
1:C:5:GLY:HA2	1:C:68:GLN:CG	2.40	0.50
2:D:217:LYS:HG3	2:D:218:ASN:ND2	2.26	0.50
1:A:62:GLY:O	1:A:66:ASN:O	2.30	0.50
1:A:96:LEU:HD11	1:C:32:VAL:CG1	2.34	0.50
2:B:230:VAL:HG23	2:B:276:VAL:HG22	1.93	0.50
2:D:194:HIS:CE1	2:D:195:LYS:HD2	2.47	0.50
2:D:291:ARG:HD2	2:D:292:TYR:CZ	2.46	0.50
2:B:69:HIS:N	2:B:69:HIS:CD2	2.80	0.50
1:C:84:LEU:HD13	1:C:146:ILE:CG1	2.37	0.50
2:D:6:LYS:C	2:D:8:VAL:H	2.15	0.50
2:D:137:SER:HA	2:D:146:VAL:HG23	1.94	0.50
2:B:6:LYS:O	2:B:7:ASP:HB2	2.11	0.50
2:B:37:THR:HG21	2:B:46:VAL:HG21	1.92	0.50
2:B:221:LEU:HD12	2:B:303:VAL:CG1	2.42	0.50
1:A:39:GLU:CA	1:A:40:GLU:CB	2.90	0.50
2:B:32:GLU:OE1	2:B:32:GLU:HA	2.10	0.50
2:D:117:ARG:HH12	2:D:170:GLU:CB	2.24	0.50
2:D:217:LYS:HE2	2:D:238:ASP:OD2	2.12	0.50
2:D:219:LEU:HD23	2:D:302:SER:C	2.32	0.50
2:B:120:CYS:O	2:B:168:SER:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:THR:C	1:C:48:ASP:H	2.14	0.50
1:C:73:ARG:O	1:C:76:GLN:N	2.45	0.50
2:D:240:TRP:CG	2:D:241:SER:N	2.79	0.50
1:C:22:CYS:O	1:C:26:TRP:HD1	1.95	0.50
1:C:101:PRO:N	1:C:104:GLN:NE2	2.59	0.50
2:D:142:ASP:N	2:D:143:PRO:CD	2.74	0.50
2:D:158:VAL:HG13	2:D:161:ASP:O	2.11	0.50
2:D:217:LYS:HG3	2:D:235:GLU:HB2	1.93	0.50
1:A:94:PRO:HD2	1:A:143:ARG:NH2	2.28	0.49
2:B:83:HIS:ND1	2:B:198:TYR:CE2	2.77	0.49
2:B:278:CYS:HB3	2:B:305:CYS:SG	2.52	0.49
1:C:71:LEU:N	1:C:71:LEU:HD23	2.27	0.49
2:D:75:LEU:HD12	2:D:75:LEU:H	1.76	0.49
1:A:164:GLY:CA	1:A:168:LEU:HD12	2.42	0.49
1:A:102:VAL:O	1:A:105:LEU:HB3	2.13	0.49
2:B:25:VAL:HG22	2:B:54:THR:HG23	1.93	0.49
2:B:181:GLU:O	2:B:181:GLU:HG2	2.11	0.49
2:D:13:LEU:HD22	2:D:82:LEU:HD22	1.91	0.49
2:B:276:VAL:HG21	2:B:284:ILE:HG12	1.93	0.49
1:C:11:TRP:CZ3	1:C:164:GLY:HA3	2.47	0.49
2:D:134:VAL:HG12	2:D:148:CYS:SG	2.53	0.49
2:D:141:SER:O	2:D:142:ASP:HB3	2.12	0.49
2:D:248:SER:HB2	2:D:292:TYR:HE1	1.78	0.49
1:C:77:GLY:O	1:C:80:PHE:HB3	2.11	0.49
2:B:105:THR:O	2:B:106:PHE:HB2	2.12	0.49
1:C:61:GLN:CG	1:C:62:GLY:N	2.76	0.49
1:A:132:SER:CB	1:A:133:PRO:CA	2.86	0.49
2:D:34:ASP:HA	2:D:36:ILE:HD11	1.94	0.49
2:D:95:LEU:HD21	2:D:122:TRP:CG	2.48	0.49
1:A:10:ALA:O	1:A:13:GLN:N	2.46	0.48
2:B:26:LEU:O	2:B:52:THR:HA	2.13	0.48
2:B:85:LYS:HD2	2:B:90:TRP:CD2	2.48	0.48
2:B:167:TYR:O	2:B:168:SER:HB3	2.13	0.48
1:C:101:PRO:CA	1:C:104:GLN:NE2	2.76	0.48
2:D:126:ILE:HG21	2:D:130:LEU:CG	2.42	0.48
1:A:89:ILE:HG22	1:A:90:PHE:CE1	2.47	0.48
2:B:138:ARG:CZ	2:B:186:ILE:CD1	2.87	0.48
1:C:58:CYS:CB	1:C:70:CYS:SG	3.01	0.48
1:C:99:ASP:O	1:C:104:GLN:NE2	2.46	0.48
2:B:109:CYS:HG	2:B:120:CYS:CB	2.25	0.48
1:C:149:SER:O	1:C:152:ALA:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:ASP:C	2:D:30:THR:HG22	2.34	0.48
2:D:188:VAL:O	2:D:202:THR:HA	2.14	0.48
1:A:93:GLU:HG3	1:A:95:SER:N	2.26	0.48
2:B:221:LEU:HD12	2:B:303:VAL:HG13	1.94	0.48
1:C:51:HIS:O	1:C:53:GLN:N	2.47	0.48
2:D:75:LEU:HD12	2:D:75:LEU:N	2.28	0.48
2:D:215:PRO:HA	2:D:298:SER:HG	1.78	0.48
1:A:79:ILE:O	1:A:83:LYS:HG3	2.13	0.48
2:B:138:ARG:NH2	2:B:186:ILE:HD11	2.27	0.48
1:A:148:ARG:HD2	1:A:151:GLN:OE1	2.12	0.48
1:A:66:ASN:HD22	1:A:67:SER:N	2.00	0.48
1:A:89:ILE:CG2	1:A:90:PHE:CD1	2.95	0.48
1:A:140:LEU:O	1:A:143:ARG:HB2	2.14	0.48
2:D:1:ILE:HG13	2:D:10:VAL:O	2.13	0.48
1:A:11:TRP:CB	1:A:165:ALA:HA	2.39	0.48
1:A:52:ILE:CD1	1:A:153:PHE:CE1	2.97	0.48
2:B:28:CYS:CB	2:B:68:CYS:SG	3.02	0.48
2:B:230:VAL:CG1	2:B:278:CYS:SG	3.02	0.48
1:C:137:TRP:CE3	1:C:138:GLN:CB	2.96	0.48
1:A:90:PHE:N	1:A:90:PHE:HD1	2.12	0.48
2:B:83:HIS:ND1	2:B:198:TYR:CD2	2.80	0.48
