



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:43 PM GMT

PDB ID : 1LL0
Title : Crystal Structure of Rabbit Muscle Glycogenin
Authors : Gibbons, B.J.; Roach, P.J.; Hurley, T.D.
Deposited on : 2002-04-26
Resolution : 3.43 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 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

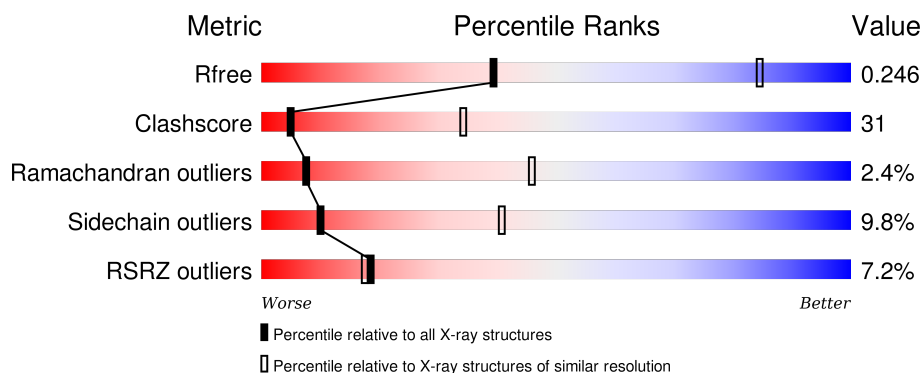
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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}	91344	1007 (3.54-3.34)
Clashscore	102246	1044 (3.52-3.36)
Ramachandran outliers	100387	1013 (3.52-3.36)
Sidechain outliers	100360	1014 (3.52-3.36)
RSRZ outliers	91569	1012 (3.54-3.34)

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

Mol	Chain	Length	Quality of chain
1	A	339	<div> <div>4%</div> <div> <div></div> <div>41%</div> <div>31%</div> <div>6%</div> <div>22%</div> </div> </div>
1	B	339	<div> <div>4%</div> <div> <div></div> <div>42%</div> <div>31%</div> <div>6%</div> <div>21%</div> </div> </div>
1	C	339	<div> <div>3%</div> <div> <div></div> <div>41%</div> <div>31%</div> <div>5%</div> <div>23%</div> </div> </div>
1	D	339	<div> <div>7%</div> <div> <div></div> <div>43%</div> <div>29%</div> <div>5%</div> <div>23%</div> </div> </div>
1	E	339	<div> <div>4%</div> <div> <div></div> <div>41%</div> <div>30%</div> <div>6%</div> <div>23%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	339	<div><div></div><div>6%</div><div>42%</div><div>30%</div><div>5%</div><div>23%</div></div>
1	G	339	<div><div></div><div>5%</div><div>41%</div><div>32%</div><div>5%</div><div>23%</div></div>
1	H	339	<div><div></div><div>6%</div><div>41%</div><div>29%</div><div>6%</div><div>23%</div></div>
1	I	339	<div><div></div><div>5%</div><div>40%</div><div>33%</div><div></div><div>22%</div></div>
1	J	339	<div><div></div><div>12%</div><div>42%</div><div>28%</div><div></div><div>26%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20736 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 GLYCOGENIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2092	1346	342	396	8			
1	B	267	Total	C	N	O	S	0	0	0
			2115	1360	350	397	8			
1	C	262	Total	C	N	O	S	0	0	0
			2077	1337	340	392	8			
1	D	261	Total	C	N	O	S	0	0	0
			2071	1333	339	392	7			
1	E	262	Total	C	N	O	S	0	0	0
			2081	1339	342	393	7			
1	F	261	Total	C	N	O	S	0	0	0
			2071	1333	339	392	7			
1	G	262	Total	C	N	O	S	0	0	0
			2079	1338	340	393	8			
1	H	260	Total	C	N	O	S	0	0	0
			2064	1327	338	391	8			
1	I	264	Total	C	N	O	S	0	0	0
			2095	1346	347	395	7			
1	J	251	Total	C	N	O	S	0	0	0
			1991	1281	327	377	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	VAL	-	EXPRESSION TAG	UNP P13280
A	-6	PRO	-	EXPRESSION TAG	UNP P13280
A	-5	ARG	-	EXPRESSION TAG	UNP P13280
A	-4	GLY	-	EXPRESSION TAG	UNP P13280
A	-3	SER	-	EXPRESSION TAG	UNP P13280
A	-2	HIS	-	EXPRESSION TAG	UNP P13280
B	-7	VAL	-	EXPRESSION TAG	UNP P13280
B	-6	PRO	-	EXPRESSION TAG	UNP P13280
B	-5	ARG	-	EXPRESSION TAG	UNP P13280

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP P13280
B	-3	SER	-	EXPRESSION TAG	UNP P13280
B	-2	HIS	-	EXPRESSION TAG	UNP P13280
C	-7	VAL	-	EXPRESSION TAG	UNP P13280
C	-6	PRO	-	EXPRESSION TAG	UNP P13280
C	-5	ARG	-	EXPRESSION TAG	UNP P13280
C	-4	GLY	-	EXPRESSION TAG	UNP P13280
C	-3	SER	-	EXPRESSION TAG	UNP P13280
C	-2	HIS	-	EXPRESSION TAG	UNP P13280
D	-7	VAL	-	EXPRESSION TAG	UNP P13280
D	-6	PRO	-	EXPRESSION TAG	UNP P13280
D	-5	ARG	-	EXPRESSION TAG	UNP P13280
D	-4	GLY	-	EXPRESSION TAG	UNP P13280
D	-3	SER	-	EXPRESSION TAG	UNP P13280
D	-2	HIS	-	EXPRESSION TAG	UNP P13280
E	-7	VAL	-	EXPRESSION TAG	UNP P13280
E	-6	PRO	-	EXPRESSION TAG	UNP P13280
E	-5	ARG	-	EXPRESSION TAG	UNP P13280
E	-4	GLY	-	EXPRESSION TAG	UNP P13280
E	-3	SER	-	EXPRESSION TAG	UNP P13280
E	-2	HIS	-	EXPRESSION TAG	UNP P13280
F	-7	VAL	-	EXPRESSION TAG	UNP P13280
F	-6	PRO	-	EXPRESSION TAG	UNP P13280
F	-5	ARG	-	EXPRESSION TAG	UNP P13280
F	-4	GLY	-	EXPRESSION TAG	UNP P13280
F	-3	SER	-	EXPRESSION TAG	UNP P13280
F	-2	HIS	-	EXPRESSION TAG	UNP P13280
G	-7	VAL	-	EXPRESSION TAG	UNP P13280
G	-6	PRO	-	EXPRESSION TAG	UNP P13280
G	-5	ARG	-	EXPRESSION TAG	UNP P13280
G	-4	GLY	-	EXPRESSION TAG	UNP P13280
G	-3	SER	-	EXPRESSION TAG	UNP P13280
G	-2	HIS	-	EXPRESSION TAG	UNP P13280
H	-7	VAL	-	EXPRESSION TAG	UNP P13280
H	-6	PRO	-	EXPRESSION TAG	UNP P13280
H	-5	ARG	-	EXPRESSION TAG	UNP P13280
H	-4	GLY	-	EXPRESSION TAG	UNP P13280
H	-3	SER	-	EXPRESSION TAG	UNP P13280
H	-2	HIS	-	EXPRESSION TAG	UNP P13280
I	-7	VAL	-	EXPRESSION TAG	UNP P13280
I	-6	PRO	-	EXPRESSION TAG	UNP P13280
I	-5	ARG	-	EXPRESSION TAG	UNP P13280

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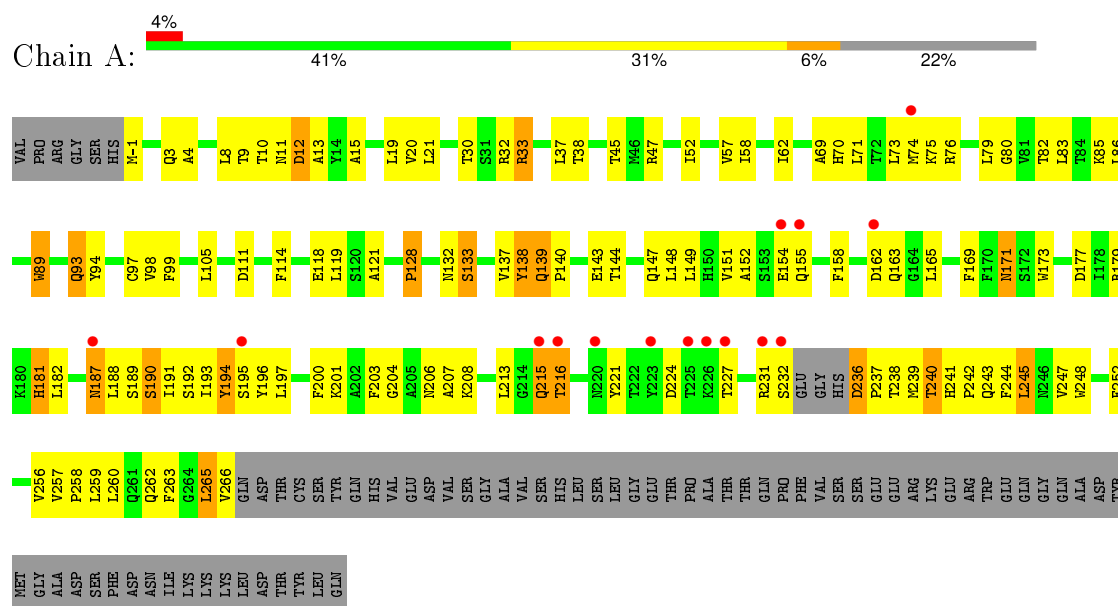
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Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	GLY	-	EXPRESSION TAG	UNP P13280
I	-3	SER	-	EXPRESSION TAG	UNP P13280
I	-2	HIS	-	EXPRESSION TAG	UNP P13280
J	-7	VAL	-	EXPRESSION TAG	UNP P13280
J	-6	PRO	-	EXPRESSION TAG	UNP P13280
J	-5	ARG	-	EXPRESSION TAG	UNP P13280
J	-4	GLY	-	EXPRESSION TAG	UNP P13280
J	-3	SER	-	EXPRESSION TAG	UNP P13280
J	-2	HIS	-	EXPRESSION TAG	UNP P13280