2:B:95:LEU:CD2	2:B:122:TRP:CD1	2.97	0.48
2:B:283:SER:HB3	2:B:305:CYS:N	2.28	0.48
2:B:224:LEU:HD23	2:B:229:GLN:O	2.14	0.48
2:D:74:VAL:HG12	2:D:74:VAL:O	2.12	0.48
1:C:86:GLY:O	1:C:87:SER:O	2.32	0.47
2:D:149:GLY:O	2:D:150:ALA:O	2.32	0.47
1:A:26:TRP:CZ2	2:B:293:TYR:CE2	3.02	0.47
2:D:32:GLU:CB	2:D:70:LYS:HZ2	2.27	0.47
2:D:194:HIS:O	2:D:195:LYS:HB2	2.15	0.47
2:D:252:CYS:O	2:D:253:VAL:HG23	2.14	0.47
1:A:89:ILE:CG2	1:A:90:PHE:CE1	2.97	0.47
1:A:97:LEU:O	1:A:100:SER:OG	2.26	0.47
1:A:145:LYS:HE3	1:A:145:LYS:HB2	1.68	0.47
2:B:212:LYS:HD2	2:B:298:SER:HA	1.95	0.47
2:B:250:THR:HG22	2:B:291:ARG:HA	1.95	0.47
1:C:74:ILE:O	1:C:78:LEU:HG	2.15	0.47
1:C:101:PRO:N	1:C:104:GLN:HE21	2.12	0.47
1:C:137:TRP:HE3	1:C:138:GLN:CB	2.26	0.47
2:D:95:LEU:HB2	2:D:201:TYR:CE1	2.49	0.47
2:D:250:THR:HG22	2:D:291:ARG:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ILE:HG21	2:B:130:LEU:HG	1.95	0.47
2:B:133:SER:HB3	2:B:191:ASP:HB2	1.95	0.47
1:C:137:TRP:HE3	1:C:138:GLN:CA	2.27	0.47
2:D:101:PRO:HA	2:D:102:LYS:HA	1.68	0.47
1:C:117:GLN:NE2	1:C:120:GLY:CA	2.77	0.47
2:D:221:LEU:CB	2:D:230:VAL:HG11	2.38	0.47
1:A:29:HIS:CG	1:A:32:VAL:HG23	2.50	0.47
1:A:158:ALA:HB1	2:B:292:TYR:CD2	2.49	0.47
2:B:33:GLU:HB3	2:B:51:LYS:HZ1	1.80	0.47
1:C:29:HIS:CB	1:C:147:LEU:HD22	2.44	0.47
2:D:28:CYS:SG	2:D:68:CYS:CB	3.01	0.47
2:B:96:LYS:N	2:B:123:LEU:O	2.28	0.47
2:B:109:CYS:SG	2:B:120:CYS:SG	3.07	0.47
2:B:126:ILE:N	2:B:126:ILE:CD1	2.77	0.47
2:D:36:ILE:HD13	2:D:50:GLY:HA2	1.96	0.47
2:D:97:ASP:OD1	2:D:104:LYS:HA	2.15	0.47
2:B:18:ASP:O	2:B:19:ALA:HB3	2.15	0.47
2:B:96:LYS:HZ1	2:B:164:GLU:HG3	1.77	0.47
2:B:126:ILE:HG22	2:B:130:LEU:CD1	2.44	0.47
1:A:97:LEU:HB2	1:A:99:ASP:OD1	2.13	0.47
1:C:1:ARG:N	1:C:1:ARG:CD	2.71	0.47
2:D:107:LEU:HD11	2:D:190:VAL:CG2	2.45	0.47
2:D:244:HIS:CD2	2:D:244:HIS:N	2.83	0.47
2:D:284:ILE:HD12	2:D:284:ILE:N	2.12	0.47
2:B:194:HIS:O	2:B:195:LYS:HB2	2.14	0.47
1:A:19:GLN:HE22	2:B:291:ARG:CD	2.25	0.46
1:A:79:ILE:HD13	1:A:113:SER:OG	2.15	0.46
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.77	0.46
1:C:24:LEU:HB3	1:C:105:LEU:HD13	1.97	0.46
1:C:137:TRP:CZ3	1:C:138:GLN:HB3	2.50	0.46
2:D:126:ILE:CG2	2:D:127:SER:N	2.77	0.46
1:C:1:ARG:H3	1:C:1:ARG:CD	2.28	0.46
1:C:77:GLY:HA3	1:C:153:PHE:CZ	2.50	0.46
2:D:26:LEU:CD1	2:D:66:TYR:CG	2.98	0.46
2:D:215:PRO:HA	2:D:216:PRO:HD3	1.79	0.46
1:A:15:GLN:NE2	1:A:15:GLN:HA	2.30	0.46
2:B:100:GLU:C	2:B:103:ASN:H	2.19	0.46
1:A:24:LEU:HD21	1:A:104:GLN:CB	2.37	0.46
1:C:75:HIS:HA	1:C:78:LEU:HD12	1.97	0.46
2:D:123:LEU:CD2	2:D:166:GLU:HB2	2.45	0.46
1:A:80:PHE:HD1	1:A:127:GLN:CG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:THR:OG1	2:B:174:ASP:OD1	2.32	0.46
1:C:98:PRO:O	1:C:103:GLY:HA3	2.16	0.46
1:C:132:SER:CB	1:C:133:PRO:CA	2.92	0.46
2:D:106:PHE:O	2:D:107:LEU:HD23	2.15	0.46
2:D:191:ASP:OD1	2:D:198:TYR:OH	2.27	0.46
2:D:211:ILE:O	2:D:296:SER:HB2	2.16	0.46
2:D:250:THR:HG22	2:D:291:ARG:CB	2.45	0.46
1:A:114:GLN:HA	1:A:114:GLN:NE2	2.30	0.46
1:A:163:HIS:CE1	2:B:245:SER:HG	2.31	0.46
1:C:58:CYS:HB3	1:C:70:CYS:HG	1.79	0.46
1:C:132:SER:HB3	1:C:133:PRO:CA	2.44	0.46
2:D:237:PRO:HD2	2:D:240:TRP:HB2	1.96	0.46
2:B:32:GLU:CG	2:B:70:LYS:NZ	2.79	0.46
2:D:156:GLU:OE1	2:D:163:LYS:HD3	2.16	0.46
2:D:251:PHE:CD2	2:D:288:ALA:HB2	2.50	0.46
1:A:15:GLN:CD	1:A:162:ALA:HB2	2.36	0.46
2:B:108:ARG:NH1	2:B:121:TRP:CE3	2.77	0.46
2:B:110:GLU:HG3	2:B:121:TRP:HZ3	1.80	0.46
2:B:112:LYS:O	2:B:113:ASN:HB3	2.15	0.46
1:C:28:ALA:HB3	1:C:105:LEU:CD2	2.45	0.46
2:D:119:THR:HA	2:D:169:VAL:O	2.16	0.46
1:A:142:LEU:CD1	1:A:146:ILE:HD11	2.43	0.46
1:A:143:ARG:O	1:A:147:LEU:HG	2.16	0.46
1:C:11:TRP:HB3	1:C:165:ALA:HA	1.97	0.46
1:C:24:LEU:HD22	1:C:105:LEU:CA	2.44	0.46
1:C:150:LEU:HD13	1:C:154:VAL:CG1	2.45	0.46
2:D:253:VAL:CB	2:D:267:VAL:HG13	2.40	0.46
1:A:89:ILE:HD13	1:A:142:LEU:HD13	1.98	0.46
2:D:65:GLN:HB2	2:D:79:LEU:HD13	1.98	0.46
1:C:117:GLN:HE21	1:C:120:GLY:HA3	1.79	0.45
2:D:82:LEU:HA	2:D:82:LEU:HD23	1.59	0.45
2:D:153:LEU:HB2	2:D:167:TYR:CE2	2.51	0.45
2:D:109:CYS:SG	2:D:205:PHE:CE2	3.10	0.45
2:D:250:THR:HG21	2:D:291:ARG:HA	1.95	0.45
2:B:109:CYS:HG	2:B:120:CYS:HB3	1.82	0.45
2:B:134:VAL:HG11	2:B:169:VAL:HG21	1.97	0.45
2:B:158:VAL:HG12	2:B:160:GLY:N	2.26	0.45
1:C:15:GLN:HB2	1:C:161:PHE:O	2.16	0.45
2:B:14:ASP:HA	2:B:85:LYS:HB2	1.98	0.45
2:B:30:THR:OG1	2:B:31:PRO:HD2	2.16	0.45
2:B:132:PHE:HE2	2:B:167:TYR:CE1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:GLU:CD	2:B:70:LYS:NZ	2.70	0.45
2:B:105:THR:O	2:B:107:LEU:N	2.40	0.45
2:D:94:ILE:HD13	2:D:194:HIS:HB2	1.98	0.45
2:B:113:ASN:OD1	2:B:115:SER:HB3	2.17	0.45
2:B:284:ILE:HD12	2:B:284:ILE:H	1.82	0.45
2:D:108:ARG:O	2:D:120:CYS:HA	2.16	0.45
2:B:100:GLU:CB	2:B:103:ASN:N	2.79	0.45
2:B:256:GLN:C	2:B:282:ALA:HB1	2.37	0.45
1:C:28:ALA:CB	1:C:105:LEU:CD2	2.94	0.45
1:C:62:GLY:O	1:C:66:ASN:O	2.35	0.45
2:D:55:ILE:CG2	2:D:56:GLN:N	2.79	0.45
2:D:119:THR:HG22	2:D:121:TRP:CH2	2.52	0.45
2:D:253:VAL:HG22	2:D:286:VAL:HG22	1.96	0.45
2:B:230:VAL:CG2	2:B:276:VAL:HG23	2.47	0.45
2:D:286:VAL:CA	2:D:300:TRP:CZ3	2.99	0.45
2:D:302:SER:HB2	2:D:304:PRO:HD3	1.99	0.45
1:C:92:GLY:HA3	1:C:139:ARG:NE	2.32	0.45
1:C:102:VAL:C	1:C:104:GLN:H	2.20	0.45
2:D:89:ILE:HD13	2:D:89:ILE:O	2.16	0.45
1:A:16:GLN:CG	1:A:17:LEU:N	2.80	0.45
1:A:35:MET:HE3	1:A:145:LYS:CE	2.25	0.45
1:A:94:PRO:HD2	1:A:143:ARG:NH1	2.32	0.45
2:B:196:LEU:HA	2:B:196:LEU:HD22	1.74	0.45
1:C:120:GLY:O	1:C:121:HIS:HB2	2.16	0.45
2:D:33:GLU:O	2:D:36:ILE:HD11	2.17	0.45
2:B:28:CYS:HB2	2:B:68:CYS:SG	2.57	0.44
1:C:50:PRO:HD2	1:C:80:PHE:CG	2.51	0.44
1:C:167:THR:C	1:C:168:LEU:HD23	2.37	0.44
2:D:282:ALA:O	2:D:305:CYS:SG	2.74	0.44
1:A:114:GLN:NE2	1:A:114:GLN:CA	2.80	0.44
2:B:64:GLY:C	2:B:79:LEU:HD12	2.38	0.44
1:C:18:SER:O	1:C:21:LEU:HB3	2.18	0.44
1:C:31:LEU:C	1:C:33:GLY:H	2.20	0.44
2:D:6:LYS:O	2:D:7:ASP:HB2	2.17	0.44
2:D:26:LEU:HD11	2:D:66:TYR:CG	2.53	0.44
1:A:11:TRP:CZ3	1:A:161:PHE:HA	2.53	0.44
2:B:42:GLN:O	2:B:43:SER:O	2.35	0.44
2:D:186:ILE:HG21	2:D:205:PHE:CE1	2.52	0.44
2:B:107:LEU:HD11	2:B:201:TYR:CB	2.42	0.44
2:B:118:PHE:CZ	2:B:171:CYS:HB2	2.53	0.44
1:C:12:THR:C	1:C:14:CYS:N	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SER:O	1:A:28:ALA:HB3	2.16	0.44
1:C:78:LEU:O	1:C:82:GLU:N	2.47	0.44
1:C:81:TYR:O	1:C:84:LEU:HB2	2.17	0.44
2:B:9:TYR:N	2:B:9:TYR:CD1	2.86	0.44
1:C:52:ILE:HD11	1:C:74:ILE:HG13	2.00	0.44
1:A:14:CYS:SG	1:A:115:LEU:HD22	2.58	0.44
2:B:32:GLU:HG3	2:B:70:LYS:CE	2.48	0.44
2:B:80:LEU:N	2:B:80:LEU:CD2	2.77	0.44
2:B:73:GLU:OE2	2:B:73:GLU:HA	2.17	0.44
2:B:225:LYS:C	2:B:227:SER:H	2.20	0.44
2:B:269:THR:C	2:B:271:LYS:H	2.21	0.44
2:D:40:LEU:HD12	2:D:41:ASP:N	2.32	0.44
2:D:95:LEU:HD21	2:D:122:TRP:CD1	2.53	0.44
2:D:97:ASP:C	2:D:99:LYS:N	2.69	0.44
2:B:28:CYS:SG	2:B:68:CYS:SG	3.13	0.44
2:B:95:LEU:HD12	2:B:201:TYR:CD1	2.53	0.44
2:B:213:PRO:O	2:B:298:SER:HB2	2.17	0.44
1:C:158:ALA:HB1	2:D:292:TYR:CD2	2.53	0.44
2:D:121:TRP:HE3	2:D:121:TRP:H	1.65	0.44
2:D:183:SER:C	2:D:184:LEU:HD23	2.38	0.44
2:D:277:ILE:H	2:D:277:ILE:HG12	1.31	0.44