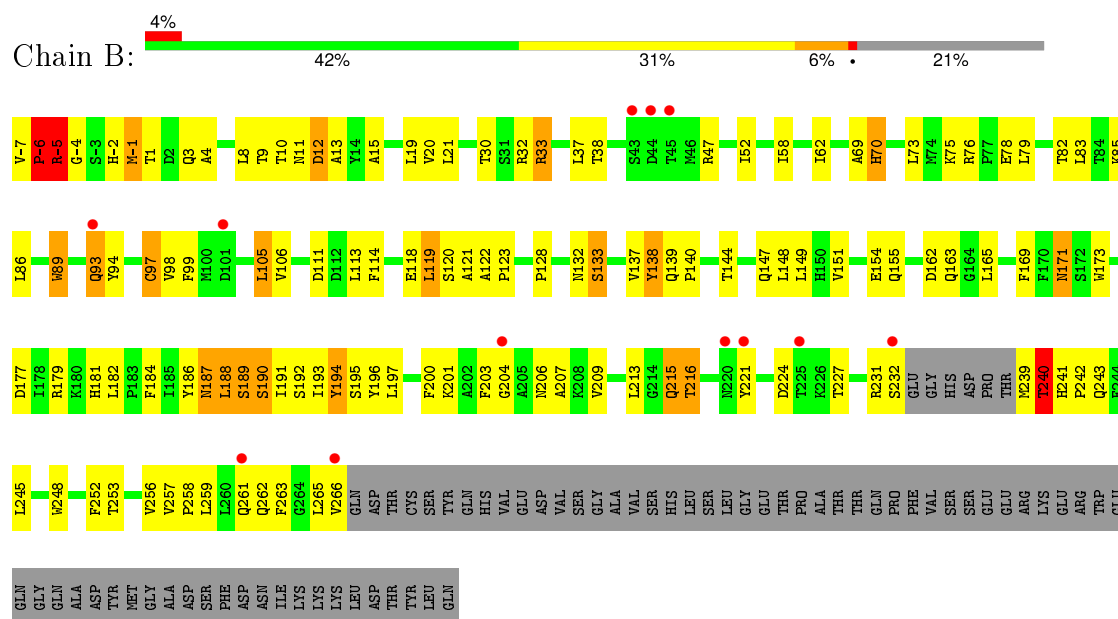
3 Residue-property plots

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

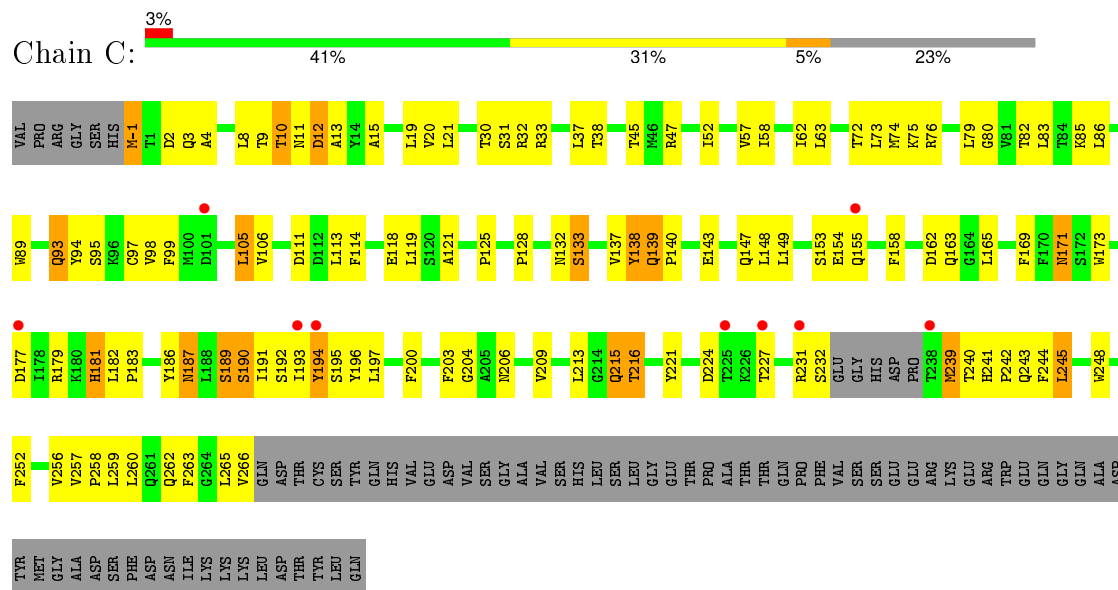
• Molecule 1: GLYCOGENIN-1



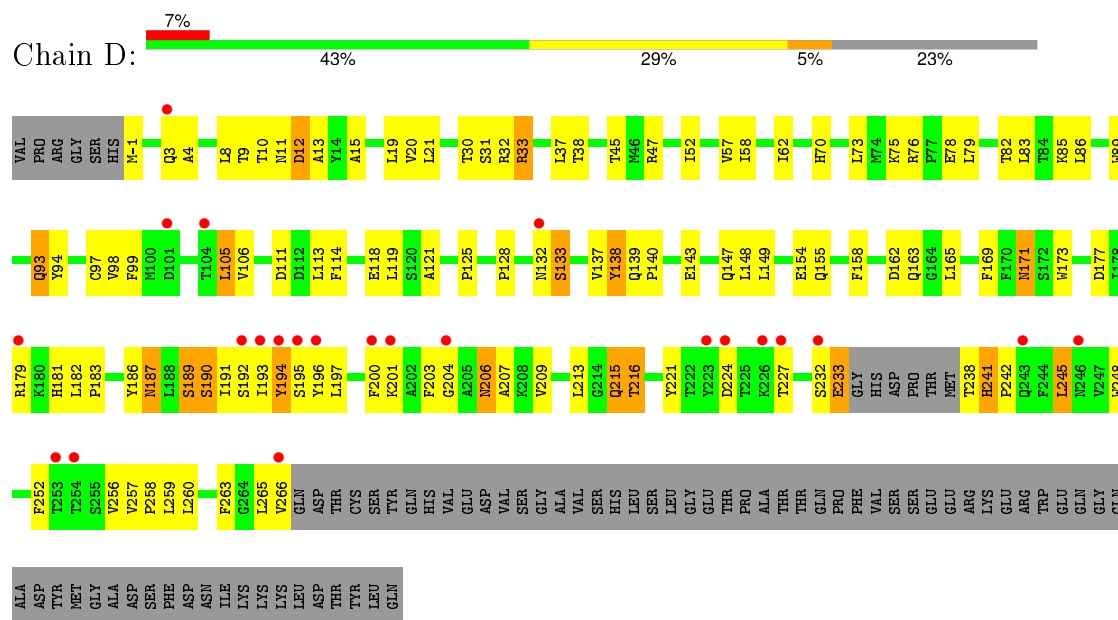
• Molecule 1: GLYCOGENIN-1



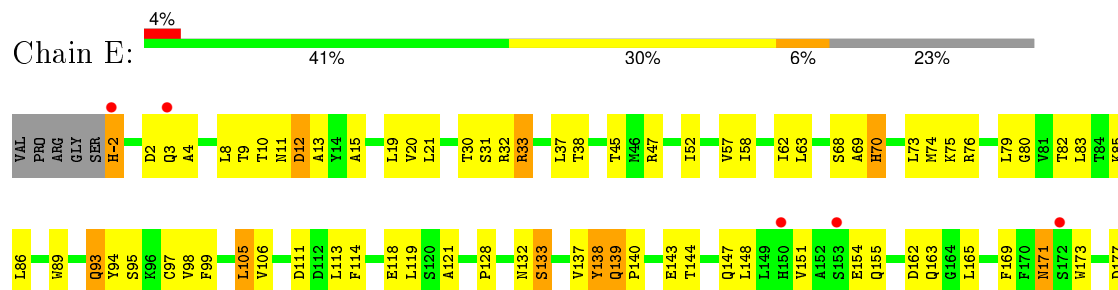
- Molecule 1: GLYCOGENIN-1

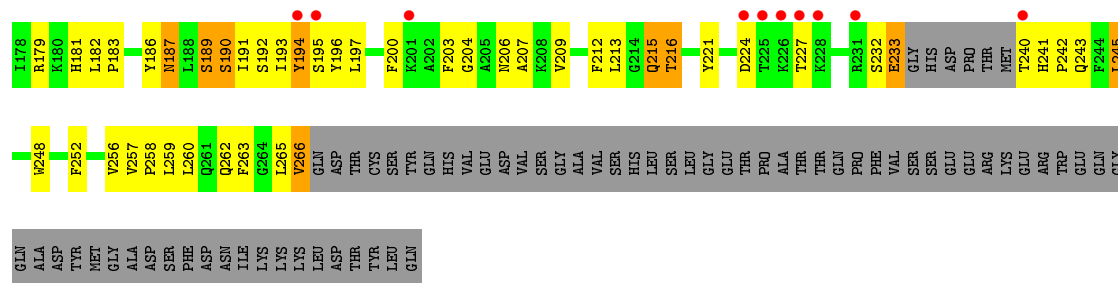


- Molecule 1: GLYCOGENIN-1

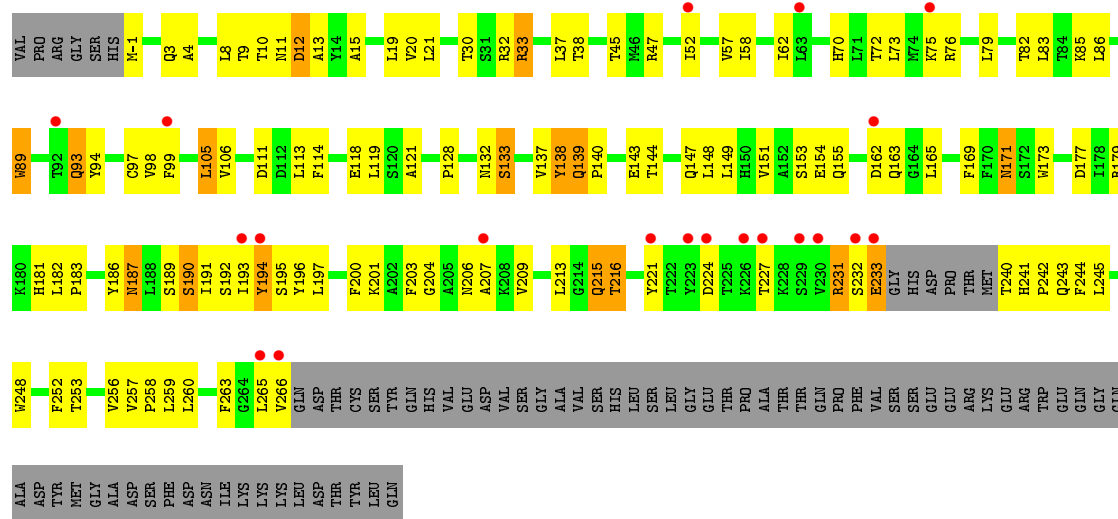


- Molecule 1: GLYCOGENIN-1

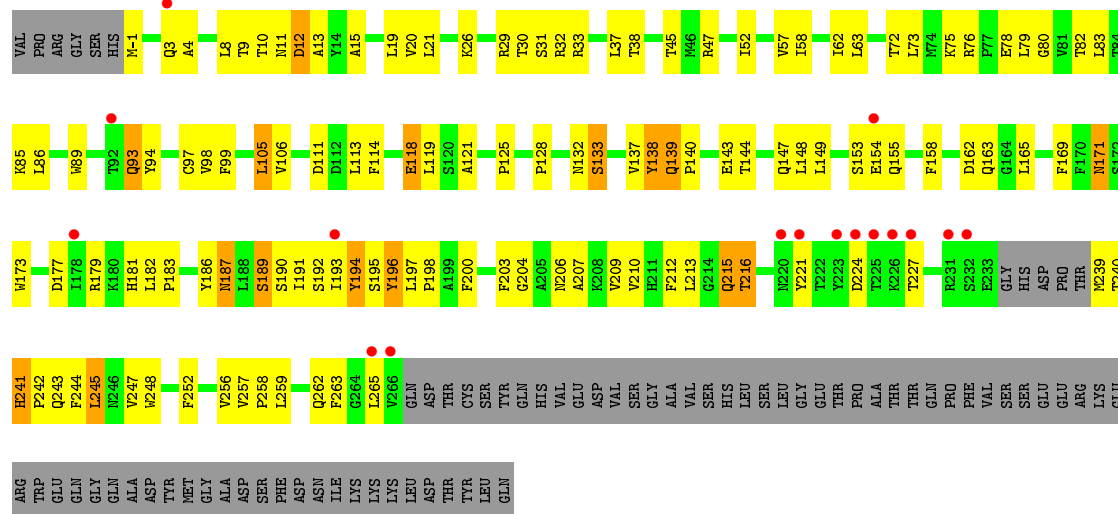




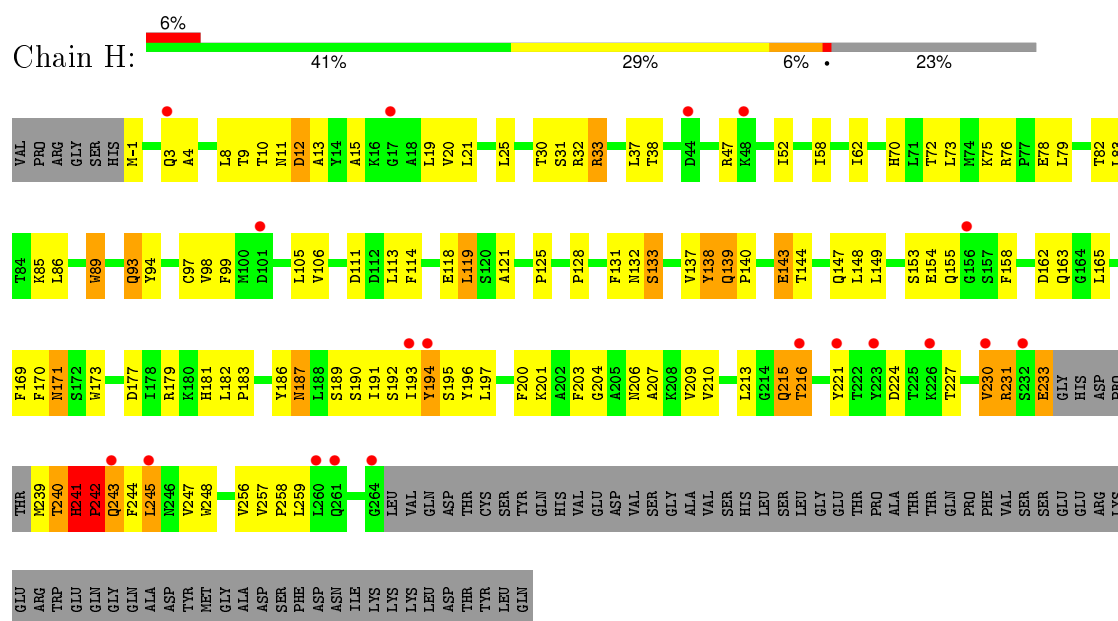
• Molecule 1: GLYCOGENIN-1



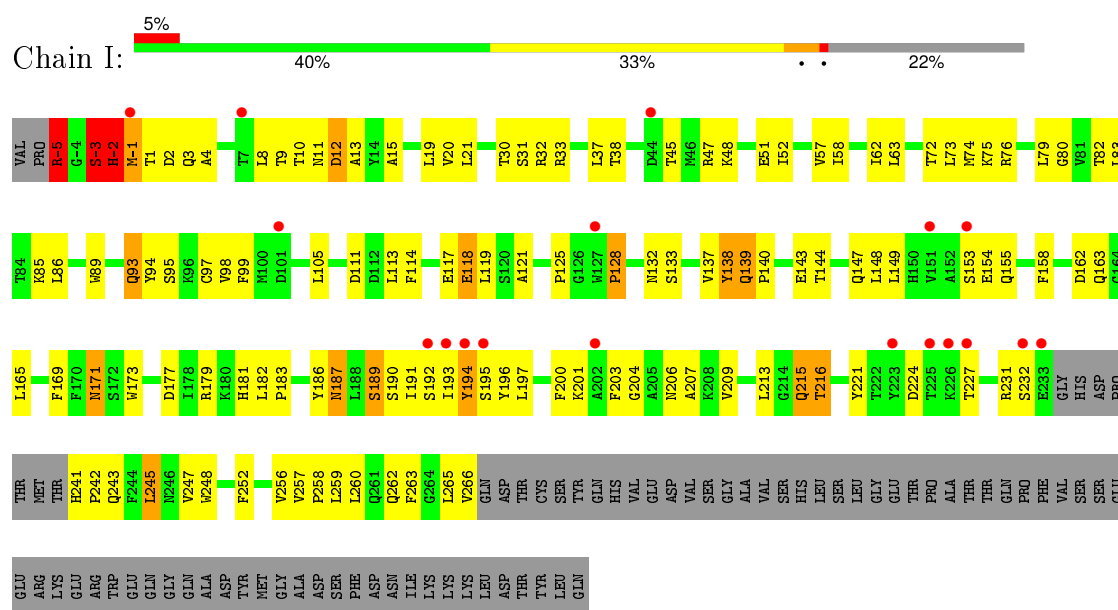
• Molecule 1: GLYCOGENIN-1



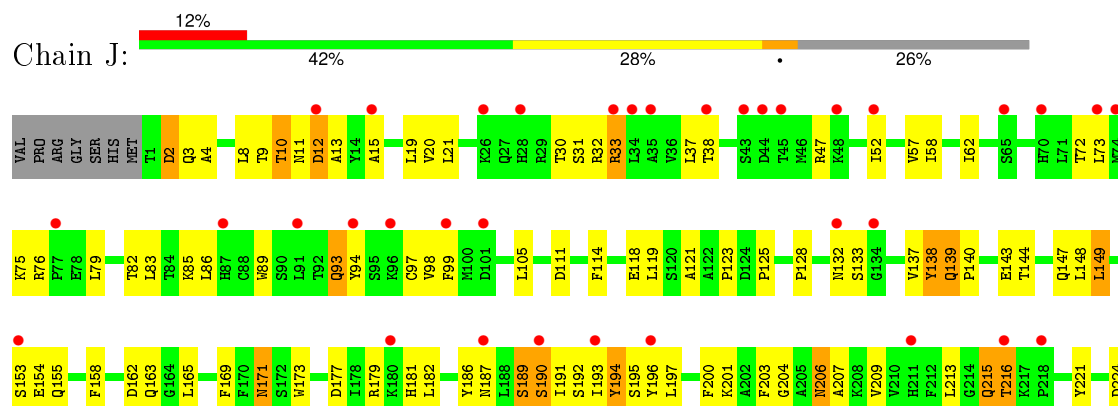
• Molecule 1: GLYCOGENIN-1



• Molecule 1: GLYCOGENIN-1



• Molecule 1: GLYCOGENIN-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.46 Å 139.46 Å 416.46 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.43 29.87 – 3.43	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.00-3.43) 95.8 (29.87-3.43)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 3.47 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.287 0.245 , 0.246	Depositor DCC
R_{free} test set	2718 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	90.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 80.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55974 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	20736	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 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	A	0.55	1/2146 (0.0%)	0.75	4/2927 (0.1%)
1	B	0.64	4/2170 (0.2%)	0.78	6/2958 (0.2%)
1	C	0.52	0/2130	0.70	2/2904 (0.1%)
1	D	0.54	0/2123	0.74	4/2893 (0.1%)
1	E	0.50	0/2135	0.71	3/2911 (0.1%)
1	F	0.52	0/2124	0.73	2/2896 (0.1%)
1	G	0.49	0/2132	0.71	2/2906 (0.1%)
1	H	0.62	2/2117 (0.1%)	0.80	8/2885 (0.3%)
1	I	0.55	2/2149 (0.1%)	0.76	5/2928 (0.2%)
1	J	0.50	0/2043	0.71	3/2787 (0.1%)
All	All	0.55	9/21269 (0.0%)	0.74	39/28995 (0.1%)

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	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	LEU	N-CA	10.90	1.68	1.46
1	H	241	HIS	C-N	8.55	1.50	1.34
1	A	188	LEU	N-CA	8.08	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	241	HIS	CA-C	6.87	1.70	1.52
1	B	120	SER	N-CA	5.77	1.57	1.46
1	B	-4	GLY	C-N	5.68	1.47	1.34
1	I	-1	MET	N-CA	5.28	1.56	1.46
1	B	97	CYS	CB-SG	-5.21	1.73	1.81
1	I	-3	SER	C-O	5.01	1.32	1.23

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	187	ASN	O-C-N	-14.53	99.45	122.70
1	A	208	LYS	N-CA-CB	11.37	131.07	110.60
1	D	187	ASN	O-C-N	-11.09	104.95	122.70
1	H	187	ASN	O-C-N	-11.06	105.00	122.70
1	G	187	ASN	O-C-N	-11.02	105.07	122.70
1	H	241	HIS	C-N-CD	-11.00	96.41	120.60
1	J	187	ASN	O-C-N	-10.84	105.36	122.70
1	I	187	ASN	O-C-N	-10.79	105.44	122.70
1	E	187	ASN	O-C-N	-10.51	105.88	122.70
1	C	187	ASN	O-C-N	-10.07	106.59	122.70
1	F	187	ASN	CA-C-N	8.06	134.93	117.20
1	I	-5	ARG	N-CA-CB	8.03	125.06	110.60
1	G	187	ASN	CA-C-N	6.89	132.37	117.20
1	B	188	LEU	N-CA-CB	-6.79	96.81	110.40
1	D	187	ASN	CA-C-N	6.79	132.14	117.20
1	H	187	ASN	CA-C-N	6.72	131.98	117.20
1	J	187	ASN	CA-C-N	6.68	131.89	117.20
1	I	187	ASN	CA-C-N	6.52	131.54	117.20
1	E	187	ASN	CA-C-N	6.41	131.30	117.20
1	H	241	HIS	CA-C-O	-6.34	106.78	120.10
1	A	188	LEU	N-CA-C	6.33	128.08	111.00
1	B	-6	PRO	CB-CA-C	6.17	127.43	112.00
1	H	241	HIS	CA-C-N	6.06	134.08	117.10
1	B	188	LEU	N-CA-C	5.98	127.15	111.00
1	D	241	HIS	CB-CA-C	-5.86	98.69	110.40
1	H	242	PRO	CA-C-N	-5.76	104.52	117.20
1	C	187	ASN	CA-C-N	5.71	129.77	117.20
1	I	-2	HIS	CB-CA-C	5.67	121.75	110.40
1	H	242	PRO	CA-N-CD	-5.64	103.60	111.50
1	B	120	SER	N-CA-CB	-5.63	102.06	110.50
1	B	119	LEU	CA-C-N	-5.55	105.00	117.20
1	J	2	ASP	CB-CG-OD1	5.37	123.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ASN	C-N-CA	-5.36	108.31	121.70
1	E	266	VAL	CA-C-O	-5.30	108.97	120.10
1	A	187	ASN	C-N-CA	-5.28	108.51	121.70
1	D	241	HIS	C-N-CD	5.24	139.41	128.40
1	H	241	HIS	N-CA-C	5.11	124.81	111.00
1	I	-1	MET	N-CA-CB	5.04	119.67	110.60
1	A	188	LEU	N-CA-CB	-5.02	100.36	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	187	ASN	Mainchain
1	D	187	ASN	Mainchain
1	E	187	ASN	Mainchain
1	F	187	ASN	Mainchain
1	G	187	ASN	Mainchain
1	H	187	ASN	Mainchain
1	I	187	ASN	Mainchain

5.2 Too-close contacts

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	2092	0	2048	155	0
1	B	2115	0	2074	157	0
1	C	2077	0	2037	144	0
1	D	2071	0	2026	109	0
1	E	2081	0	2034	127	0
1	F	2071	0	2026	119	0
1	G	2079	0	2036	137	0
1	H	2064	0	2016	122	0
1	I	2095	0	2048	140	0
1	J	1991	0	1946	100	0
All	All	20736	0	20291	1274	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 31.