1:A:11:TRP:O	1:A:15:GLN:N	2.32	0.43
2:B:126:ILE:CG2	2:B:130:LEU:HG	2.47	0.43
2:D:64:GLY:CA	2:D:196:LEU:HD11	2.47	0.43
2:D:228:ARG:O	2:D:278:CYS:N	2.51	0.43
1:A:104:GLN:O	1:A:107:ALA:HB3	2.18	0.43
2:D:16:TYR:CE2	2:D:59:GLU:OE2	2.72	0.43
2:D:117:ARG:HH11	2:D:170:GLU:HG3	1.78	0.43
2:B:119:THR:HB	2:B:121:TRP:CH2	2.52	0.43
1:C:49:VAL:CB	1:C:80:PHE:CE2	2.96	0.43
2:D:69:HIS:CE1	2:D:74:VAL:HG22	2.54	0.43
2:D:281:ASN:HB3	2:D:282:ALA:H	1.61	0.43
1:A:120:GLY:O	1:A:122:HIS:N	2.51	0.43
2:B:63:ALA:HB2	2:B:82:LEU:HD21	2.00	0.43
2:B:252:CYS:O	2:B:300:TRP:HZ3	2.00	0.43
1:C:150:LEU:HD12	1:C:151:GLN:N	2.33	0.43
1:A:63:LEU:HA	1:A:63:LEU:HD23	1.72	0.43
2:D:117:ARG:HH21	2:D:172:GLN:CB	2.28	0.43
2:D:122:TRP:CH2	2:D:169:VAL:CG1	3.01	0.43
2:B:126:ILE:HD12	2:B:126:ILE:H	1.81	0.43
2:B:236:TYR:CB	2:B:244:HIS:CE1	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:SER:O	2:D:45:GLU:CB	2.67	0.43
2:D:219:LEU:O	2:D:303:VAL:HG21	2.19	0.43
1:C:96:LEU:HD23	1:C:96:LEU:HA	1.75	0.43
2:D:64:GLY:HA2	2:D:196:LEU:HD11	2.00	0.43
1:A:29:HIS:HE1	1:A:31:LEU:HB2	1.84	0.43
1:A:89:ILE:CD1	1:A:142:LEU:CD1	2.96	0.43
1:A:114:GLN:HE21	1:A:114:GLN:N	2.16	0.43
1:A:150:LEU:HD11	1:A:154:VAL:CG1	2.48	0.43
2:B:129:ASP:HB3	2:B:195:LYS:HG3	2.01	0.43
2:B:255:VAL:O	2:B:256:GLN:HB3	2.18	0.43
1:C:13:GLN:H	1:C:13:GLN:HG3	1.67	0.43
1:C:75:HIS:CD2	1:C:75:HIS:C	2.92	0.43
1:C:112:LEU:HD12	1:C:112:LEU:C	2.36	0.43
1:A:135:GLN:HA	1:A:136:PRO:HD3	1.34	0.42
2:D:124:THR:OG1	2:D:126:ILE:HB	2.19	0.42
1:A:80:PHE:CE2	1:A:84:LEU:HD11	2.55	0.42
1:A:136:PRO:O	1:A:140:LEU:HB2	2.20	0.42
2:B:8:VAL:HG22	2:B:79:LEU:HB3	2.00	0.42
2:B:86:GLU:O	2:B:89:ILE:HG23	2.18	0.42
2:B:221:LEU:CD1	2:B:303:VAL:CG1	2.97	0.42
1:A:29:HIS:HB3	1:A:32:VAL:HG23	2.01	0.42
1:A:159:ARG:HB3	2:B:246:TYR:CD2	2.54	0.42
2:B:95:LEU:CD2	2:B:122:TRP:HD1	2.32	0.42
2:B:182:GLU:OE2	2:B:207:ILE:HB	2.19	0.42
2:D:291:ARG:HD2	2:D:292:TYR:CE2	2.54	0.42
1:A:11:TRP:O	1:A:15:GLN:HB2	2.20	0.42
1:A:79:ILE:CD1	1:A:113:SER:CB	2.97	0.42
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.81	0.42
2:B:17:PRO:O	2:B:18:ASP:HB2	2.20	0.42
2:B:278:CYS:CB	2:B:305:CYS:SG	3.08	0.42
1:C:11:TRP:CD2	1:C:164:GLY:HA3	2.55	0.42
1:C:70:CYS:O	1:C:73:ARG:HB3	2.19	0.42
1:C:159:ARG:HB3	2:D:246:TYR:O	2.19	0.42
2:D:28:CYS:SG	2:D:30:THR:CG2	3.07	0.42
2:D:231:GLU:HA	2:D:274:ALA:O	2.19	0.42
2:B:224:LEU:O	2:B:225:LYS:CB	2.67	0.42
1:C:47:ASN:O	1:C:48:ASP:O	2.37	0.42
1:A:15:GLN:HE21	1:A:162:ALA:H	1.66	0.42
1:A:54:CYS:HG	2:B:177:CYS:CB	2.33	0.42
2:B:134:VAL:CG1	2:B:148:CYS:SG	3.08	0.42
2:D:4:LEU:HA	2:D:4:LEU:HD12	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:CYS:CB	1:A:70:CYS:SG	3.07	0.42
2:B:303:VAL:HG22	2:B:304:PRO:CD	2.46	0.42
1:A:96:LEU:CD1	1:C:32:VAL:CG1	2.95	0.42
1:A:130:SER:O	1:A:131:LEU:HG	2.20	0.42
2:B:36:ILE:HD12	2:B:36:ILE:N	2.34	0.42
2:B:100:GLU:CB	2:B:103:ASN:HA	2.50	0.42
2:B:152:THR:CG2	2:B:153:LEU:N	2.80	0.42
1:C:115:LEU:HA	1:C:115:LEU:HD23	1.79	0.42
2:D:91:SER:OG	2:D:199:GLU:OE2	2.26	0.42
2:D:109:CYS:SG	2:D:120:CYS:SG	3.14	0.42
2:D:252:CYS:SG	2:D:253:VAL:N	2.93	0.42
1:C:102:VAL:C	1:C:104:GLN:N	2.72	0.42
1:A:24:LEU:HD23	1:A:105:LEU:N	2.35	0.41
2:B:85:LYS:HD2	2:B:90:TRP:CH2	2.55	0.41
1:C:137:TRP:HZ3	1:C:138:GLN:HB3	1.86	0.41
1:C:145:LYS:HE3	1:C:145:LYS:HB3	1.67	0.41
2:D:117:ARG:HE	2:D:172:GLN:HB2	1.85	0.41
2:D:198:TYR:CD2	2:D:198:TYR:O	2.73	0.41
2:D:273:SER:O	2:D:274:ALA:HB2	2.20	0.41
2:B:189:MET:HB3	2:B:200:GLN:OE1	2.19	0.41
2:D:81:LEU:HD23	2:D:81:LEU:HA	1.78	0.41
1:C:49:VAL:HB	1:C:80:PHE:CD2	2.54	0.41
1:C:97:LEU:HD12	1:C:97:LEU:HA	1.59	0.41
1:C:100:SER:CB	1:C:101:PRO:CD	2.98	0.41
2:D:57:VAL:HA	2:D:62:ASP:HB3	2.02	0.41
2:D:81:LEU:HD13	2:D:193:VAL:HG11	2.02	0.41
2:D:157:ARG:HB2	2:D:158:VAL:H	1.68	0.41
1:A:119:GLU:C	1:A:121:HIS:N	2.72	0.41
2:B:236:TYR:HB2	2:B:244:HIS:CE1	2.56	0.41
1:C:97:LEU:HD12	1:C:98:PRO:HD3	2.02	0.41
2:D:36:ILE:HD13	2:D:50:GLY:CA	2.50	0.41
2:B:17:PRO:HD3	2:B:58:LYS:O	2.20	0.41
2:B:92:THR:O	2:B:94:ILE:N	2.53	0.41
1:C:102:VAL:O	1:C:105:LEU:HB2	2.21	0.41
1:C:135:GLN:O	1:C:138:GLN:HG3	2.21	0.41
1:A:70:CYS:SG	1:A:74:ILE:HD12	2.61	0.41
1:A:97:LEU:N	1:A:97:LEU:CD1	2.78	0.41
1:C:92:GLY:O	1:C:95:SER:HA	2.21	0.41
1:C:100:SER:OG	1:C:101:PRO:HD2	2.21	0.41
1:C:137:TRP:CE3	1:C:138:GLN:CG	3.03	0.41
1:A:36:ASP:CA	1:A:37:LEU:CB	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:TRP:CH2	2:B:4:LEU:HD12	2.56	0.41
2:B:14:ASP:C	2:B:15:TRP:CG	2.93	0.41
1:C:54:CYS:HA	2:D:177:CYS:SG	2.61	0.41
2:D:40:LEU:HD12	2:D:41:ASP:H	1.86	0.41
2:D:177:CYS:SG	2:D:177:CYS:O	2.78	0.41
2:D:217:LYS:HD2	2:D:218:ASN:HD21	1.86	0.41
1:A:32:VAL:HG21	1:A:144:PHE:CE1	2.56	0.41
1:A:142:LEU:HD13	1:A:146:ILE:CD1	2.45	0.41
2:B:28:CYS:HA	2:B:68:CYS:SG	2.61	0.41
2:B:38:TRP:HA	2:B:67:THR:O	2.21	0.41
2:B:94:ILE:HB	2:B:199:GLU:OE1	2.21	0.41
2:B:123:LEU:HD21	2:B:166:GLU:HG3	2.02	0.41
2:B:230:VAL:HG13	2:B:278:CYS:SG	2.60	0.41
2:B:236:TYR:OH	2:B:249:LEU:N	2.44	0.41
2:B:251:PHE:CE2	2:B:288:ALA:HB2	2.56	0.41
1:C:137:TRP:CE3	1:C:138:GLN:HG2	2.51	0.41
2:D:83:HIS:NE2	2:D:90:TRP:CE3	2.89	0.41
2:D:94:ILE:HD11	2:D:194:HIS:CB	2.50	0.41
2:D:107:LEU:HD11	2:D:190:VAL:HG23	2.02	0.41
2:D:270:ASP:HB3	2:D:291:ARG:CZ	2.51	0.41
1:A:52:ILE:HG23	1:A:52:ILE:HD13	1.73	0.41
1:A:70:CYS:O	1:A:73:ARG:N	2.53	0.41
2:B:94:ILE:HG22	2:B:95:LEU:N	2.35	0.41
2:B:182:GLU:HB2	2:B:206:PHE:CD2	2.56	0.41
2:B:184:LEU:HD23	2:B:184:LEU:HA	1.93	0.41
2:B:208:ARG:HG3	2:B:209:ASP:N	2.36	0.41
2:B:230:VAL:CG2	2:B:276:VAL:CG2	2.99	0.41
1:C:61:GLN:C	1:C:63:LEU:H	2.24	0.41
2:D:16:TYR:HA	2:D:17:PRO:HA	1.20	0.41
2:D:221:LEU:CB	2:D:230:VAL:CG1	2.97	0.41
2:B:207:ILE:HA	2:B:210:ILE:HG12	2.03	0.40
2:B:213:PRO:O	2:B:298:SER:CB	2.69	0.40
1:C:74:ILE:O	1:C:153:PHE:HZ	2.04	0.40
1:C:79:ILE:HA	1:C:82:GLU:HG2	2.03	0.40
1:C:140:LEU:O	1:C:143:ARG:HB2	2.21	0.40
2:D:83:HIS:CD2	2:D:90:TRP:CE3	3.09	0.40
2:D:253:VAL:CA	2:D:286:VAL:HG22	2.35	0.40
1:A:90:PHE:HA	1:A:143:ARG:NE	2.37	0.40
1:A:93:GLU:CG	1:A:94:PRO:HA	2.46	0.40
2:B:67:THR:CG2	2:B:74:VAL:CG2	2.97	0.40
2:B:126:ILE:HG22	2:B:130:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:THR:HB	2:D:43:SER:O	2.21	0.40
2:D:79:LEU:HD12	2:D:79:LEU:HA	1.89	0.40
2:D:103:ASN:O	2:D:105:THR:HG23	2.21	0.40
2:D:218:ASN:ND2	2:D:235:GLU:OE2	2.55	0.40
2:D:231:GLU:CG	2:D:275:THR:CG2	2.94	0.40
2:B:111:ALA:O	2:B:211:ILE:HA	2.21	0.40
2:B:221:LEU:HD23	2:B:221:LEU:HA	1.72	0.40
2:D:97:ASP:O	2:D:98:GLN:C	2.60	0.40
2:D:129:ASP:HB3	2:D:195:LYS:HG3	2.03	0.40
1:A:31:LEU:N	1:A:31:LEU:HD23	2.36	0.40
2:B:59:GLU:OE1	2:B:60:PHE:HD1	2.04	0.40
2:D:132:PHE:HB2	2:D:151:ALA:HB3	2.00	0.40
1:A:32:VAL:HG11	1:A:144:PHE:CD1	2.56	0.40
1:A:54:CYS:SG	2:B:177:CYS:CB	3.09	0.40
2:B:16:TYR:CG	2:B:17:PRO:CD	2.89	0.40
2:B:113:ASN:ND2	2:B:239:THR:O	2.52	0.40
2:B:153:LEU:HA	2:B:167:TYR:CD2	2.57	0.40
2:D:26:LEU:CD1	2:D:66:TYR:CB	3.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:SER:OG	1:C:132:SER:OG[3_655]	2.08	0.12