All (1274) 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:B:188:LEU:N	1:B:188:LEU:CA	1.68	1.52
1:A:193:ILE:CB	1:A:240:THR:HG21	1.55	1.37
1:B:200:PHE:CE2	1:B:240:THR:HB	1.58	1.36
1:A:193:ILE:HB	1:A:240:THR:CG2	1.57	1.32
1:C:200:PHE:CE2	1:C:240:THR:HB	1.66	1.30
1:B:200:PHE:CZ	1:B:240:THR:HB	1.72	1.24
1:C:193:ILE:HB	1:C:240:THR:CG2	1.67	1.23
1:B:261:GLN:CA	1:B:266:VAL:HG12	1.69	1.21
1:C:193:ILE:CB	1:C:240:THR:HG21	1.73	1.16
1:A:193:ILE:HD12	1:A:240:THR:HG23	1.25	1.13
1:E:240:THR:HG23	1:E:242:PRO:HD2	1.23	1.13
1:A:231:ARG:HG3	1:A:232:SER:H	1.11	1.12
1:B:261:GLN:HA	1:B:266:VAL:HG12	1.11	1.08
1:G:240:THR:HG22	1:G:241:HIS:H	0.93	1.08
1:J:194:TYR:HA	1:J:197:LEU:HD13	1.36	1.08
1:A:193:ILE:HG22	1:A:200:PHE:CD1	1.89	1.07
1:G:194:TYR:HA	1:G:197:LEU:HD13	1.34	1.06
1:C:194:TYR:HA	1:C:197:LEU:HD13	1.31	1.04
1:I:194:TYR:HA	1:I:197:LEU:HD13	1.37	1.04
1:E:194:TYR:HA	1:E:197:LEU:HD13	1.35	1.04
1:B:194:TYR:HA	1:B:197:LEU:HD13	1.33	1.04
1:H:194:TYR:HA	1:H:197:LEU:HD13	1.37	1.03
1:A:194:TYR:HA	1:A:197:LEU:HD13	1.35	1.03
1:G:240:THR:HG22	1:G:241:HIS:N	1.70	1.02
1:C:193:ILE:HD13	1:C:240:THR:HG23	1.40	1.01
1:B:261:GLN:CB	1:B:266:VAL:HG12	1.90	1.01
1:F:215:GLN:HG2	1:F:216:THR:H	1.25	1.01
1:A:240:THR:HG23	1:A:241:HIS:H	1.24	1.01
1:F:194:TYR:HA	1:F:197:LEU:HD13	1.38	1.00
1:B:231:ARG:HG3	1:B:232:SER:H	1.25	1.00
1:D:194:TYR:HA	1:D:197:LEU:HD13	1.38	0.99
1:B:200:PHE:CE2	1:B:240:THR:CB	2.45	0.99
1:B:261:GLN:HG2	1:B:266:VAL:HB	1.44	0.99
1:B:215:GLN:HG2	1:B:216:THR:H	1.26	0.98
1:A:215:GLN:HG2	1:A:216:THR:H	1.27	0.98
1:J:231:ARG:HG3	1:J:232:SER:H	1.27	0.98
1:C:239:MET:O	1:C:243:GLN:HB2	1.64	0.97
1:G:215:GLN:HG2	1:G:216:THR:H	1.30	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLN:HA	1:B:266:VAL:CG1	1.95	0.97
1:E:80:GLY:HA3	1:G:262:GLN:NE2	1.80	0.97
1:J:215:GLN:HG2	1:J:216:THR:H	1.27	0.96
1:C:215:GLN:HG2	1:C:216:THR:H	1.29	0.96
1:I:215:GLN:HG2	1:I:216:THR:H	1.27	0.96
1:D:215:GLN:HG2	1:D:216:THR:H	1.31	0.95
1:G:240:THR:CG2	1:G:241:HIS:H	1.77	0.94
1:A:193:ILE:HB	1:A:240:THR:CB	1.97	0.94
1:C:240:THR:O	1:C:243:GLN:HB3	1.68	0.94
1:B:240:THR:O	1:B:243:GLN:HB3	1.67	0.94
1:E:190:SER:HB2	1:E:241:HIS:CE1	2.03	0.94
1:B:261:GLN:HG2	1:B:266:VAL:CB	1.98	0.94
1:H:215:GLN:HG2	1:H:216:THR:H	1.31	0.94
1:E:215:GLN:HG2	1:E:216:THR:H	1.30	0.94
1:F:231:ARG:HG3	1:F:233:GLU:H	1.32	0.93
1:F:231:ARG:HG3	1:F:232:SER:H	1.31	0.93
1:C:262:GLN:NE2	1:I:80:GLY:HA3	1.82	0.92
1:C:231:ARG:HG3	1:C:232:SER:H	1.31	0.92
1:C:262:GLN:HE22	1:I:80:GLY:HA3	1.34	0.92
1:A:193:ILE:CG1	1:A:240:THR:HG21	1.99	0.92
1:C:239:MET:HB3	1:C:242:PRO:HD2	1.52	0.92
1:A:193:ILE:HB	1:A:240:THR:HG21	0.91	0.91
1:G:212:PHE:CE2	1:G:245:LEU:HD13	2.06	0.91
1:F:215:GLN:HG2	1:F:216:THR:N	1.87	0.90
1:B:187:ASN:C	1:B:188:LEU:CA	2.39	0.90
1:F:190:SER:HB2	1:F:241:HIS:NE2	1.87	0.89
1:C:200:PHE:CE2	1:C:240:THR:CB	2.53	0.89
1:I:93:GLN:HE21	1:I:93:GLN:H	1.20	0.89
1:E:80:GLY:HA3	1:G:262:GLN:HE22	1.38	0.89
1:A:193:ILE:HD12	1:A:240:THR:CG2	2.02	0.88
1:H:93:GLN:H	1:H:93:GLN:HE21	1.21	0.88
1:I:215:GLN:HG2	1:I:216:THR:N	1.89	0.88
1:J:32:ARG:HG3	1:J:114:PHE:CE1	2.10	0.87
1:B:215:GLN:HG2	1:B:216:THR:N	1.88	0.87
1:C:193:ILE:HD13	1:C:240:THR:CG2	2.04	0.86
1:I:48:LYS:HA	1:I:51:GLU:HG3	1.57	0.86
1:B:240:THR:O	1:B:243:GLN:CB	2.22	0.86
1:I:32:ARG:HG3	1:I:114:PHE:CE1	2.10	0.86
1:C:200:PHE:CZ	1:C:240:THR:CB	2.59	0.86
1:A:260:LEU:HB3	1:A:266:VAL:CG2	2.05	0.86
1:C:200:PHE:CZ	1:C:240:THR:OG1	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:GLN:HG2	1:H:216:THR:N	1.91	0.85
1:J:93:GLN:HE21	1:J:93:GLN:H	1.21	0.85
1:A:93:GLN:H	1:A:93:GLN:HE21	1.24	0.85
1:B:188:LEU:N	1:B:188:LEU:CB	2.40	0.85
1:F:32:ARG:HG3	1:F:114:PHE:CE1	2.11	0.85
1:E:190:SER:CB	1:E:241:HIS:CE1	2.60	0.85
1:B:241:HIS:HB3	1:B:242:PRO:HD3	1.59	0.84
1:B:32:ARG:HG3	1:B:114:PHE:CE1	2.13	0.84
1:D:3:GLN:HB2	1:D:32:ARG:HD2	1.59	0.84
1:F:93:GLN:H	1:F:93:GLN:HE21	1.21	0.84
1:D:215:GLN:HG2	1:D:216:THR:N	1.93	0.83
1:G:215:GLN:HG2	1:G:216:THR:N	1.93	0.83
1:A:215:GLN:HG2	1:A:216:THR:N	1.91	0.83
1:C:32:ARG:HG3	1:C:114:PHE:CE1	2.12	0.83
1:G:193:ILE:HD13	1:G:241:HIS:HB3	1.60	0.83
1:J:215:GLN:HG2	1:J:216:THR:N	1.92	0.83
1:A:231:ARG:CG	1:A:232:SER:H	1.90	0.83
1:D:93:GLN:H	1:D:93:GLN:HE21	1.23	0.82
1:H:32:ARG:HG3	1:H:114:PHE:CE1	2.14	0.82
1:G:93:GLN:HE21	1:G:93:GLN:H	1.25	0.82
1:C:200:PHE:CZ	1:C:240:THR:HB	2.14	0.82
1:E:32:ARG:HG3	1:E:114:PHE:CE1	2.14	0.82
1:A:80:GLY:HA3	1:I:262:GLN:NE2	1.94	0.82
1:B:93:GLN:HE21	1:B:93:GLN:H	1.25	0.82
1:A:32:ARG:HG3	1:A:114:PHE:CE1	2.14	0.82
1:H:3:GLN:HB2	1:H:32:ARG:HD2	1.62	0.82
1:H:119:LEU:HG	1:H:170:PHE:CG	2.15	0.82
1:C:215:GLN:HG2	1:C:216:THR:N	1.94	0.81
1:E:215:GLN:HG2	1:E:216:THR:N	1.94	0.81
1:G:32:ARG:HG3	1:G:114:PHE:CE1	2.14	0.81
1:E:93:GLN:HE21	1:E:93:GLN:H	1.28	0.81
1:B:231:ARG:HG3	1:B:232:SER:N	1.95	0.81
1:A:47:ARG:HH11	1:A:47:ARG:HG2	1.44	0.81
1:J:241:HIS:HB3	1:J:242:PRO:HD3	1.62	0.81
1:C:52:ILE:HG23	1:I:74:MET:HE1	1.62	0.81
1:A:240:THR:OG1	1:A:244:PHE:HE1	1.62	0.81
1:C:241:HIS:HB3	1:C:242:PRO:HD3	1.61	0.81
1:D:32:ARG:HG3	1:D:114:PHE:CE1	2.16	0.81
1:D:190:SER:HB2	1:D:241:HIS:CD2	2.14	0.81
1:D:98:VAL:HG22	1:D:137:VAL:HG22	1.63	0.81
1:D:47:ARG:HH11	1:D:47:ARG:HG2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:OD1	1:A:237:PRO:HD2	1.82	0.80
1:G:241:HIS:ND1	1:G:241:HIS:C	2.35	0.80
1:B:200:PHE:CZ	1:B:240:THR:CB	2.63	0.80
1:C:240:THR:OG1	1:C:244:PHE:CE1	2.34	0.80
1:G:240:THR:HB	1:G:242:PRO:HD2	1.63	0.80
1:H:47:ARG:HG2	1:H:47:ARG:HH11	1.43	0.80
1:A:231:ARG:HG3	1:A:232:SER:N	1.94	0.80
1:B:3:GLN:HB2	1:B:32:ARG:HD2	1.61	0.80
1:B:-5:ARG:HG3	1:B:-5:ARG:O	1.79	0.80
1:E:97:CYS:HB2	1:E:138:TYR:CE2	2.16	0.80
1:G:212:PHE:CE2	1:G:245:LEU:CD1	2.64	0.79
1:H:243:GLN:O	1:H:247:VAL:HG23	1.83	0.79
1:A:240:THR:HG23	1:A:241:HIS:N	1.96	0.79
1:A:240:THR:OG1	1:A:244:PHE:CE1	2.35	0.79
1:F:98:VAL:HG22	1:F:137:VAL:HG22	1.64	0.79
1:G:47:ARG:HH11	1:G:47:ARG:HG2	1.47	0.79
1:C:193:ILE:HB	1:C:240:THR:HG21	0.85	0.79
1:B:47:ARG:HG2	1:B:47:ARG:HH11	1.46	0.79
1:C:93:GLN:HE21	1:C:93:GLN:H	1.26	0.79
1:A:240:THR:CG2	1:A:241:HIS:H	1.95	0.79
1:I:3:GLN:HB2	1:I:32:ARG:HD2	1.65	0.79
1:E:3:GLN:HB2	1:E:32:ARG:HD2	1.62	0.78
1:F:97:CYS:HB2	1:F:138:TYR:CE2	2.18	0.78
1:G:97:CYS:HB2	1:G:138:TYR:CE2	2.18	0.78
1:E:233:GLU:HA	1:E:233:GLU:OE1	1.82	0.78
1:G:3:GLN:HB2	1:G:32:ARG:HD2	1.64	0.78
1:H:231:ARG:HD2	1:H:233:GLU:OE2	1.84	0.78
1:J:47:ARG:HH11	1:J:47:ARG:HG2	1.46	0.78
1:E:190:SER:HB2	1:E:241:HIS:ND1	1.98	0.78
1:H:97:CYS:HB2	1:H:138:TYR:CE2	2.19	0.78
1:D:132:ASN:HD22	1:D:163:GLN:HE22	1.32	0.78
1:C:47:ARG:HG2	1:C:47:ARG:HH11	1.49	0.78
1:F:216:THR:HB	1:F:221:TYR:HE1	1.49	0.78
1:I:97:CYS:HB2	1:I:138:TYR:CE2	2.19	0.78
1:I:98:VAL:HG22	1:I:137:VAL:HG22	1.64	0.78
1:C:97:CYS:HB2	1:C:138:TYR:CE2	2.19	0.78
1:B:231:ARG:CG	1:B:232:SER:H	1.96	0.78
1:J:97:CYS:HB2	1:J:138:TYR:CE2	2.19	0.78
1:B:132:ASN:HD22	1:B:163:GLN:HE22	1.31	0.77
1:E:47:ARG:HH11	1:E:47:ARG:HG2	1.49	0.77
1:H:230:VAL:O	1:H:231:ARG:HG2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:CYS:HB2	1:A:138:TYR:CE2	2.18	0.77
1:C:263:PHE:CE2	1:I:63:LEU:HD13	2.18	0.77
1:A:3:GLN:HB2	1:A:32:ARG:HD2	1.65	0.77
1:C:3:GLN:HB2	1:C:32:ARG:HD2	1.67	0.77
1:B:97:CYS:HB2	1:B:138:TYR:CE2	2.20	0.77
1:J:231:ARG:HG3	1:J:232:SER:N	2.00	0.77
1:F:231:ARG:HG3	1:F:232:SER:N	2.00	0.77
1:I:132:ASN:HD22	1:I:163:GLN:HE22	1.32	0.77
1:E:132:ASN:HD22	1:E:163:GLN:HE22	1.31	0.77
1:B:-1:MET:HB2	1:B:32:ARG:HD3	1.66	0.76
1:F:231:ARG:CG	1:F:232:SER:H	1.98	0.76
1:H:98:VAL:HG22	1:H:137:VAL:HG22	1.67	0.76
1:B:261:GLN:HG2	1:B:266:VAL:CG1	2.15	0.76
1:B:216:THR:HB	1:B:221:TYR:HE1	1.50	0.76
1:A:132:ASN:HD22	1:A:163:GLN:HE22	1.31	0.76
1:D:97:CYS:HB2	1:D:138:TYR:CE2	2.20	0.76
1:J:132:ASN:HD22	1:J:163:GLN:HE22	1.34	0.76
1:F:190:SER:CB	1:F:241:HIS:NE2	2.49	0.76
1:E:216:THR:HB	1:E:221:TYR:HE1	1.51	0.75
1:A:193:ILE:CD1	1:A:240:THR:HG23	2.11	0.75
1:G:241:HIS:C	1:G:241:HIS:HD1	1.89	0.75
1:A:241:HIS:HB3	1:A:242:PRO:HD3	1.68	0.75
1:C:132:ASN:HD22	1:C:163:GLN:HE22	1.34	0.75
1:A:262:GLN:HE22	1:G:80:GLY:HA3	1.48	0.75
1:H:216:THR:HB	1:H:221:TYR:HE1	1.51	0.75
1:D:190:SER:HB2	1:D:241:HIS:NE2	2.02	0.75
1:G:193:ILE:CD1	1:G:241:HIS:HB3	2.17	0.75
1:B:9:THR:CG2	1:B:38:THR:HG22	2.17	0.75
1:A:240:THR:O	1:A:243:GLN:HB3	1.86	0.75
1:J:231:ARG:CG	1:J:232:SER:H	1.99	0.75
1:J:216:THR:HB	1:J:221:TYR:HE1	1.52	0.75
1:A:9:THR:CG2	1:A:38:THR:HG22	2.17	0.75
1:D:9:THR:CG2	1:D:38:THR:HG22	2.17	0.75
1:G:193:ILE:HD13	1:G:241:HIS:CB	2.17	0.74
1:B:98:VAL:HG22	1:B:137:VAL:HG22	1.69	0.74
1:F:47:ARG:HH11	1:F:47:ARG:HG2	1.51	0.74
1:A:98:VAL:HG22	1:A:137:VAL:HG22	1.70	0.74
1:A:200:PHE:CE2	1:A:240:THR:HB	2.22	0.74
1:F:132:ASN:HD22	1:F:163:GLN:HE22	1.34	0.74
1:G:9:THR:CG2	1:G:38:THR:HG22	2.17	0.74
1:J:9:THR:CG2	1:J:38:THR:HG22	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:ALA:HA	1:I:182:LEU:HD12	1.69	0.74
1:G:186:TYR:O	1:G:209:VAL:HB	1.87	0.74
1:B:132:ASN:HA	1:B:163:GLN:NE2	2.03	0.74
1:J:257:VAL:HB	1:J:258:PRO:HD3	1.69	0.73
1:F:93:GLN:N	1:F:93:GLN:HE21	1.86	0.73
1:F:9:THR:CG2	1:F:38:THR:HG22	2.17	0.73
1:C:231:ARG:CG	1:C:232:SER:H	2.01	0.73
1:F:93:GLN:H	1:F:93:GLN:NE2	1.86	0.73
1:B:257:VAL:HB	1:B:258:PRO:HD3	1.69	0.73
1:F:132:ASN:HA	1:F:163:GLN:NE2	2.03	0.73
1:B:193:ILE:O	1:B:240:THR:HG21	1.88	0.73
1:G:132:ASN:HD22	1:G:163:GLN:HE22	1.35	0.73
1:I:216:THR:HB	1:I:221:TYR:HE1	1.54	0.73
1:I:93:GLN:H	1:I:93:GLN:NE2	1.87	0.73
1:H:132:ASN:HD22	1:H:163:GLN:HE22	1.36	0.73
1:C:216:THR:HB	1:C:221:TYR:HE1	1.54	0.73
1:B:-7:VAL:C	1:B:-5:ARG:H	1.91	0.73
1:I:9:THR:CG2	1:I:38:THR:HG22	2.19	0.73
1:D:216:THR:HB	1:D:221:TYR:HE1	1.52	0.73
1:J:93:GLN:NE2	1:J:93:GLN:H	1.87	0.73
1:D:132:ASN:HA	1:D:163:GLN:NE2	2.04	0.73
1:B:261:GLN:CB	1:B:266:VAL:CG1	2.67	0.72
1:H:9:THR:CG2	1:H:38:THR:HG22	2.19	0.72
1:C:80:GLY:HA3	1:E:262:GLN:NE2	2.04	0.72
1:A:241:HIS:NE2	1:A:245:LEU:HD11	2.04	0.72
1:A:260:LEU:HB3	1:A:266:VAL:HG23	1.70	0.72
1:A:193:ILE:CG1	1:A:240:THR:CG2	2.67	0.72
1:F:193:ILE:HG22	1:F:200:PHE:CD1	2.25	0.72
1:I:257:VAL:HB	1:I:258:PRO:HD3	1.72	0.72
1:G:98:VAL:HG22	1:G:137:VAL:HG22	1.70	0.72
1:H:47:ARG:NH1	1:H:47:ARG:HG2	2.02	0.72
1:J:47:ARG:NH1	1:J:47:ARG:HG2	2.05	0.72
1:C:132:ASN:HA	1:C:163:GLN:NE2	2.04	0.72
1:C:231:ARG:HG3	1:C:232:SER:N	2.04	0.71
1:B:47:ARG:NH1	1:B:47:ARG:HG2	2.05	0.71
1:C:121:ALA:HA	1:C:182:LEU:HD12	1.72	0.71
1:J:98:VAL:HG22	1:J:137:VAL:HG22	1.70	0.71
1:C:193:ILE:HG22	1:C:200:PHE:CD1	2.26	0.71
1:I:93:GLN:HE21	1:I:93:GLN:N	1.87	0.71
1:A:260:LEU:CB	1:A:266:VAL:CG2	2.68	0.71
1:I:231:ARG:HG3	1:I:232:SER:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:ASN:HA	1:I:163:GLN:NE2	2.05	0.71
1:B:85:LYS:HE3	1:B:99:PHE:CE2	2.25	0.71
1:H:257:VAL:HB	1:H:258:PRO:HD3	1.71	0.71
1:C:9:THR:CG2	1:C:38:THR:HG22	2.20	0.71
1:G:216:THR:HB	1:G:221:TYR:HE1	1.53	0.71
1:J:132:ASN:HA	1:J:163:GLN:NE2	2.06	0.71
1:J:121:ALA:HA	1:J:182:LEU:HD12	1.71	0.71
1:D:93:GLN:H	1:D:93:GLN:NE2	1.89	0.71
1:D:47:ARG:HG2	1:D:47:ARG:NH1	2.05	0.71
1:G:257:VAL:HB	1:G:258:PRO:HD3	1.72	0.71
1:C:98:VAL:HG22	1:C:137:VAL:HG22	1.72	0.71