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	157/178 (88%)	118 (75%)	21 (13%)	18 (12%)	0 1
1	C	153/178 (86%)	108 (71%)	23 (15%)	22 (14%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	294/306 (96%)	236 (80%)	38 (13%)	20 (7%)	1 3
2	D	292/306 (95%)	234 (80%)	37 (13%)	21 (7%)	1 3
All	All	896/968 (93%)	696 (78%)	119 (13%)	81 (9%)	1 1

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	94	PRO
1	A	129	PRO
1	A	130	SER
1	A	132	SER
2	B	16	TYR
2	B	17	PRO
2	B	19	ALA
2	B	43	SER
2	B	78	SER
2	B	93	ASP
2	B	99	LYS
2	B	101	PRO
2	B	225	LYS
2	B	280	LYS
1	C	8	SER
1	C	11	TRP
1	C	35	MET
1	C	48	ASP
1	C	54	CYS
1	C	87	SER
1	C	133	PRO
1	C	134	SER
2	D	45	GLU
2	D	98	GLN
2	D	99	LYS
2	D	100	GLU
2	D	150	ALA
2	D	157	ARG
2	D	159	ARG
2	D	177	CYS
2	D	178	PRO
2	D	281	ASN
1	A	67	SER

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Mol	Chain	Res	Type
1	A	120	GLY
2	B	98	GLN
2	B	103	ASN
2	B	141	SER
2	B	161	ASP
2	B	281	ASN
2	B	295	SER
1	C	10	ALA
1	C	32	VAL
1	C	46	THR
1	C	103	GLY
1	C	132	SER
2	D	71	GLY
2	D	101	PRO
2	D	282	ALA
1	A	87	SER
1	C	36	ASP
2	D	78	SER
2	D	161	ASP
2	D	179	ALA
2	D	304	PRO
1	A	4	PRO
1	A	95	SER
1	A	119	GLU
1	A	131	LEU
1	A	136	PRO
2	B	150	ALA
2	B	195	LYS
1	C	7	SER
1	C	30	PRO
1	C	121	HIS
1	C	131	LEU
1	C	135	GLN
1	A	118	PRO
1	A	126	GLN
1	A	135	GLN
1	A	153	PHE
1	C	74	ILE
1	A	109	LEU
2	B	113	ASN
1	C	92	GLY
2	D	213	PRO