1:E:85:LYS:HE3	1:E:99:PHE:CE2	2.26	0.71
1:A:47:ARG:NH1	1:A:47:ARG:HG2	2.04	0.71
1:D:257:VAL:HB	1:D:258:PRO:HD3	1.73	0.71
1:H:93:GLN:H	1:H:93:GLN:NE2	1.89	0.70
1:E:98:VAL:HG22	1:E:137:VAL:HG22	1.71	0.70
1:B:261:GLN:CG	1:B:266:VAL:HG12	2.21	0.70
1:G:85:LYS:HE3	1:G:99:PHE:CE2	2.27	0.70
1:H:93:GLN:N	1:H:93:GLN:HE21	1.90	0.70
1:G:121:ALA:HA	1:G:182:LEU:HD12	1.73	0.70
1:A:132:ASN:HA	1:A:163:GLN:NE2	2.06	0.70
1:I:186:TYR:O	1:I:209:VAL:HB	1.91	0.70
1:A:85:LYS:HE3	1:A:99:PHE:CE2	2.27	0.70
1:J:93:GLN:N	1:J:93:GLN:HE21	1.89	0.70
1:D:93:GLN:HE21	1:D:93:GLN:N	1.90	0.70
1:C:74:MET:HE1	1:E:52:ILE:HG23	1.72	0.70
1:B:261:GLN:CA	1:B:266:VAL:CG1	2.60	0.70
1:I:2:ASP:O	1:I:94:TYR:HA	1.92	0.70
1:G:47:ARG:HG2	1:G:47:ARG:NH1	2.04	0.70
1:C:47:ARG:HG2	1:C:47:ARG:NH1	2.06	0.70
1:D:121:ALA:HA	1:D:182:LEU:HD12	1.74	0.70
1:A:216:THR:HB	1:A:221:TYR:HE1	1.54	0.70
1:B:93:GLN:HE21	1:B:93:GLN:N	1.90	0.70
1:F:3:GLN:HB2	1:F:32:ARG:HD2	1.72	0.69
1:E:121:ALA:HA	1:E:182:LEU:HD12	1.74	0.69
1:H:85:LYS:HE3	1:H:99:PHE:CE2	2.27	0.69
1:F:190:SER:CB	1:F:241:HIS:CE1	2.76	0.69
1:B:93:GLN:NE2	1:B:93:GLN:H	1.90	0.69
1:B:193:ILE:HG22	1:B:200:PHE:CD1	2.27	0.69
1:E:233:GLU:CA	1:E:233:GLU:OE1	2.40	0.69
1:E:132:ASN:HA	1:E:163:GLN:NE2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:VAL:HB	1:F:258:PRO:HD3	1.73	0.69
1:E:193:ILE:HG22	1:E:200:PHE:CD1	2.28	0.69
1:H:62:ILE:HD12	1:H:73:LEU:HD22	1.75	0.69
1:J:193:ILE:HG22	1:J:200:PHE:CD1	2.27	0.69
1:B:121:ALA:HA	1:B:182:LEU:HD12	1.74	0.69
1:A:93:GLN:H	1:A:93:GLN:NE2	1.89	0.69
1:E:47:ARG:HG2	1:E:47:ARG:NH1	2.06	0.69
1:D:85:LYS:HE3	1:D:99:PHE:CE2	2.28	0.69
1:F:121:ALA:HA	1:F:182:LEU:HD12	1.74	0.69
1:H:186:TYR:O	1:H:209:VAL:HB	1.91	0.69
1:C:85:LYS:HE3	1:C:99:PHE:CE2	2.28	0.69
1:E:186:TYR:O	1:E:209:VAL:HB	1.93	0.69
1:A:262:GLN:NE2	1:G:80:GLY:HA3	2.07	0.69
1:A:193:ILE:CD1	1:A:240:THR:CG2	2.69	0.69
1:C:240:THR:HG23	1:C:241:HIS:N	2.08	0.69
1:E:240:THR:CG2	1:E:242:PRO:HD2	2.15	0.69
1:E:257:VAL:HB	1:E:258:PRO:HD3	1.74	0.68
1:F:241:HIS:CE1	1:F:244:PHE:HD1	2.11	0.68
1:E:9:THR:CG2	1:E:38:THR:HG22	2.22	0.68
1:A:93:GLN:N	1:A:93:GLN:HE21	1.90	0.68
1:I:85:LYS:HE3	1:I:99:PHE:CE2	2.28	0.68
1:H:132:ASN:HA	1:H:163:GLN:NE2	2.09	0.68
1:A:257:VAL:HB	1:A:258:PRO:HD3	1.74	0.68
1:J:85:LYS:HE3	1:J:99:PHE:CE2	2.28	0.68
1:A:121:ALA:HA	1:A:182:LEU:HD12	1.76	0.68
1:F:62:ILE:HD12	1:F:73:LEU:HD22	1.73	0.68
1:G:193:ILE:HG22	1:G:200:PHE:CD1	2.30	0.67
1:E:-2:HIS:ND1	1:E:-2:HIS:N	2.42	0.67
1:C:257:VAL:HB	1:C:258:PRO:HD3	1.74	0.67
1:G:93:GLN:NE2	1:G:93:GLN:H	1.92	0.67
1:F:47:ARG:HG2	1:F:47:ARG:NH1	2.08	0.67
1:I:62:ILE:HD12	1:I:73:LEU:HD22	1.76	0.67
1:F:186:TYR:O	1:F:209:VAL:HB	1.95	0.67
1:C:240:THR:O	1:C:243:GLN:CB	2.41	0.67
1:I:1:THR:HA	1:I:33:ARG:HD2	1.76	0.67
1:C:93:GLN:NE2	1:C:93:GLN:H	1.92	0.67
1:D:62:ILE:HD12	1:D:73:LEU:HD22	1.76	0.67
1:I:193:ILE:HG22	1:I:200:PHE:CD1	2.30	0.67
1:D:241:HIS:ND1	1:D:245:LEU:CD1	2.58	0.67
1:C:93:GLN:HE21	1:C:93:GLN:N	1.92	0.67
1:J:62:ILE:HD12	1:J:73:LEU:HD22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:CD1	1:C:240:THR:CG2	2.73	0.67
1:G:132:ASN:HA	1:G:163:GLN:NE2	2.10	0.67
1:H:193:ILE:HG22	1:H:200:PHE:CD1	2.30	0.66
1:A:193:ILE:HG22	1:A:200:PHE:CE1	2.30	0.66
1:F:193:ILE:HD13	1:F:241:HIS:HB2	1.76	0.66
1:B:216:THR:HB	1:B:221:TYR:CE1	2.31	0.66
1:H:240:THR:HG23	1:H:242:PRO:HD2	1.78	0.66
1:E:93:GLN:NE2	1:E:93:GLN:H	1.93	0.66
1:G:221:TYR:CD2	1:G:245:LEU:HD23	2.31	0.66
1:G:93:GLN:HE21	1:G:93:GLN:N	1.94	0.66
1:E:93:GLN:HE21	1:E:93:GLN:N	1.94	0.66
1:F:216:THR:HB	1:F:221:TYR:CE1	2.30	0.66
1:C:263:PHE:CZ	1:I:63:LEU:HD22	2.31	0.66
1:C:200:PHE:CD2	1:C:240:THR:HB	2.28	0.65
1:H:216:THR:HB	1:H:221:TYR:CE1	2.31	0.65
1:D:193:ILE:HG22	1:D:200:PHE:CD1	2.31	0.65
1:C:186:TYR:O	1:C:209:VAL:HB	1.95	0.65
1:B:200:PHE:CE2	1:B:240:THR:CG2	2.79	0.65
1:A:193:ILE:CB	1:A:240:THR:CG2	2.39	0.65
1:C:240:THR:HG23	1:C:241:HIS:H	1.59	0.65
1:E:132:ASN:HD22	1:E:163:GLN:NE2	1.94	0.65
1:F:190:SER:HB2	1:F:241:HIS:CE1	2.31	0.65
1:J:216:THR:HB	1:J:221:TYR:CE1	2.31	0.65
1:G:52:ILE:HG21	1:G:259:LEU:HD11	1.78	0.65
1:C:193:ILE:CD1	1:C:240:THR:HG23	2.21	0.64
1:I:1:MET:HB3	1:I:2:ASP:OD1	1.96	0.64
1:E:52:ILE:HG21	1:E:259:LEU:HD11	1.80	0.64
1:H:118:GLU:HB2	1:H:139:GLN:NE2	2.12	0.64
1:G:241:HIS:HE1	1:G:245:LEU:HD22	1.61	0.64
1:G:193:ILE:CD1	1:G:241:HIS:CB	2.75	0.64
1:D:216:THR:HB	1:D:221:TYR:CE1	2.32	0.64
1:A:80:GLY:HA3	1:I:262:GLN:HE22	1.61	0.64
1:E:260:LEU:HB3	1:E:266:VAL:HG23	1.79	0.64
1:D:132:ASN:HD22	1:D:163:GLN:NE2	1.95	0.64
1:B:62:ILE:HD12	1:B:73:LEU:HD22	1.80	0.64
1:E:240:THR:O	1:E:243:GLN:CB	2.46	0.64
1:J:52:ILE:HG21	1:J:259:LEU:HD11	1.79	0.64
1:C:200:PHE:CE1	1:C:204:GLY:HA3	2.33	0.63
1:A:132:ASN:HD22	1:A:163:GLN:NE2	1.95	0.63
1:J:4:ALA:HB2	1:J:33:ARG:HB2	1.81	0.63
1:J:3:GLN:HB2	1:J:32:ARG:HD2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-7:VAL:O	1:B:-5:ARG:N	2.31	0.63
1:C:240:THR:OG1	1:C:244:PHE:HE1	1.79	0.63
1:I:216:THR:HB	1:I:221:TYR:CE1	2.33	0.63
1:B:132:ASN:HD22	1:B:163:GLN:NE2	1.96	0.63
1:D:186:TYR:O	1:D:209:VAL:HB	1.99	0.63
1:E:62:ILE:HD12	1:E:73:LEU:HD22	1.79	0.63
1:F:85:LYS:HE3	1:F:99:PHE:CE2	2.34	0.63
1:H:200:PHE:CD1	1:H:204:GLY:HA3	2.34	0.63
1:A:216:THR:HB	1:A:221:TYR:CE1	2.33	0.63
1:G:216:THR:HB	1:G:221:TYR:CE1	2.34	0.63
1:G:221:TYR:CE2	1:G:245:LEU:HD23	2.34	0.63
1:E:216:THR:HB	1:E:221:TYR:CE1	2.31	0.63
1:A:62:ILE:HD12	1:A:73:LEU:HD22	1.81	0.63
1:E:194:TYR:C	1:E:194:TYR:CD2	2.72	0.62
1:F:194:TYR:CD2	1:F:194:TYR:C	2.72	0.62
1:D:241:HIS:HD1	1:D:245:LEU:CD1	2.11	0.62
1:I:194:TYR:CD2	1:I:194:TYR:C	2.72	0.62
1:I:231:ARG:HG3	1:I:232:SER:N	2.14	0.62
1:B:200:PHE:CD2	1:B:240:THR:CG2	2.81	0.62
1:A:194:TYR:CD2	1:A:194:TYR:C	2.73	0.62
1:B:261:GLN:HG2	1:B:266:VAL:HG12	1.79	0.62
1:C:216:THR:HB	1:C:221:TYR:CE1	2.34	0.62
1:C:200:PHE:CD1	1:C:204:GLY:HA3	2.35	0.62
1:I:200:PHE:CE1	1:I:204:GLY:HA3	2.35	0.62
1:B:186:TYR:O	1:B:209:VAL:HB	1.98	0.62
1:F:194:TYR:HD2	1:F:194:TYR:C	2.03	0.62
1:H:210:VAL:HG22	1:H:244:PHE:CE1	2.35	0.62
1:J:200:PHE:CD1	1:J:204:GLY:HA3	2.35	0.62
1:C:52:ILE:HG21	1:C:259:LEU:HD11	1.82	0.62
1:C:9:THR:HG23	1:C:9:THR:O	2.00	0.62
1:G:194:TYR:C	1:G:194:TYR:CD2	2.73	0.62
1:I:215:GLN:CG	1:I:216:THR:H	2.09	0.62
1:I:-1:MET:CB	1:I:2:ASP:OD1	2.47	0.62
1:E:4:ALA:HB2	1:E:33:ARG:HB2	1.82	0.62
1:G:240:THR:HB	1:G:242:PRO:CD	2.30	0.62
1:A:194:TYR:HD2	1:A:194:TYR:C	2.04	0.62
1:A:241:HIS:CD2	1:A:245:LEU:CD1	2.82	0.61
1:H:194:TYR:C	1:H:194:TYR:HD2	2.03	0.61
1:E:200:PHE:CD1	1:E:204:GLY:HA3	2.35	0.61
1:A:200:PHE:CD1	1:A:204:GLY:HA3	2.35	0.61
1:G:200:PHE:CD1	1:G:204:GLY:HA3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:PHE:CD1	1:I:204:GLY:HA3	2.35	0.61
1:E:194:TYR:HD2	1:E:194:TYR:C	2.03	0.61
1:H:194:TYR:CD2	1:H:194:TYR:C	2.72	0.61
1:C:200:PHE:CE1	1:C:240:THR:OG1	2.51	0.61
1:J:194:TYR:C	1:J:194:TYR:HD2	2.04	0.61
1:I:194:TYR:HD2	1:I:194:TYR:C	2.03	0.61
1:G:62:ILE:HD12	1:G:73:LEU:HD22	1.82	0.61
1:G:9:THR:HG23	1:G:9:THR:O	2.01	0.61
1:A:193:ILE:HG21	1:A:240:THR:OG1	2.01	0.61
1:E:97:CYS:HB2	1:E:138:TYR:HE2	1.64	0.61
1:G:243:GLN:O	1:G:247:VAL:HG23	2.01	0.61
1:J:194:TYR:CD2	1:J:194:TYR:C	2.73	0.60
1:E:58:ILE:H	1:E:58:ILE:HD12	1.66	0.60
1:F:52:ILE:HG21	1:F:259:LEU:HD11	1.82	0.60
1:A:9:THR:HG23	1:A:9:THR:O	2.02	0.60
1:B:4:ALA:HB2	1:B:33:ARG:HB2	1.83	0.60
1:B:187:ASN:O	1:B:188:LEU:CA	2.48	0.60
1:A:200:PHE:CE1	1:A:204:GLY:HA3	2.36	0.60
1:H:200:PHE:CE1	1:H:204:GLY:HA3	2.37	0.60
1:C:194:TYR:HD2	1:C:194:TYR:C	2.05	0.60
1:H:97:CYS:HB2	1:H:138:TYR:HE2	1.65	0.60
1:A:177:ASP:OD1	1:A:179:ARG:HB2	2.01	0.60
1:D:200:PHE:CD1	1:D:204:GLY:HA3	2.36	0.60
1:A:215:GLN:CG	1:A:216:THR:H	2.11	0.60
1:I:132:ASN:HD22	1:I:163:GLN:NE2	1.97	0.60
1:B:-1:MET:CB	1:B:32:ARG:HD3	2.32	0.60
1:J:58:ILE:HD12	1:J:58:ILE:H	1.67	0.60
1:F:58:ILE:HD12	1:F:58:ILE:H	1.67	0.60
1:J:186:TYR:O	1:J:209:VAL:HB	2.01	0.60
1:A:187:ASN:OD1	1:A:187:ASN:O	2.19	0.60
1:C:194:TYR:C	1:C:194:TYR:CD2	2.74	0.60
1:G:194:TYR:C	1:G:194:TYR:HD2	2.04	0.60
1:D:241:HIS:ND1	1:D:245:LEU:HD12	2.17	0.60
1:I:58:ILE:HD12	1:I:58:ILE:H	1.66	0.60
1:C:80:GLY:HA3	1:E:262:GLN:HE22	1.65	0.60
1:I:-5:ARG:HH12	1:I:-2:HIS:CE1	2.20	0.60
1:H:132:ASN:HD22	1:H:163:GLN:NE2	2.00	0.59
1:B:194:TYR:C	1:B:194:TYR:CD2	2.75	0.59
1:H:4:ALA:HB2	1:H:33:ARG:HB2	1.83	0.59
1:A:231:ARG:O	1:A:232:SER:CB	2.51	0.59
1:B:9:THR:HG23	1:B:9:THR:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ASN:C	1:E:171:ASN:HD22	2.06	0.59
1:A:193:ILE:CG2	1:A:240:THR:OG1	2.50	0.59
1:G:240:THR:CG2	1:G:242:PRO:HD3	2.33	0.59
1:D:194:TYR:C	1:D:194:TYR:CD2	2.76	0.59
1:D:143:GLU:O	1:D:147:GLN:HG2	2.03	0.59
1:A:171:ASN:HD22	1:A:171:ASN:C	2.04	0.59
1:I:9:THR:O	1:I:9:THR:HG23	2.02	0.59
1:D:194:TYR:HD2	1:D:194:TYR:C	2.06	0.59
1:D:200:PHE:CE1	1:D:204:GLY:HA3	2.37	0.59
1:G:132:ASN:HD22	1:G:163:GLN:NE2	2.00	0.59
1:D:9:THR:O	1:D:9:THR:HG23	2.03	0.59
1:J:177:ASP:OD1	1:J:179:ARG:HB2	2.03	0.59
1:G:200:PHE:CE1	1:G:204:GLY:HA3	2.37	0.59
1:D:241:HIS:ND1	1:D:245:LEU:HD11	2.17	0.59
1:D:224:ASP:OD1	1:D:227:THR:HG23	2.02	0.59
1:E:240:THR:O	1:E:243:GLN:HB3	2.01	0.58
1:B:215:GLN:CG	1:B:216:THR:H	2.08	0.58
1:B:200:PHE:CD1	1:B:204:GLY:HA3	2.37	0.58
1:F:9:THR:O	1:F:9:THR:HG23	2.03	0.58
1:C:58:ILE:H	1:C:58:ILE:HD12	1.66	0.58
1:I:-5:ARG:NH1	1:I:-2:HIS:CE1	2.71	0.58
1:B:261:GLN:CG	1:B:266:VAL:CG1	2.79	0.58
1:F:97:CYS:HB2	1:F:138:TYR:HE2	1.66	0.58
1:B:193:ILE:O	1:B:240:THR:CG2	2.52	0.58
1:J:132:ASN:HD22	1:J:163:GLN:NE2	1.99	0.58
1:G:58:ILE:H	1:G:58:ILE:HD12	1.68	0.58
1:B:194:TYR:C	1:B:194:TYR:HD2	2.07	0.58
1:G:221:TYR:CE2	1:G:245:LEU:CD2	2.86	0.58
1:J:200:PHE:CE1	1:J:204:GLY:HA3	2.38	0.58
1:B:-6:PRO:O	1:B:-5:ARG:C	2.42	0.58
1:E:9:THR:O	1:E:9:THR:HG23	2.04	0.58
1:B:262:GLN:HG2	1:B:263:PHE:CD1	2.39	0.58
1:B:200:PHE:CD2	1:B:240:THR:HG21	2.39	0.58
1:D:241:HIS:N	1:D:242:PRO:CD	2.66	0.58
1:E:200:PHE:CE1	1:E:204:GLY:HA3	2.38	0.58
1:F:231:ARG:CG	1:F:232:SER:N	2.64	0.58
1:E:63:LEU:HD13	1:G:263:PHE:CE2	2.39	0.58
1:H:75:LYS:HG3	1:H:76:ARG:HG3	1.84	0.58
1:C:52:ILE:HA	1:I:74:MET:HE1	1.86	0.58
1:C:82:THR:HG23	1:C:162:ASP:HA	1.86	0.58
1:B:189:SER:HB2	1:B:213:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:215:GLN:CG	1:G:216:THR:H	2.12	0.57
1:H:52:ILE:HG21	1:H:259:LEU:HD11	1.84	0.57
1:A:82:THR:HG23	1:A:162:ASP:HA	1.86	0.57
1:A:231:ARG:O	1:A:232:SER:HB2	2.03	0.57
1:I:52:ILE:HG21	1:I:259:LEU:HD11	1.85	0.57
1:H:230:VAL:O	1:H:231:ARG:CG	2.50	0.57
1:B:52:ILE:HG21	1:B:259:LEU:HD11	1.87	0.57
1:F:200:PHE:CD1	1:F:204:GLY:HA3	2.39	0.57
1:C:132:ASN:HD22	1:C:163:GLN:NE2	2.00	0.57
1:I:231:ARG:CG	1:I:232:SER:H	2.17	0.57
1:C:193:ILE:CB	1:C:240:THR:CG2	2.55	0.57
1:J:215:GLN:CG	1:J:216:THR:H	2.08	0.57
1:A:58:ILE:H	1:A:58:ILE:HD12	1.70	0.57
1:H:3:GLN:CB	1:H:32:ARG:HD2	2.35	0.57
1:D:52:ILE:HG21	1:D:259:LEU:HD11	1.87	0.57
1:G:240:THR:HG22	1:G:242:PRO:HD3	1.87	0.57
1:F:32:ARG:HG2	1:F:32:ARG:HH11	1.70	0.57
1:G:177:ASP:OD1	1:G:179:ARG:HB2	2.05	0.57
1:D:215:GLN:CG	1:D:216:THR:H	2.12	0.57
1:H:210:VAL:HG21	1:H:244:PHE:CD1	2.40	0.57
1:J:20:VAL:HG21	1:J:248:TRP:CZ2	2.40	0.57
1:B:177:ASP:OD1	1:B:179:ARG:HB2	2.05	0.57
1:E:86:LEU:HD11	1:E:165:LEU:HD23	1.87	0.57
1:F:143:GLU:O	1:F:147:GLN:HG2	2.05	0.56
1:C:62:ILE:HD12	1:C:73:LEU:HD22	1.87	0.56
1:B:200:PHE:CE1	1:B:204:GLY:HA3	2.40	0.56
1:E:-2:HIS:HA	1:E:31:SER:O	2.05	0.56
1:I:125:PRO:O	1:J:125:PRO:O	2.22	0.56
1:H:82:THR:HG23	1:H:162:ASP:HA	1.87	0.56
1:A:241:HIS:CD2	1:A:245:LEU:HD11	2.40	0.56
1:B:-7:VAL:C	1:B:-5:ARG:N	2.58	0.56
1:F:132:ASN:HD22	1:F:163:GLN:NE2	2.00	0.56
1:J:82:THR:HG23	1:J:162:ASP:HA	1.86	0.56
1:I:183:PRO:HD2	1:I:186:TYR:CD2	2.41	0.56
1:I:177:ASP:OD1	1:I:179:ARG:HB2	2.06	0.56
1:F:86:LEU:HD11	1:F:165:LEU:HD23	1.87	0.56
1:F:171:ASN:C	1:F:171:ASN:HD22	2.08	0.56
1:G:75:LYS:HG3	1:G:76:ARG:HG3	1.88	0.56
1:B:75:LYS:HG3	1:B:76:ARG:HG3	1.85	0.56
1:A:190:SER:HA	1:A:193:ILE:HG12	1.88	0.56
1:E:232:SER:O	1:E:233:GLU:C	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:CYS:HB2	1:C:138:TYR:HE2	1.69	0.56
1:C:263:PHE:CZ	1:I:63:LEU:HD13	2.40	0.56
1:D:58:ILE:H	1:D:58:ILE:HD12	1.71	0.56
1:F:193:ILE:CD1	1:F:241:HIS:HB2	2.36	0.56
1:I:97:CYS:HB2	1:I:138:TYR:HE2	1.70	0.56
1:D:82:THR:HG23	1:D:162:ASP:HA	1.88	0.56
1:D:148:LEU:HD23	1:D:169:PHE:CD2	2.41	0.56
1:D:171:ASN:C	1:D:171:ASN:HD22	2.09	0.56
1:A:240:THR:O	1:A:243:GLN:CB	2.54	0.56
1:F:241:HIS:ND1	1:F:244:PHE:HD1	2.04	0.56
1:I:4:ALA:HB2	1:I:33:ARG:HB2	1.88	0.56
1:B:144:THR:HA	1:B:147:GLN:HG3	1.87	0.56
1:B:86:LEU:HD11	1:B:165:LEU:HD23	1.87	0.56
1:F:113:LEU:HD21	1:F:186:TYR:CD1	2.40	0.55
1:H:177:ASP:OD1	1:H:179:ARG:HB2	2.05	0.55
1:E:143:GLU:O	1:E:147:GLN:HG2	2.06	0.55
1:G:171:ASN:HD22	1:G:171:ASN:C	2.09	0.55
1:I:171:ASN:HD22	1:I:171:ASN:C	2.08	0.55
1:C:240:THR:CG2	1:C:241:HIS:H	2.20	0.55
1:E:183:PRO:HD2	1:E:186:TYR:CD2	2.41	0.55
1:J:171:ASN:C	1:J:171:ASN:HD22	2.08	0.55
1:F:200:PHE:CE1	1:F:204:GLY:HA3	2.40	0.55
1:I:48:LYS:CA	1:I:51:GLU:HG3	2.33	0.55
1:B:82:THR:HG23	1:B:162:ASP:HA	1.89	0.55
1:B:97:CYS:HB2	1:B:138:TYR:HE2	1.69	0.55
1:C:148:LEU:HD23	1:C:169:PHE:CD2	2.41	0.55
1:A:52:ILE:HG21	1:A:259:LEU:HD11	1.88	0.55
1:C:143:GLU:O	1:C:147:GLN:HG2	2.06	0.55
1:H:171:ASN:HD22	1:H:171:ASN:C	2.10	0.55
1:D:97:CYS:HB2	1:D:138:TYR:HE2	1.70	0.55
1:D:86:LEU:HD11	1:D:165:LEU:HD23	1.89	0.55
1:E:215:GLN:CG	1:E:216:THR:H	2.12	0.55
1:H:119:LEU:HG	1:H:170:PHE:CB	2.37	0.55
1:F:75:LYS:HG3	1:F:76:ARG:HG3	1.88	0.55
1:B:193:ILE:HB	1:B:240:THR:OG1	2.07	0.55
1:B:266:VAL:HG23	1:B:266:VAL:O	2.07	0.55
1:B:-7:VAL:HG13	1:B:-7:VAL:O	2.07	0.55
1:B:224:ASP:OD1	1:B:227:THR:HG23	2.07	0.55
1:F:82:THR:HG23	1:F:162:ASP:HA	1.88	0.55
1:I:82:THR:HG23	1:I:162:ASP:HA	1.88	0.55
1:H:20:VAL:HG21	1:H:248:TRP:CZ2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASN:HD22	1:B:171:ASN:C	2.09	0.55
1:F:215:GLN:CG	1:F:216:THR:H	2.07	0.54
1:H:215:GLN:CG	1:H:216:THR:H	2.12	0.54
1:H:32:ARG:HG2	1:H:32:ARG:HH11	1.71	0.54
1:G:143:GLU:O	1:G:147:GLN:HG2	2.08	0.54
1:D:241:HIS:CB	1:D:242:PRO:HD3	2.38	0.54
1:E:74:MET:HE2	1:G:52:ILE:HG23	1.88	0.54
1:F:177:ASP:OD1	1:F:179:ARG:HB2	2.06	0.54
1:I:20:VAL:HG21	1:I:248:TRP:CZ2	2.42	0.54
1:B:76:ARG:HG2	1:B:76:ARG:HH11	1.73	0.54
1:C:75:LYS:HG3	1:C:76:ARG:HG3	1.89	0.54
1:E:82:THR:HG23	1:E:162:ASP:HA	1.89	0.54
1:A:75:LYS:HG3	1:A:76:ARG:HG3	1.89	0.54
1:A:32:ARG:HH11	1:A:32:ARG:HG2	1.72	0.54
1:H:9:THR:HG23	1:H:9:THR:O	2.08	0.54
1:F:224:ASP:OD1	1:F:227:THR:HG23	2.08	0.54
1:J:231:ARG:CG	1:J:232:SER:N	2.67	0.54
1:B:58:ILE:HD12	1:B:58:ILE:H	1.73	0.54
1:E:32:ARG:HG2	1:E:32:ARG:HH11	1.73	0.54
1:J:52:ILE:HG21	1:J:259:LEU:CD1	2.37	0.54
1:G:76:ARG:HH11	1:G:76:ARG:HG2	1.72	0.54
1:C:12:ASP:O	1:C:15:ALA:HB3	2.08	0.54
1:G:86:LEU:HD11	1:G:165:LEU:HD23	1.89	0.54
1:H:243:GLN:OE1	1:H:243:GLN:O	2.25	0.54
1:I:128:PRO:CG	1:J:123:PRO:HG2	2.38	0.54
1:G:82:THR:HG23	1:G:162:ASP:HA	1.90	0.54
1:G:148:LEU:HD23	1:G:169:PHE:CD2	2.43	0.54
1:I:32:ARG:HG2	1:I:32:ARG:HH11	1.73	0.53
1:G:183:PRO:HD2	1:G:186:TYR:CD2	2.42	0.53
1:G:76:ARG:NH1	1:G:76:ARG:HG2	2.23	0.53
1:J:86:LEU:HD11	1:J:165:LEU:HD23	1.89	0.53
1:J:148:LEU:HD23	1:J:169:PHE:CD2	2.43	0.53
1:I:86:LEU:HD11	1:I:165:LEU:HD23	1.90	0.53
1:B:32:ARG:HG2	1:B:32:ARG:HH11	1.73	0.53
1:D:241:HIS:CE1	1:D:245:LEU:HD11	2.43	0.53
1:J:75:LYS:HG3	1:J:76:ARG:HG3	1.90	0.53
1:I:2:ASP:OD1	1:I:3:GLN:N	2.42	0.53
1:E:75:LYS:HG3	1:E:76:ARG:HG3	1.89	0.53
1:C:52:ILE:HA	1:I:74:MET:CE	2.38	0.53
1:A:20:VAL:HG21	1:A:248:TRP:CZ2	2.43	0.53
1:H:58:ILE:H	1:H:58:ILE:HD12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:LEU:HD21	1:I:186:TYR:CD1	2.44	0.53
1:J:213:LEU:HD23	1:J:213:LEU:H	1.74	0.53
1:C:171:ASN:HD22	1:C:171:ASN:C	2.12	0.53
1:A:8:LEU:HD12	1:A:37:LEU:O	2.09	0.53
1:I:143:GLU:O	1:I:147:GLN:HG2	2.08	0.53
1:A:86:LEU:HD11	1:A:165:LEU:HD23	1.91	0.53
1:E:2:HIS:N	1:E:31:SER:HB2	2.24	0.53
1:D:177:ASP:OD1	1:D:179:ARG:HB2	2.09	0.53
1:C:86:LEU:HD11	1:C:165:LEU:HD23	1.90	0.53
1:J:215:GLN:HG2	1:J:216:THR:OG1	2.09	0.53
1:C:213:LEU:H	1:C:213:LEU:HD23	1.73	0.53
1:I:148:LEU:HD23	1:I:169:PHE:CD2	2.43	0.53
1:F:190:SER:HB3	1:F:241:HIS:CE1	2.42	0.53
1:I:215:GLN:HG2	1:I:216:THR:OG1	2.09	0.53
1:I:241:HIS:HB3	1:I:242:PRO:HD3	1.91	0.53
1:G:97:CYS:HB2	1:G:138:TYR:HE2	1.68	0.53
1:H:148:LEU:HD23	1:H:169:PHE:CD2	2.43	0.53
1:A:4:ALA:HB2	1:A:33:ARG:HB2	1.89	0.53
1:G:113:LEU:HD21	1:G:186:TYR:CD1	2.44	0.52
1:J:12:ASP:O	1:J:15:ALA:HB3	2.09	0.52
1:H:118:GLU:HB2	1:H:139:GLN:HE21	1.73	0.52
1:D:113:LEU:HD21	1:D:186:TYR:CD1	2.44	0.52
1:H:86:LEU:HD11	1:H:165:LEU:HD23	1.90	0.52
1:J:143:GLU:O	1:J:147:GLN:HG2	2.08	0.52
1:J:8:LEU:HD12	1:J:9:THR:H	1.74	0.52
1:E:183:PRO:HD2	1:E:186:TYR:CE2	2.45	0.52
1:F:183:PRO:HD2	1:F:186:TYR:CD2	2.44	0.52
1:H:240:THR:HG23	1:H:242:PRO:CD	2.39	0.52
1:H:94:TYR:O	1:H:140:PRO:HG2	2.10	0.52
1:G:215:GLN:HG2	1:G:216:THR:OG1	2.09	0.52
1:F:8:LEU:HD12	1:F:9:THR:H	1.73	0.52
1:C:8:LEU:HD12	1:C:9:THR:H	1.75	0.52
1:C:76:ARG:HG2	1:C:76:ARG:HH11	1.75	0.52
1:C:76:ARG:HG2	1:C:76:ARG:NH1	2.24	0.52
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.74	0.52
1:D:94:TYR:O	1:D:140:PRO:HG2	2.10	0.52
1:C:260:LEU:HB3	1:C:266:VAL:HG23	1.91	0.52
1:A:94:TYR:O	1:A:140:PRO:HG2	2.09	0.52
1:H:8:LEU:HD12	1:H:9:THR:H	1.74	0.52
1:B:20:VAL:HG21	1:B:248:TRP:CZ2	2.43	0.52
1:I:12:ASP:O	1:I:15:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:LEU:H	1:H:213:LEU:HD23	1.75	0.52
1:H:183:PRO:HD2	1:H:186:TYR:CD2	2.44	0.52
1:C:63:LEU:HD13	1:E:263:PHE:CE2	2.44	0.52
1:B:-5:ARG:HD2	1:B:-2:HIS:HD2	1.74	0.52
1:A:97:CYS:HB2	1:A:138:TYR:HE2	1.69	0.52
1:A:74:MET:HE2	1:I:52:ILE:HG23	1.92	0.52
1:F:193:ILE:HG12	1:F:241:HIS:ND1	2.25	0.52
1:H:119:LEU:HG	1:H:170:PHE:CD2	2.44	0.52
1:J:8:LEU:HD12	1:J:37:LEU:O	2.10	0.52
1:H:113:LEU:HD21	1:H:186:TYR:CD1	2.44	0.52
1:E:76:ARG:HG2	1:E:76:ARG:HH11	1.74	0.52
1:C:177:ASP:OD1	1:C:179:ARG:HB2	2.10	0.52
1:D:32:ARG:HG2	1:D:32:ARG:HH11	1.74	0.52
1:I:8:LEU:HD12	1:I:9:THR:H	1.75	0.52
1:I:75:LYS:HG3	1:I:76:ARG:HG3	1.91	0.52
1:A:173:TRP:O	1:A:181:HIS:HE1	1.93	0.52
1:F:4:ALA:HB2	1:F:33:ARG:HB2	1.92	0.52
1:B:257:VAL:HG12	1:B:261:GLN:CD	2.30	0.52
1:G:242:PRO:O	1:G:245:LEU:N	2.42	0.52
1:J:3:GLN:HB3	1:J:114:PHE:CE2	2.45	0.52
1:A:260:LEU:HB2	1:A:266:VAL:HG21	1.90	0.52
1:G:8:LEU:HD12	1:G:37:LEU:O	2.10	0.52
1:B:76:ARG:HG2	1:B:76:ARG:NH1	2.25	0.52
1:I:76:ARG:HH11	1:I:76:ARG:HG2	1.74	0.52
1:G:224:ASP:OD1	1:G:227:THR:HG23	2.10	0.52
1:E:177:ASP:OD1	1:E:179:ARG:HB2	2.10	0.51
1:J:9:THR:O	1:J:9:THR:HG23	2.10	0.51
1:I:183:PRO:HD2	1:I:186:TYR:CE2	2.45	0.51
1:F:20:VAL:HG21	1:F:248:TRP:CZ2	2.45	0.51
1:G:4:ALA:HB2	1:G:33:ARG:HB2	1.91	0.51
1:B:215:GLN:HG2	1:B:216:THR:OG1	2.11	0.51
1:J:32:ARG:HH11	1:J:32:ARG:HG2	1.75	0.51
1:D:241:HIS:HB3	1:D:242:PRO:CD	2.40	0.51
1:C:215:GLN:HG2	1:C:216:THR:OG1	2.10	0.51
1:A:11:ASN:OD1	1:A:13:ALA:N	2.42	0.51
1:A:8:LEU:HD12	1:A:9:THR:H	1.76	0.51
1:G:8:LEU:HD12	1:G:9:THR:H	1.74	0.51
1:I:213:LEU:HD23	1:I:213:LEU:H	1.75	0.51
1:G:125:PRO:O	1:H:125:PRO:O	2.29	0.51
1:C:240:THR:CG2	1:C:241:HIS:N	2.73	0.51
1:F:215:GLN:HG2	1:F:216:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:ASP:O	1:I:94:TYR:CA	2.58	0.51
1:H:183:PRO:HD2	1:H:186:TYR:CE2	2.46	0.51
1:I:76:ARG:NH1	1:I:76:ARG:HG2	2.25	0.51
1:F:148:LEU:HD23	1:F:169:PHE:CD2	2.45	0.51
1:C:4:ALA:HB2	1:C:33:ARG:HB2	1.93	0.51
1:E:76:ARG:NH1	1:E:76:ARG:HG2	2.26	0.51
1:B:187:ASN:O	1:B:187:ASN:OD1	2.27	0.51
1:I:94:TYR:O	1:I:140:PRO:HG2	2.10	0.51
1:E:189:SER:HB2	1:E:213:LEU:HD21	1.92	0.51
1:I:11:ASN:OD1	1:I:13:ALA:N	2.43	0.51
1:D:12:ASP:O	1:D:15:ALA:HB3	2.11	0.51
1:D:241:HIS:HB3	1:D:242:PRO:HD3	1.92	0.51
1:E:58:ILE:N	1:E:58:ILE:HD12	2.25	0.51
1:A:76:ARG:NH1	1:A:76:ARG:HG2	2.25	0.51
1:C:20:VAL:HG21	1:C:248:TRP:CZ2	2.45	0.51
1:E:148:LEU:HD23	1:E:169:PHE:CD2	2.46	0.51
1:B:241:HIS:HB3	1:B:242:PRO:CD	2.36	0.51
1:H:121:ALA:HA	1:H:182:LEU:HD12	1.92	0.51
1:J:97:CYS:HB2	1:J:138:TYR:HE2	1.71	0.51
1:J:19:LEU:HD13	1:J:256:VAL:HG13	1.93	0.51
1:H:37:LEU:HD23	1:H:58:ILE:HB	1.93	0.51
1:A:238:THR:HG22	1:A:238:THR:O	2.10	0.51
1:H:215:GLN:HG2	1:H:216:THR:OG1	2.10	0.50
1:H:76:ARG:HG2	1:H:76:ARG:HH11	1.76	0.50
1:J:11:ASN:OD1	1:J:13:ALA:N	2.41	0.50
1:E:12:ASP:O	1:E:15:ALA:HB3	2.11	0.50
1:E:113:LEU:HD21	1:E:186:TYR:CD1	2.45	0.50
1:E:260:LEU:HB3	1:E:266:VAL:CG2	2.40	0.50
1:I:-3:SER:O	1:I:-2:HIS:HB3	2.12	0.50
1:I:-5:ARG:CD	1:I:-5:ARG:O	2.60	0.50
1:G:20:VAL:HG21	1:G:248:TRP:CZ2	2.46	0.50
1:F:94:TYR:O	1:F:140:PRO:HG2	2.11	0.50
1:C:11:ASN:OD1	1:C:13:ALA:N	2.43	0.50
1:C:190:SER:HB2	1:C:241:HIS:ND1	2.26	0.50
1:J:58:ILE:HD12	1:J:58:ILE:N	2.26	0.50
1:E:213:LEU:H	1:E:213:LEU:HD23	1.76	0.50
1:G:183:PRO:HD2	1:G:186:TYR:CE2	2.46	0.50
1:E:8:LEU:HD12	1:E:9:THR:H	1.76	0.50
1:D:20:VAL:HG21	1:D:248:TRP:CZ2	2.47	0.50
1:D:260:LEU:HB3	1:D:266:VAL:HG23	1.94	0.50
1:B:8:LEU:HD12	1:B:9:THR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:GLU:O	1:H:147:GLN:HG2	2.10	0.50
1:D:76:ARG:HH11	1:D:76:ARG:HG2	1.76	0.50
1:B:192:SER:HA	1:B:195:SER:HB3	1.93	0.50
1:C:58:ILE:HD12	1:C:58:ILE:N	2.27	0.50
1:F:183:PRO:HD2	1:F:186:TYR:CE2	2.46	0.50
1:D:75:LYS:HG3	1:D:76:ARG:HG3	1.93	0.50
1:D:189:SER:HB2	1:D:213:LEU:HD21	1.94	0.50
1:H:11:ASN:OD1	1:H:13:ALA:N	2.44	0.50
1:F:213:LEU:HD23	1:F:213:LEU:H	1.76	0.50
1:A:224:ASP:OD1	1:A:227:THR:HG23	2.12	0.50
1:F:12:ASP:O	1:F:15:ALA:HB3	2.12	0.50
1:I:133:SER:H	1:I:163:GLN:HE21	1.60	0.50
1:F:58:ILE:HD12	1:F:58:ILE:N	2.27	0.50
1:G:12:ASP:O	1:G:15:ALA:HB3	2.12	0.50
1:G:173:TRP:O	1:G:181:HIS:HE1	1.95	0.50
1:B:184:PHE:O	1:B:188:LEU:N	2.45	0.49
1:E:215:GLN:HG2	1:E:216:THR:OG1	2.12	0.49
1:A:37:LEU:HD23	1:A:58:ILE:HB	1.94	0.49
1:I:128:PRO:HG2	1:J:123:PRO:HG2	1.94	0.49
1:J:224:ASP:OD1	1:J:227:THR:HG23	2.12	0.49
1:I:193:ILE:HA	1:I:200:PHE:HB2	1.94	0.49
1:C:215:GLN:CG	1:C:216:THR:H	2.11	0.49
1:I:52:ILE:HG21	1:I:259:LEU:CD1	2.42	0.49
1:C:63:LEU:HD22	1:E:263:PHE:CZ	2.46	0.49
1:F:37:LEU:HD23	1:F:58:ILE:HB	1.94	0.49
1:G:52:ILE:HG21	1:G:259:LEU:CD1	2.42	0.49
1:H:210:VAL:CG2	1:H:244:PHE:CD1	2.96	0.49
1:H:224:ASP:OD1	1:H:227:THR:HG23	2.12	0.49
1:B:94:TYR:O	1:B:140:PRO:HG2	2.12	0.49
1:D:8:LEU:HD12	1:D:9:THR:H	1.76	0.49
1:B:144:THR:O	1:B:147:GLN:HB2	2.13	0.49
1:A:45:THR:CG2	1:A:265:LEU:HD23	2.43	0.49
1:B:231:ARG:CG	1:B:232:SER:N	2.63	0.49
1:E:52:ILE:HG21	1:E:259:LEU:CD1	2.42	0.49