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Mol	Chain	Res	Type
1	C	102	VAL
2	D	94	ILE
2	D	253	VAL
2	B	143	PRO
2	D	17	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/151 (86%)	94 (72%)	36 (28%)	0	1
1	C	125/151 (83%)	82 (66%)	43 (34%)	0	0
2	B	263/277 (95%)	196 (74%)	67 (26%)	0	1
2	D	259/277 (94%)	191 (74%)	68 (26%)	0	1
All	All	777/856 (91%)	563 (72%)	214 (28%)	0	1

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	THR
1	A	15	GLN
1	A	17	LEU
1	A	18	SER
1	A	34	HIS
1	A	37	LEU
1	A	52	ILE
1	A	54	CYS
1	A	58	CYS
1	A	65	ASP
1	A	66	ASN
1	A	70	CYS
1	A	79	ILE
1	A	82	GLU
1	A	87	SER

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Mol	Chain	Res	Type
1	A	90	PHE
1	A	91	THR
1	A	97	LEU
1	A	99	ASP
1	A	109	LEU
1	A	110	LEU
1	A	114	GLN
1	A	117	GLN
1	A	121	HIS
1	A	122	HIS
1	A	123	TRP
1	A	130	SER
1	A	132	SER
1	A	140	LEU
1	A	141	LEU
1	A	142	LEU
1	A	145	LYS
1	A	148	ARG
1	A	167	THR
1	A	168	LEU
2	B	1	ILE
2	B	4	LEU
2	B	5	LYS
2	B	6	LYS
2	B	13	LEU
2	B	15	TRP
2	B	17	PRO
2	B	26	LEU
2	B	29	ASP
2	B	32	GLU
2	B	33	GLU
2	B	37	THR
2	B	44	SER
2	B	52	THR
2	B	59	GLU
2	B	65	GLN
2	B	68	CYS
2	B	69	HIS
2	B	70	LYS
2	B	74	VAL
2	B	80	LEU
2	B	84	LYS

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Mol	Chain	Res	Type
2	B	85	LYS
2	B	89	ILE
2	B	99	LYS
2	B	108	ARG
2	B	109	CYS
2	B	127	SER
2	B	128	THR
2	B	131	THR
2	B	134	VAL
2	B	135	LYS
2	B	140	SER
2	B	147	THR
2	B	153	LEU
2	B	154	SER
2	B	166	GLU
2	B	169	VAL
2	B	173	GLU
2	B	175	SER
2	B	177	CYS
2	B	182	GLU
2	B	186	ILE
2	B	187	GLU
2	B	196	LEU
2	B	200	GLN
2	B	203	SER
2	B	204	SER
2	B	207	ILE
2	B	212	LYS
2	B	222	LYS
2	B	227	SER
2	B	233	SER
2	B	239	THR
2	B	250	THR
2	B	254	GLN
2	B	266	ARG
2	B	275	THR
2	B	277	ILE
2	B	279	ARG
2	B	285	SER
2	B	296	SER
2	B	299	GLU
2	B	302	SER

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Mol	Chain	Res	Type
2	B	303	VAL
2	B	305	CYS
2	B	306	SER
1	C	1	ARG
1	C	3	VAL
1	C	8	SER
1	C	12	THR
1	C	13	GLN
1	C	14	CYS
1	C	16	GLN
1	C	17	LEU
1	C	20	LYS
1	C	24	LEU
1	C	31	LEU
1	C	32	VAL
1	C	36	ASP
1	C	49	VAL
1	C	58	CYS
1	C	59	ASP
1	C	66	ASN
1	C	68	GLN
1	C	71	LEU
1	C	72	GLN
1	C	74	ILE
1	C	82	GLU
1	C	88	ASP
1	C	93	GLU
1	C	95	SER
1	C	97	LEU
1	C	100	SER
1	C	105	LEU
1	C	106	HIS
1	C	108	SER
1	C	110	LEU
1	C	112	LEU
1	C	131	LEU
1	C	132	SER
1	C	138	GLN
1	C	141	LEU
1	C	145	LYS
1	C	146	ILE
1	C	147	LEU