1:B:213:LEU:HD23	1:B:213:LEU:H	1.77	0.49
1:F:76:ARG:HG2	1:F:76:ARG:HH11	1.78	0.49
1:G:11:ASN:OD1	1:G:13:ALA:N	2.42	0.49
1:H:12:ASP:O	1:H:15:ALA:HB3	2.13	0.49
1:D:190:SER:CB	1:D:241:HIS:NE2	2.75	0.49
1:G:58:ILE:HD12	1:G:58:ILE:N	2.28	0.49
1:J:37:LEU:HD23	1:J:58:ILE:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ARG:NH1	1:D:76:ARG:HG2	2.28	0.49
1:F:189:SER:HB2	1:F:213:LEU:HD21	1.95	0.49
1:A:200:PHE:CD2	1:A:240:THR:HB	2.48	0.49
1:D:37:LEU:HD23	1:D:58:ILE:HB	1.93	0.49
1:E:8:LEU:HD12	1:E:37:LEU:O	2.11	0.49
1:A:148:LEU:HD23	1:A:169:PHE:CD2	2.47	0.49
1:F:241:HIS:CE1	1:F:244:PHE:CD1	2.97	0.49
1:H:76:ARG:NH1	1:H:76:ARG:HG2	2.28	0.49
1:J:76:ARG:NH1	1:J:76:ARG:HG2	2.28	0.49
1:F:260:LEU:HB3	1:F:266:VAL:HG23	1.93	0.49
1:J:94:TYR:O	1:J:140:PRO:HG2	2.12	0.49
1:F:52:ILE:HG21	1:F:259:LEU:CD1	2.43	0.49
1:D:213:LEU:HD23	1:D:213:LEU:H	1.78	0.49
1:G:94:TYR:O	1:G:140:PRO:HG2	2.12	0.49
1:A:239:MET:O	1:A:243:GLN:HB2	2.12	0.48
1:E:241:HIS:CD2	1:E:245:LEU:CD1	2.96	0.48
1:A:58:ILE:HD12	1:A:58:ILE:N	2.28	0.48
1:H:210:VAL:CG2	1:H:244:PHE:CE1	2.95	0.48
1:A:143:GLU:O	1:A:147:GLN:HG2	2.13	0.48
1:A:213:LEU:H	1:A:213:LEU:HD23	1.78	0.48
1:G:31:SER:OG	1:G:32:ARG:NH1	2.47	0.48
1:C:3:GLN:CB	1:C:32:ARG:HD2	2.40	0.48
1:F:133:SER:H	1:F:163:GLN:HE21	1.61	0.48
1:J:76:ARG:HG2	1:J:76:ARG:HH11	1.77	0.48
1:J:173:TRP:O	1:J:181:HIS:HE1	1.95	0.48
1:A:190:SER:HA	1:A:193:ILE:CD1	2.43	0.48
1:F:190:SER:HB2	1:F:241:HIS:CD2	2.49	0.48
1:A:9:THR:HG21	1:A:38:THR:HG22	1.95	0.48
1:I:58:ILE:N	1:I:58:ILE:HD12	2.28	0.48
1:H:239:MET:C	1:H:240:THR:O	2.51	0.48
1:B:1:THR:HA	1:B:33:ARG:HD2	1.95	0.48
1:F:192:SER:HA	1:F:195:SER:HB3	1.95	0.48
1:E:240:THR:O	1:E:243:GLN:HB2	2.13	0.48
1:I:1:MET:O	1:I:33:ARG:HG2	2.14	0.48
1:C:19:LEU:HD13	1:C:256:VAL:HG13	1.96	0.48
1:E:86:LEU:HD11	1:E:165:LEU:CD2	2.43	0.48
1:I:260:LEU:HB3	1:I:266:VAL:HG23	1.94	0.48
1:D:11:ASN:OD1	1:D:13:ALA:N	2.44	0.48
1:F:252:PHE:O	1:F:257:VAL:HG23	2.13	0.48
1:G:32:ARG:HH11	1:G:32:ARG:HG2	1.78	0.48
1:I:19:LEU:HD13	1:I:256:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:HIS:ND1	1:G:241:HIS:O	2.33	0.48
1:D:193:ILE:HA	1:D:200:PHE:HB2	1.96	0.48
1:E:47:ARG:CG	1:E:47:ARG:HH11	2.23	0.48
1:F:173:TRP:O	1:F:181:HIS:HE1	1.97	0.48
1:C:191:ILE:HG13	1:C:192:SER:N	2.29	0.48
1:E:94:TYR:O	1:E:140:PRO:HG2	2.12	0.48
1:I:173:TRP:O	1:I:181:HIS:HE1	1.97	0.48
1:D:78:GLU:N	1:D:78:GLU:OE2	2.32	0.48
1:G:193:ILE:HA	1:G:200:PHE:HB2	1.96	0.48
1:B:133:SER:H	1:B:163:GLN:HE21	1.62	0.48
1:C:183:PRO:HD2	1:C:186:TYR:CE2	2.48	0.48
1:I:-5:ARG:NH2	1:I:-2:HIS:CE1	2.82	0.48
1:A:191:ILE:HG13	1:A:192:SER:N	2.28	0.48
1:E:224:ASP:OD1	1:E:227:THR:HG23	2.13	0.48
1:C:262:GLN:HE22	1:I:80:GLY:CA	2.15	0.48
1:G:47:ARG:CG	1:G:47:ARG:HH11	2.22	0.48
1:D:133:SER:H	1:D:163:GLN:HE21	1.60	0.48
1:C:74:MET:HE1	1:E:52:ILE:HA	1.96	0.48
1:D:183:PRO:HD2	1:D:186:TYR:CD2	2.49	0.48
1:C:32:ARG:HH11	1:C:32:ARG:HG2	1.79	0.47
1:F:8:LEU:HD12	1:F:37:LEU:O	2.14	0.47
1:F:76:ARG:HG2	1:F:76:ARG:NH1	2.29	0.47
1:B:19:LEU:HD13	1:B:256:VAL:HG13	1.95	0.47
1:C:193:ILE:HA	1:C:200:PHE:HB2	1.95	0.47
1:A:215:GLN:HG2	1:A:216:THR:OG1	2.13	0.47
1:G:45:THR:HG22	1:G:263:PHE:HB3	1.96	0.47
1:I:45:THR:HG22	1:I:263:PHE:HB3	1.96	0.47
1:C:94:TYR:O	1:C:140:PRO:HG2	2.13	0.47
1:G:37:LEU:HD23	1:G:58:ILE:HB	1.95	0.47
1:H:52:ILE:HG21	1:H:259:LEU:CD1	2.44	0.47
1:B:86:LEU:HD11	1:B:165:LEU:CD2	2.45	0.47
1:B:191:ILE:O	1:B:195:SER:N	2.47	0.47
1:I:224:ASP:OD1	1:I:227:THR:HG23	2.13	0.47
1:H:192:SER:HA	1:H:195:SER:HB3	1.96	0.47
1:A:241:HIS:HB3	1:A:242:PRO:CD	2.43	0.47
1:D:215:GLN:HG2	1:D:216:THR:OG1	2.14	0.47
1:I:37:LEU:HD23	1:I:58:ILE:HB	1.95	0.47
1:F:86:LEU:HD11	1:F:165:LEU:CD2	2.44	0.47
1:F:191:ILE:HG13	1:F:192:SER:N	2.29	0.47
1:D:192:SER:HA	1:D:195:SER:HB3	1.95	0.47
1:E:193:ILE:HA	1:E:200:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:HIS:O	1:D:242:PRO:C	2.47	0.47
1:C:183:PRO:HD2	1:C:186:TYR:CD2	2.50	0.47
1:A:45:THR:HG22	1:A:263:PHE:HB3	1.97	0.47
1:E:191:ILE:HG13	1:E:192:SER:N	2.29	0.47
1:E:2:ASP:O	1:E:95:SER:N	2.40	0.47
1:F:45:THR:HG22	1:F:263:PHE:HB3	1.94	0.47
1:C:173:TRP:O	1:C:181:HIS:HE1	1.96	0.47
1:A:139:GLN:HE21	1:A:139:GLN:HB2	1.53	0.47
1:A:193:ILE:HD12	1:A:241:HIS:N	2.30	0.47
1:I:2:ASP:OD1	1:I:3:GLN:HG3	2.13	0.47
1:B:-7:VAL:HA	1:B:-6:PRO:HD2	1.66	0.47
1:G:133:SER:H	1:G:163:GLN:HE21	1.63	0.47
1:G:212:PHE:CD2	1:G:245:LEU:CD1	2.98	0.47
1:I:47:ARG:O	1:I:51:GLU:HG2	2.14	0.47
1:H:119:LEU:HD11	1:H:131:PHE:CZ	2.50	0.47
1:D:8:LEU:HD12	1:D:37:LEU:O	2.15	0.47
1:H:19:LEU:HD13	1:H:256:VAL:HG13	1.95	0.47
1:A:19:LEU:HD13	1:A:256:VAL:HG13	1.97	0.47
1:H:191:ILE:O	1:H:195:SER:N	2.47	0.47
1:D:191:ILE:HG13	1:D:192:SER:N	2.28	0.47
1:J:191:ILE:O	1:J:195:SER:N	2.47	0.47
1:A:12:ASP:O	1:A:15:ALA:HB3	2.14	0.47
1:B:11:ASN:OD1	1:B:13:ALA:N	2.45	0.47
1:D:31:SER:OG	1:D:32:ARG:NH1	2.48	0.47
1:G:213:LEU:HD23	1:G:213:LEU:H	1.79	0.47
1:E:20:VAL:HG21	1:E:248:TRP:CZ2	2.48	0.47
1:D:173:TRP:O	1:D:181:HIS:HE1	1.98	0.47
1:D:252:PHE:O	1:D:257:VAL:HG23	2.15	0.47
1:A:252:PHE:O	1:A:257:VAL:HG23	2.14	0.47
1:J:62:ILE:CD1	1:J:73:LEU:HD22	2.43	0.47
1:G:86:LEU:HD11	1:G:165:LEU:CD2	2.45	0.47
1:B:191:ILE:HG13	1:B:192:SER:N	2.28	0.47
1:C:192:SER:HA	1:C:195:SER:HB3	1.97	0.47
1:G:72:THR:HG23	1:G:153:SER:HB2	1.97	0.47
1:C:52:ILE:CG2	1:I:74:MET:HE1	2.38	0.47
1:B:-5:ARG:HD2	1:B:-2:HIS:CD2	2.50	0.47
1:C:9:THR:HG21	1:C:38:THR:HG22	1.97	0.47
1:E:63:LEU:HD22	1:G:263:PHE:CZ	2.49	0.47
1:A:76:ARG:HD2	1:A:152:ALA:O	2.15	0.47
1:B:148:LEU:HD23	1:B:169:PHE:CD2	2.50	0.47
1:E:173:TRP:O	1:E:181:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLN:HB3	1:B:266:VAL:CG1	2.44	0.46
1:J:241:HIS:HB3	1:J:242:PRO:CD	2.40	0.46
1:C:113:LEU:HD21	1:C:186:TYR:CD1	2.51	0.46
1:D:30:THR:HA	1:D:111:ASP:OD2	2.14	0.46
1:A:241:HIS:CD2	1:A:245:LEU:HD12	2.50	0.46
1:G:245:LEU:HA	1:G:245:LEU:HD12	1.74	0.46
1:E:80:GLY:CA	1:G:262:GLN:HE22	2.18	0.46
1:B:37:LEU:HD23	1:B:58:ILE:HB	1.98	0.46
1:I:231:ARG:CG	1:I:232:SER:N	2.77	0.46
1:F:19:LEU:HD13	1:F:256:VAL:HG13	1.98	0.46
1:E:11:ASN:OD1	1:E:13:ALA:N	2.44	0.46
1:A:206:ASN:O	1:A:207:ALA:C	2.54	0.46
1:F:149:LEU:HA	1:F:149:LEU:HD12	1.78	0.46
1:F:62:ILE:CD1	1:F:73:LEU:HD22	2.43	0.46
1:D:183:PRO:HD2	1:D:186:TYR:CE2	2.50	0.46
1:B:189:SER:HB2	1:B:213:LEU:CD2	2.44	0.46
1:A:94:TYR:O	1:A:140:PRO:CG	2.63	0.46
1:B:149:LEU:HA	1:B:149:LEU:HD12	1.78	0.46
1:F:193:ILE:HA	1:F:200:PHE:HB2	1.96	0.46
1:D:193:ILE:HD12	1:D:194:TYR:HB3	1.97	0.46
1:H:31:SER:OG	1:H:32:ARG:NH1	2.49	0.46
1:D:9:THR:HG21	1:D:38:THR:HG22	1.97	0.46
1:B:173:TRP:O	1:B:181:HIS:HE1	1.97	0.46
1:D:19:LEU:HD13	1:D:256:VAL:HG13	1.98	0.46
1:J:30:THR:HA	1:J:111:ASP:OD2	2.16	0.46
1:B:206:ASN:O	1:B:207:ALA:C	2.54	0.46
1:B:190:SER:HB2	1:B:241:HIS:ND1	2.30	0.46
1:A:240:THR:CG2	1:A:241:HIS:N	2.64	0.46
1:G:212:PHE:CD2	1:G:245:LEU:HD13	2.47	0.46
1:F:241:HIS:O	1:F:242:PRO:C	2.53	0.46
1:E:37:LEU:HD23	1:E:58:ILE:HB	1.97	0.46
1:E:45:THR:HG22	1:E:263:PHE:HB3	1.98	0.46
1:A:193:ILE:HB	1:A:240:THR:OG1	2.15	0.46
1:C:241:HIS:HB3	1:C:242:PRO:CD	2.36	0.46
1:D:241:HIS:CB	1:D:242:PRO:CD	2.93	0.46
1:B:-5:ARG:NH1	1:B:-2:HIS:HD2	2.14	0.46
1:H:144:THR:O	1:H:147:GLN:HB2	2.15	0.46
1:B:122:ALA:HB3	1:B:187:ASN:HB3	1.98	0.46
1:D:58:ILE:N	1:D:58:ILE:HD12	2.30	0.46
1:F:224:ASP:HB3	1:F:227:THR:OG1	2.16	0.46
1:J:144:THR:O	1:J:147:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:TRP:O	1:H:181:HIS:HE1	1.99	0.46
1:B:9:THR:HG21	1:B:38:THR:HG22	1.96	0.46
1:A:192:SER:HA	1:A:195:SER:HB3	1.98	0.46
1:I:191:ILE:HG13	1:I:192:SER:N	2.29	0.46
1:G:193:ILE:CD1	1:G:241:HIS:HB2	2.46	0.46
1:A:260:LEU:CB	1:A:266:VAL:HG23	2.40	0.46
1:B:259:LEU:O	1:B:263:PHE:HD1	1.99	0.46
1:J:191:ILE:HG13	1:J:192:SER:N	2.30	0.46
1:J:79:LEU:O	1:J:83:LEU:HG	2.16	0.46
1:F:139:GLN:HE21	1:F:139:GLN:HB2	1.60	0.46
1:A:193:ILE:C	1:A:240:THR:HG21	2.36	0.46
1:B:262:GLN:HG2	1:B:263:PHE:CE1	2.50	0.46
1:C:191:ILE:O	1:C:195:SER:N	2.49	0.46
1:I:30:THR:HA	1:I:111:ASP:OD2	2.16	0.46
1:B:193:ILE:HA	1:B:200:PHE:HB2	1.98	0.45
1:A:193:ILE:HA	1:A:200:PHE:HB2	1.97	0.45
1:G:212:PHE:HE2	1:G:245:LEU:HD13	1.74	0.45
1:A:171:ASN:ND2	1:A:171:ASN:C	2.70	0.45
1:C:189:SER:HB2	1:C:213:LEU:HD21	1.97	0.45
1:D:191:ILE:O	1:D:195:SER:N	2.49	0.45
1:A:79:LEU:O	1:A:83:LEU:HG	2.15	0.45
1:J:193:ILE:HA	1:J:200:PHE:HB2	1.98	0.45
1:I:193:ILE:HD12	1:I:194:TYR:HB3	1.97	0.45
1:H:191:ILE:HG13	1:H:192:SER:N	2.30	0.45
1:I:192:SER:HA	1:I:195:SER:HB3	1.98	0.45
1:H:193:ILE:HD12	1:H:194:TYR:HB3	1.98	0.45
1:F:193:ILE:HD12	1:F:194:TYR:HB3	1.98	0.45
1:E:133:SER:H	1:E:163:GLN:HE21	1.63	0.45
1:D:4:ALA:HB2	1:D:33:ARG:HB2	1.98	0.45
1:B:240:THR:O	1:B:243:GLN:HB2	2.12	0.45
1:F:242:PRO:O	1:F:243:GLN:C	2.55	0.45
1:C:133:SER:H	1:C:163:GLN:HE21	1.64	0.45
1:F:9:THR:HG21	1:F:38:THR:HG22	1.98	0.45
1:E:144:THR:O	1:E:147:GLN:HB2	2.17	0.45
1:G:224:ASP:HB3	1:G:227:THR:OG1	2.16	0.45
1:E:192:SER:HA	1:E:195:SER:HB3	1.98	0.45
1:B:193:ILE:HD12	1:B:194:TYR:HB3	1.97	0.45
1:B:257:VAL:HG12	1:B:261:GLN:HG3	1.97	0.45
1:J:192:SER:HA	1:J:195:SER:HB3	1.97	0.45
1:F:11:ASN:OD1	1:F:13:ALA:N	2.48	0.45
1:B:187:ASN:O	1:B:188:LEU:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:PRO:O	1:B:243:GLN:C	2.55	0.45
1:H:193:ILE:HA	1:H:200:PHE:HB2	1.98	0.45
1:E:241:HIS:CD2	1:E:245:LEU:HD12	2.52	0.45
1:H:121:ALA:HB3	1:H:131:PHE:HB2	1.98	0.45
1:J:133:SER:H	1:J:163:GLN:HE21	1.63	0.45
1:H:133:SER:H	1:H:163:GLN:HE21	1.65	0.45
1:H:58:ILE:HD12	1:H:58:ILE:N	2.31	0.45
1:H:86:LEU:HD11	1:H:165:LEU:CD2	2.46	0.45
1:J:224:ASP:HB3	1:J:227:THR:OG1	2.17	0.45
1:A:3:GLN:CB	1:A:32:ARG:HD2	2.41	0.45
1:D:241:HIS:HD1	1:D:245:LEU:HD11	1.76	0.45
1:A:133:SER:H	1:A:163:GLN:HE21	1.65	0.45
1:H:8:LEU:HD12	1:H:37:LEU:O	2.16	0.45
1:J:20:VAL:HG21	1:J:248:TRP:CE2	2.51	0.45
1:I:57:VAL:HG12	1:I:57:VAL:O	2.15	0.45
1:I:47:ARG:O	1:I:51:GLU:CG	2.65	0.45
1:D:132:ASN:ND2	1:D:163:GLN:NE2	2.65	0.45
1:A:62:ILE:CD1	1:A:73:LEU:HD22	2.46	0.45
1:F:144:THR:O	1:F:147:GLN:HB2	2.15	0.45
1:H:189:SER:HB2	1:H:213:LEU:HD21	1.99	0.45
1:A:260:LEU:CB	1:A:266:VAL:HG21	2.46	0.45
1:H:119:LEU:HD23	1:H:170:PHE:CE2	2.51	0.45
1:C:52:ILE:HG21	1:C:259:LEU:CD1	2.46	0.45
1:D:86:LEU:HD11	1:D:165:LEU:CD2	2.47	0.45
1:C:86:LEU:HD11	1:C:165:LEU:CD2	2.47	0.45
1:H:79:LEU:O	1:H:83:LEU:HG	2.17	0.45
1:G:241:HIS:CE1	1:G:245:LEU:HD22	2.46	0.45
1:D:3:GLN:CB	1:D:32:ARG:HD2	2.39	0.45
1:E:132:ASN:ND2	1:E:163:GLN:NE2	2.63	0.45
1:E:256:VAL:O	1:E:257:VAL:C	2.56	0.45
1:D:62:ILE:CD1	1:D:73:LEU:HD22	2.46	0.45
1:I:-5:ARG:HH22	1:I:-2:HIS:CE1	2.34	0.45
1:D:105:LEU:HD23	1:D:106:VAL:N	2.32	0.45
1:A:242:PRO:O	1:A:243:GLN:C	2.55	0.44
1:I:8:LEU:HD12	1:I:37:LEU:O	2.17	0.44
1:E:206:ASN:O	1:E:207:ALA:C	2.55	0.44
1:D:149:LEU:HD12	1:D:149:LEU:HA	1.74	0.44
1:A:200:PHE:CE2	1:A:240:THR:CB	2.97	0.44
1:F:194:TYR:O	1:F:194:TYR:HD2	1.99	0.44
1:G:252:PHE:O	1:G:257:VAL:HG23	2.17	0.44
1:B:259:LEU:O	1:B:263:PHE:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:79:LEU:O	1:I:83:LEU:HG	2.18	0.44
1:B:12:ASP:O	1:B:15:ALA:HB3	2.18	0.44
1:B:78:GLU:N	1:B:78:GLU:OE2	2.34	0.44
1:D:45:THR:HG22	1:D:263:PHE:HB3	1.98	0.44
1:J:193:ILE:HD12	1:J:194:TYR:HB3	1.99	0.44
1:J:86:LEU:HD11	1:J:165:LEU:CD2	2.47	0.44
1:D:79:LEU:O	1:D:83:LEU:HG	2.17	0.44
1:G:206:ASN:O	1:G:207:ALA:C	2.56	0.44
1:G:149:LEU:HD12	1:G:149:LEU:HA	1.74	0.44
1:E:171:ASN:ND2	1:E:171:ASN:C	2.70	0.44
1:D:206:ASN:O	1:D:207:ALA:C	2.55	0.44
1:G:191:ILE:HG13	1:G:192:SER:N	2.31	0.44
1:B:-5:ARG:NH1	1:B:-2:HIS:CD2	2.85	0.44
1:A:132:ASN:ND2	1:A:163:GLN:NE2	2.63	0.44
1:A:151:VAL:HG21	1:A:169:PHE:HD2	1.82	0.44
1:H:206:ASN:O	1:H:207:ALA:C	2.55	0.44
1:E:193:ILE:HD12	1:E:194:TYR:HB3	2.00	0.44
1:F:47:ARG:CG	1:F:47:ARG:HH11	2.25	0.44
1:G:9:THR:HG21	1:G:38:THR:HG22	1.96	0.44
1:C:193:ILE:HD12	1:C:194:TYR:HB3	1.99	0.44
1:H:194:TYR:O	1:H:194:TYR:HD2	2.01	0.44
1:H:200:PHE:O	1:H:204:GLY:N	2.45	0.44
1:B:58:ILE:HD12	1:B:58:ILE:N	2.32	0.44
1:I:252:PHE:O	1:I:257:VAL:HG23	2.18	0.44
1:I:86:LEU:HD11	1:I:165:LEU:CD2	2.47	0.44
1:C:224:ASP:OD1	1:C:227:THR:HG23	2.18	0.44
1:G:30:THR:HA	1:G:111:ASP:OD2	2.18	0.44
1:B:188:LEU:HD11	1:B:193:ILE:HG23	1.99	0.44
1:B:224:ASP:HB3	1:B:227:THR:OG1	2.18	0.44
1:A:263:PHE:CE2	1:G:63:LEU:HD13	2.52	0.44
1:G:192:SER:HA	1:G:195:SER:HB3	1.98	0.44
1:I:72:THR:HG23	1:I:153:SER:HB2	2.00	0.44
1:H:30:THR:HA	1:H:111:ASP:OD2	2.18	0.44
1:F:79:LEU:O	1:F:83:LEU:HG	2.18	0.44
1:G:78:GLU:OE2	1:G:78:GLU:N	2.35	0.44
1:C:242:PRO:O	1:C:243:GLN:C	2.56	0.44
1:F:190:SER:HB3	1:F:241:HIS:NE2	2.28	0.44
1:D:224:ASP:HB3	1:D:227:THR:OG1	2.17	0.44
1:G:193:ILE:HD12	1:G:194:TYR:HB3	1.99	0.43
1:E:31:SER:OG	1:E:32:ARG:NH1	2.51	0.43
1:B:8:LEU:HD12	1:B:37:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:LEU:HD12	1:F:9:THR:N	2.32	0.43
1:A:256:VAL:O	1:A:257:VAL:C	2.56	0.43
1:G:189:SER:HB2	1:G:213:LEU:HD21	2.00	0.43
1:B:52:ILE:HG21	1:B:259:LEU:CD1	2.47	0.43
1:A:86:LEU:HD11	1:A:165:LEU:CD2	2.48	0.43
1:B:265:LEU:HG	1:B:265:LEU:O	2.18	0.43
1:A:200:PHE:CZ	1:A:240:THR:OG1	2.71	0.43
1:F:232:SER:O	1:F:233:GLU:C	2.57	0.43
1:I:132:ASN:ND2	1:I:163:GLN:NE2	2.66	0.43
1:C:8:LEU:HD12	1:C:37:LEU:O	2.18	0.43
1:F:256:VAL:O	1:F:257:VAL:C	2.56	0.43
1:B:30:THR:HA	1:B:111:ASP:OD2	2.18	0.43
1:H:72:THR:HG23	1:H:153:SER:HB2	2.00	0.43
1:G:210:VAL:HG21	1:G:244:PHE:CD2	2.53	0.43
1:A:71:LEU:O	1:A:74:MET:HB2	2.18	0.43
1:I:2:ASP:O	1:I:95:SER:N	2.49	0.43
1:H:8:LEU:HD12	1:H:9:THR:N	2.34	0.43
1:E:19:LEU:HD13	1:E:256:VAL:HG13	1.99	0.43
1:C:193:ILE:CG1	1:C:240:THR:CG2	2.96	0.43
1:A:47:ARG:CG	1:A:47:ARG:HH11	2.20	0.43
1:H:89:TRP:CE2	1:H:138:TYR:HD1	2.37	0.43
1:I:8:LEU:HD12	1:I:9:THR:N	2.33	0.43
1:C:37:LEU:HD23	1:C:58:ILE:HB	1.99	0.43
1:H:239:MET:O	1:H:240:THR:O	2.37	0.43
1:F:191:ILE:O	1:F:195:SER:N	2.50	0.43
1:E:191:ILE:O	1:E:195:SER:N	2.51	0.43
1:I:191:ILE:O	1:I:195:SER:N	2.50	0.43
1:D:57:VAL:O	1:D:57:VAL:HG12	2.18	0.43
1:I:194:TYR:HD2	1:I:194:TYR:O	2.02	0.43
1:F:32:ARG:HG2	1:F:32:ARG:NH1	2.33	0.43
1:C:52:ILE:HD13	1:I:74:MET:HE3	2.01	0.43
1:C:57:VAL:O	1:C:57:VAL:HG12	2.19	0.43
1:E:242:PRO:O	1:E:243:GLN:C	2.56	0.43
1:E:212:PHE:CD2	1:E:241:HIS:CE1	3.07	0.43
1:G:3:GLN:CB	1:G:32:ARG:HD2	2.40	0.43
1:I:242:PRO:O	1:I:243:GLN:C	2.56	0.43
1:C:63:LEU:HD13	1:E:263:PHE:CZ	2.54	0.43
1:C:224:ASP:HB3	1:C:227:THR:OG1	2.19	0.43
1:A:128:PRO:CG	1:B:123:PRO:HG2	2.49	0.43
1:A:243:GLN:O	1:A:247:VAL:HG23	2.18	0.43
1:A:224:ASP:HB3	1:A:227:THR:OG1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-1:MET:HB3	1:C:2:ASP:OD1	2.18	0.43
1:B:257:VAL:HB	1:B:258:PRO:CD	2.44	0.43
1:E:194:TYR:O	1:E:194:TYR:HD2	2.01	0.43
1:D:197:LEU:O	1:D:201:LYS:HG3	2.19	0.43
1:J:256:VAL:O	1:J:257:VAL:C	2.57	0.43
1:F:94:TYR:O	1:F:140:PRO:CG	2.66	0.43
1:C:79:LEU:O	1:C:83:LEU:HG	2.19	0.43
1:C:72:THR:HG23	1:C:153:SER:HB2	2.01	0.43
1:A:149:LEU:HD12	1:A:149:LEU:HA	1.78	0.43
1:H:197:LEU:O	1:H:201:LYS:HG3	2.19	0.42
1:E:241:HIS:CD2	1:E:245:LEU:HD11	2.54	0.42
1:F:206:ASN:O	1:F:207:ALA:C	2.56	0.42
1:J:149:LEU:HA	1:J:149:LEU:HD12	1.81	0.42
1:A:200:PHE:CZ	1:A:240:THR:CB	3.02	0.42
1:J:193:ILE:C	1:J:193:ILE:HD12	2.40	0.42
1:H:62:ILE:CD1	1:H:73:LEU:HD22	2.45	0.42
1:H:20:VAL:HG21	1:H:248:TRP:CE2	2.54	0.42
1:C:149:LEU:HD12	1:C:149:LEU:HA	1.74	0.42
1:I:256:VAL:O	1:I:257:VAL:C	2.56	0.42
1:G:19:LEU:HD13	1:G:256:VAL:HG13	2.01	0.42
1:I:62:ILE:CD1	1:I:73:LEU:HD22	2.44	0.42
1:G:118:GLU:HB2	1:G:139:GLN:NE2	2.34	0.42
1:C:31:SER:OG	1:C:32:ARG:NH1	2.52	0.42
1:H:94:TYR:O	1:H:140:PRO:CG	2.68	0.42
1:F:151:VAL:HG21	1:F:169:PHE:HD2	1.84	0.42
1:E:79:LEU:O	1:E:83:LEU:HG	2.19	0.42
1:E:57:VAL:O	1:E:57:VAL:HG12	2.19	0.42
1:C:158:PHE:CD1	1:C:158:PHE:C	2.92	0.42
1:C:190:SER:HB2	1:C:241:HIS:CE1	2.54	0.42
1:F:3:GLN:CB	1:F:32:ARG:HD2	2.45	0.42
1:E:-2:HIS:HA	1:E:31:SER:HB2	2.01	0.42
1:J:243:GLN:O	1:J:247:VAL:HG23	2.20	0.42
1:H:256:VAL:O	1:H:257:VAL:C	2.58	0.42
1:B:113:LEU:HD21	1:B:186:TYR:CD1	2.54	0.42
1:J:171:ASN:C	1:J:171:ASN:ND2	2.73	0.42
1:A:52:ILE:HG21	1:A:259:LEU:CD1	2.49	0.42
1:C:10:THR:O	1:C:11:ASN:HB3	2.20	0.42
1:G:139:GLN:HE21	1:G:139:GLN:HB2	1.59	0.42
1:C:105:LEU:HD23	1:C:106:VAL:N	2.34	0.42
1:B:239:MET:O	1:B:243:GLN:HB2	2.19	0.42
1:G:8:LEU:HD12	1:G:9:THR:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:THR:HA	1:E:111:ASP:OD2	2.19	0.42
1:H:25:LEU:CD2	1:H:106:VAL:HG21	2.50	0.42
1:J:72:THR:HG23	1:J:153:SER:HB2	2.01	0.42
1:G:57:VAL:HG12	1:G:57:VAL:O	2.19	0.42
1:J:31:SER:OG	1:J:32:ARG:NH1	2.53	0.42
1:H:32:ARG:HG2	1:H:32:ARG:NH1	2.34	0.42
1:J:132:ASN:ND2	1:J:163:GLN:NE2	2.66	0.42
1:I:20:VAL:HG21	1:I:248:TRP:CE2	2.55	0.42
1:D:94:TYR:O	1:D:140:PRO:CG	2.67	0.42
1:G:94:TYR:O	1:G:140:PRO:CG	2.67	0.42
1:I:158:PHE:C	1:I:158:PHE:CD1	2.93	0.42
1:I:197:LEU:O	1:I:201:LYS:HG3	2.19	0.42
1:A:89:TRP:CE2	1:A:138:TYR:HD1	2.38	0.42
1:G:105:LEU:HD23	1:G:106:VAL:N	2.34	0.42
1:H:78:GLU:OE2	1:H:78:GLU:N	2.35	0.42
1:H:193:ILE:C	1:H:193:ILE:HD12	2.40	0.42
1:F:240:THR:O	1:F:243:GLN:HB2	2.20	0.42
1:G:144:THR:O	1:G:147:GLN:HB2	2.20	0.42
1:J:189:SER:HB2	1:J:213:LEU:HD21	2.02	0.42
1:I:189:SER:HB2	1:I:213:LEU:HD21	2.01	0.42
1:J:10:THR:O	1:J:11:ASN:HB3	2.20	0.42
1:E:94:TYR:O	1:E:140:PRO:CG	2.67	0.42
1:G:191:ILE:O	1:G:195:SER:N	2.49	0.42
1:F:72:THR:HG23	1:F:153:SER:HB2	2.01	0.42
1:G:212:PHE:CE2	1:G:245:LEU:HD12	2.53	0.42
1:J:190:SER:HB2	1:J:241:HIS:ND1	2.35	0.42
1:J:206:ASN:O	1:J:207:ALA:C	2.59	0.42
1:J:139:GLN:HB2	1:J:139:GLN:HE21	1.57	0.42
1:I:221:TYR:CD2	1:I:245:LEU:HD22	2.55	0.41
1:C:132:ASN:ND2	1:C:163:GLN:NE2	2.66	0.41
1:F:253:THR:HA	1:F:257:VAL:HG23	2.02	0.41
1:C:256:VAL:O	1:C:257:VAL:C	2.57	0.41
1:C:125:PRO:O	1:D:125:PRO:O	2.38	0.41
1:A:69:ALA:O	1:A:70:HIS:C	2.59	0.41
1:F:89:TRP:CE2	1:F:138:TYR:HD1	2.38	0.41
1:G:62:ILE:CD1	1:G:73:LEU:HD22	2.48	0.41
1:F:105:LEU:HD23	1:F:106:VAL:N	2.35	0.41
1:A:190:SER:HA	1:A:193:ILE:CG1	2.50	0.41
1:A:194:TYR:O	1:A:194:TYR:HD2	2.02	0.41
1:E:3:GLN:CB	1:E:32:ARG:HD2	2.43	0.41
1:E:105:LEU:HD23	1:E:106:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:57:VAL:O	1:J:57:VAL:HG12	2.20	0.41
1:G:256:VAL:O	1:G:257:VAL:C	2.57	0.41
1:G:26:LYS:O	1:G:29:ARG:N	2.49	0.41
1:I:31:SER:OG	1:I:32:ARG:NH1	2.54	0.41
1:C:45:THR:HG22	1:C:263:PHE:HB3	2.01	0.41
1:F:171:ASN:ND2	1:F:171:ASN:C	2.73	0.41
1:B:69:ALA:O	1:B:70:HIS:C	2.59	0.41
1:A:57:VAL:O	1:A:57:VAL:HG12	2.19	0.41
1:B:252:PHE:O	1:B:257:VAL:HG23	2.20	0.41
1:I:-1:MET:HB2	1:I:2:ASP:OD1	2.20	0.41
1:J:257:VAL:HB	1:J:258:PRO:CD	2.45	0.41
1:G:79:LEU:O	1:G:83:LEU:HG	2.20	0.41
1:F:57:VAL:O	1:F:57:VAL:HG12	2.21	0.41
1:A:138:TYR:N	1:A:138:TYR:CD2	2.89	0.41
1:H:9:THR:HG21	1:H:38:THR:HG22	2.00	0.41
1:I:118:GLU:HB2	1:I:139:GLN:NE2	2.35	0.41
1:C:30:THR:HA	1:C:111:ASP:OD2	2.20	0.41
1:E:139:GLN:HE21	1:E:139:GLN:HB2	1.55	0.41
1:C:221:TYR:CD2	1:C:245:LEU:HD22	2.56	0.41
1:I:-1:MET:O	1:I:33:ARG:CG	2.69	0.41
1:B:132:ASN:ND2	1:B:163:GLN:NE2	2.66	0.41
1:C:252:PHE:O	1:C:257:VAL:HG23	2.21	0.41
1:D:171:ASN:C	1:D:171:ASN:ND2	2.73	0.41
1:E:69:ALA:O	1:E:70:HIS:C	2.59	0.41
1:B:253:THR:HA	1:B:257:VAL:HG23	2.02	0.41
1:I:200:PHE:O	1:I:204:GLY:N	2.44	0.41
1:H:119:LEU:CG	1:H:170:PHE:CD2	3.04	0.41
1:H:47:ARG:CG	1:H:47:ARG:HH11	2.21	0.41
1:B:89:TRP:CE2	1:B:138:TYR:HD1	2.39	0.41
1:D:138:TYR:H	1:D:138:TYR:HD2	1.69	0.41
1:A:8:LEU:HD12	1:A:9:THR:N	2.35	0.41
1:J:253:THR:HA	1:J:257:VAL:HG23	2.03	0.41
1:I:9:THR:HG21	1:I:38:THR:HG22	1.99	0.41
1:I:144:THR:O	1:I:147:GLN:HB2	2.21	0.41
1:B:20:VAL:HG21	1:B:248:TRP:CE2	2.56	0.41
1:H:224:ASP:HB3	1:H:227:THR:OG1	2.20	0.41
1:G:196:TYR:C	1:G:198:PRO:HD2	2.42	0.41
1:G:158:PHE:CD1	1:G:158:PHE:C	2.94	0.41
1:J:242:PRO:O	1:J:243:GLN:C	2.59	0.41
1:B:62:ILE:CD1	1:B:73:LEU:HD22	2.49	0.41
1:I:-5:ARG:CZ	1:I:-2:HIS:CE1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:THR:O	1:A:147:GLN:HB2	2.21	0.41
1:F:30:THR:HA	1:F:111:ASP:OD2	2.21	0.41
1:D:232:SER:O	1:D:233:GLU:C	2.60	0.41
1:I:149:LEU:HA	1:I:149:LEU:HD12	1.78	0.41
1:J:197:LEU:O	1:J:201:LYS:HG3	2.21	0.40
1:H:138:TYR:N	1:H:138:TYR:CD2	2.89	0.40
1:D:138:TYR:CD2	1:D:138:TYR:N	2.89	0.40
1:E:257:VAL:O	1:E:258:PRO:C	2.59	0.40
1:I:171:ASN:ND2	1:I:171:ASN:C	2.72	0.40
1:C:2:ASP:O	1:C:95:SER:N	2.47	0.40
1:I:117:GLU:O	1:I:118:GLU:C	2.59	0.40
1:H:158:PHE:CD1	1:H:158:PHE:C	2.95	0.40
1:I:94:TYR:O	1:I:140:PRO:CG	2.69	0.40
1:D:8:LEU:HD12	1:D:9:THR:N	2.37	0.40
1:H:171:ASN:ND2	1:H:171:ASN:C	2.74	0.40
1:B:105:LEU:HD23	1:B:106:VAL:N	2.36	0.40
1:A:30:THR:HA	1:A:111:ASP:OD2	2.20	0.40
1:H:149:LEU:HD12	1:H:149:LEU:HA	1.80	0.40
1:C:139:GLN:HE21	1:C:139:GLN:HB2	1.55	0.40
1:D:158:PHE:C	1:D:158:PHE:CD1	2.93	0.40
1:B:79:LEU:O	1:B:83:LEU:HG	2.21	0.40
1:B:188:LEU:HD11	1:B:193:ILE:CG2	2.51	0.40
1:B:197:LEU:O	1:B:201:LYS:HG3	2.21	0.40
1:A:197:LEU:O	1:A:201:LYS:HG3	2.21	0.40
1:H:231:ARG:CD	1:H:233:GLU:OE2	2.61	0.40
1:H:240:THR:OG1	1:H:241:HIS:N	2.54	0.40
1:I:206:ASN:O	1:I:207:ALA:C	2.59	0.40
1:J:158:PHE:CD1	1:J:158:PHE:C	2.95	0.40
1:G:193:ILE:HD11	1:G:241:HIS:HB3	2.00	0.40
1:F:197:LEU:O	1:F:201:LYS:HG3	2.21	0.40
1:E:-2:HIS:CA	1:E:31:SER:HB2	2.51	0.40
1:B:8:LEU:HD12	1:B:9:THR:N	2.37	0.40
1:G:257:VAL:O	1:G:258:PRO:C	2.60	0.40
1:D:52:ILE:HG21	1:D:259:LEU:CD1	2.49	0.40
1:B:94:TYR:O	1:B:140:PRO:CG	2.68	0.40
1:E:224:ASP:HB3	1:E:227:THR:OG1	2.21	0.40
1:B:151:VAL:HG21	1:B:169:PHE:HD2	1.86	0.40
1:A:158:PHE:C	1:A:158:PHE:CD1	2.95	0.40
1:A:193:ILE:CA	1:A:240:THR:HG21	2.40	0.40
1:H:221:TYR:CD2	1:H:245:LEU:HD22	2.57	0.40
1:I:138:TYR:CD2	1:I:138:TYR:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:ASN:ND2	1:G:163:GLN:NE2	2.67	0.40
1:F:253:THR:HA	1:F:257:VAL:CG2	2.52	0.40
1:E:252:PHE:O	1:E:257:VAL:HG23	2.21	0.40
1:I:243:GLN:O	1:I:247:VAL:HG23	2.21	0.40
1:E:151:VAL:HG21	1:E:169:PHE:HD2	1.86	0.40
1:C:11:ASN:C	1:C:11:ASN:OD1	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/339 (77%)	223 (86%)	31 (12%)	6 (2%)	8	47
1	B	263/339 (78%)	223 (85%)	31 (12%)	9 (3%)	5	37
1	C	258/339 (76%)	220 (85%)	33 (13%)	5 (2%)	10	50
1	D	256/339 (76%)	219 (86%)	31 (12%)	6 (2%)	8	47
1	E	258/339 (76%)	224 (87%)	28 (11%)	6 (2%)	8	47
1	F	257/339 (76%)	221 (86%)	29 (11%)	7 (3%)	6	43
1	G	258/339 (76%)	225 (87%)	28 (11%)	5 (2%)	10	50
1	H	256/339 (76%)	221 (86%)	26 (10%)	9 (4%)	4	37
1	I	260/339 (77%)	226 (87%)	30 (12%)	4 (2%)	13	55
1	J	247/339 (73%)	213 (86%)	30 (12%)	4 (2%)	12	54
All	All	2573/3390 (76%)	2215 (86%)	297 (12%)	61 (2%)	7	46