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Mol	Chain	Res	Type
1	C	148	ARG
1	C	150	LEU
1	C	159	ARG
1	C	168	LEU
2	D	5	LYS
2	D	6	LYS
2	D	13	LEU
2	D	14	ASP
2	D	22	GLU
2	D	27	THR
2	D	30	THR
2	D	32	GLU
2	D	34	ASP
2	D	36	ILE
2	D	43	SER
2	D	49	SER
2	D	55	ILE
2	D	65	GLN
2	D	70	LYS
2	D	73	GLU
2	D	78	SER
2	D	84	LYS
2	D	89	ILE
2	D	92	THR
2	D	95	LEU
2	D	100	GLU
2	D	117	ARG
2	D	120	CYS
2	D	121	TRP
2	D	123	LEU
2	D	124	THR
2	D	131	THR
2	D	137	SER
2	D	148	CYS
2	D	152	THR
2	D	153	LEU
2	D	157	ARG
2	D	165	TYR
2	D	166	GLU
2	D	169	VAL
2	D	170	GLU
2	D	182	GLU

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Mol	Chain	Res	Type
2	D	184	LEU
2	D	189	MET
2	D	195	LYS
2	D	196	LEU
2	D	197	LYS
2	D	198	TYR
2	D	204	SER
2	D	210	ILE
2	D	218	ASN
2	D	219	LEU
2	D	221	LEU
2	D	222	LYS
2	D	224	LEU
2	D	225	LYS
2	D	227	SER
2	D	229	GLN
2	D	232	VAL
2	D	242	THR
2	D	245	SER
2	D	250	THR
2	D	254	GLN
2	D	267	VAL
2	D	277	ILE
2	D	278	CYS
2	D	279	ARG
2	D	281	ASN
2	D	284	ILE
2	D	298	SER
2	D	302	SER
2	D	305	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	53	GLN
1	A	66	ASN
1	A	68	GLN
1	A	72	GLN
1	A	114	GLN
1	A	117	GLN
1	A	121	HIS

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Mol	Chain	Res	Type
1	A	122	HIS
2	B	220	GLN
2	B	244	HIS
1	C	16	GLN
1	C	19	GLN
1	C	29	HIS
1	C	66	ASN
1	C	75	HIS
1	C	104	GLN
1	C	117	GLN
2	D	144	GLN
2	D	218	ASN
2	D	244	HIS
2	D	281	ASN

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

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	B	5001	-	4,4,4	2.26	2 (50%)	6,6,6	1.68	2 (33%)
5	MAN	D	1281	-	11,11,12	1.98	3 (27%)	15,15,17	1.94	6 (40%)
3	PO4	D	5002	-	4,4,4	2.62	2 (50%)	6,6,6	1.03	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	D	1281	-	-	1/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5002	PO4	P-O1	4.27	1.60	1.50
5	D	1281	MAN	C2-C3	3.47	1.57	1.52
3	B	5001	PO4	P-O1	3.38	1.58	1.50
5	D	1281	MAN	C4-C3	2.87	1.59	1.52
5	D	1281	MAN	C4-C5	2.26	1.57	1.53
3	B	5001	PO4	P-O2	2.15	1.61	1.54
3	D	5002	PO4	P-O3	2.09	1.60	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1281	MAN	O5-C5-C6	3.84	113.22	107.20
5	D	1281	MAN	C2-C3-C4	3.51	116.97	110.89
3	B	5001	PO4	O3-P-O2	2.59	116.29	107.97
5	D	1281	MAN	C3-C4-C5	2.39	114.49	110.24
5	D	1281	MAN	O2-C2-C1	2.32	113.90	109.15
5	D	1281	MAN	O2-C2-C3	2.26	114.67	110.14
3	B	5001	PO4	O4-P-O2	2.10	114.71	107.97
5	D	1281	MAN	C1-C2-C3	2.08	112.22	109.67
3	D	5002	PO4	O4-P-O3	2.05	114.56	107.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1281	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1281	MAN	1	0

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	A	161/178 (90%)	-0.05	5 (3%) 49 44	38, 72, 123, 140	0
1	C	159/178 (89%)	0.10	13 (8%) 11 9	51, 76, 121, 136	0
2	B	298/306 (97%)	-0.22	2 (0%) 87 87	41, 63, 92, 108	0
2	D	296/306 (96%)	-0.11	7 (2%) 59 56	48, 73, 114, 132	0
All	All	914/968 (94%)	-0.10	27 (2%) 50 45	38, 70, 114, 140	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	226	ASN	3.9
1	A	122	HIS	3.5
1	C	120	GLY	3.2
2	D	305	CYS	3.1
2	D	160	GLY	3.1
2	D	161	ASP	3.0
1	C	121	HIS	3.0
2	D	140	SER	3.0
1	C	37	LEU	2.9
1	C	122	HIS	2.9
2	B	161	ASP	2.7
2	B	99	LYS	2.6
2	D	227	SER	2.6
2	D	225	LYS	2.5
1	C	44	GLU	2.4
1	C	118	PRO	2.3
1	A	120	GLY	2.3
1	C	7	SER	2.3
1	C	129	PRO	2.2
1	A	98	PRO	2.2
1	A	119	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	45	THR	2.2
1	C	130	SER	2.1
1	C	70	CYS	2.1
1	A	121	HIS	2.1
1	C	31	LEU	2.0
1	C	46	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	D	1281	11/12	0.80	0.24	128,130,133,133	0
3	PO4	D	5002	5/5	0.88	0.17	126,129,132,132	0
4	K	D	5003	1/1	0.92	0.08	76,76,76,76	0
4	K	B	5004	1/1	0.95	0.07	73,73,73,73	0
3	PO4	B	5001	5/5	0.98	0.11	88,91,91,94	0

6.5 Other polymers (i)

There are no such residues in this entry.