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	240	THR

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Mol	Chain	Res	Type
1	H	241	HIS
1	A	128	PRO
1	A	190	SER
1	A	215	GLN
1	B	-6	PRO
1	B	128	PRO
1	B	215	GLN
1	C	128	PRO
1	C	215	GLN
1	D	128	PRO
1	D	215	GLN
1	E	128	PRO
1	E	215	GLN
1	F	128	PRO
1	F	215	GLN
1	G	128	PRO
1	G	215	GLN
1	H	128	PRO
1	I	128	PRO
1	I	215	GLN
1	J	215	GLN
1	B	-5	ARG
1	F	231	ARG
1	H	215	GLN
1	J	128	PRO
1	A	118	GLU
1	A	240	THR
1	B	118	GLU
1	B	190	SER
1	B	240	THR
1	C	118	GLU
1	C	190	SER
1	D	118	GLU
1	D	190	SER
1	E	118	GLU
1	E	190	SER
1	F	118	GLU
1	G	118	GLU
1	H	190	SER
1	I	118	GLU
1	I	190	SER
1	J	118	GLU

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Mol	Chain	Res	Type
1	J	190	SER
1	C	133	SER
1	D	70	HIS
1	D	133	SER
1	F	70	HIS
1	F	133	SER
1	F	190	SER
1	G	133	SER
1	G	190	SER
1	H	70	HIS
1	H	133	SER
1	H	230	VAL
1	H	231	ARG
1	A	133	SER
1	B	70	HIS
1	B	133	SER
1	E	70	HIS
1	E	133	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/299 (78%)	211 (90%)	23 (10%)	10	41
1	B	236/299 (79%)	214 (91%)	22 (9%)	11	44
1	C	232/299 (78%)	209 (90%)	23 (10%)	10	40
1	D	231/299 (77%)	207 (90%)	24 (10%)	9	38
1	E	232/299 (78%)	209 (90%)	23 (10%)	10	40
1	F	231/299 (77%)	210 (91%)	21 (9%)	12	45
1	G	232/299 (78%)	210 (90%)	22 (10%)	11	42
1	H	230/299 (77%)	206 (90%)	24 (10%)	9	38
1	I	233/299 (78%)	211 (91%)	22 (9%)	11	43
1	J	222/299 (74%)	200 (90%)	22 (10%)	10	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2313/2990 (77%)	2087 (90%)	226 (10%)	10	41

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	10	THR
1	A	12	ASP
1	A	21	LEU
1	A	33	ARG
1	A	89	TRP
1	A	93	GLN
1	A	105	LEU
1	A	119	LEU
1	A	138	TYR
1	A	139	GLN
1	A	154	GLU
1	A	155	GLN
1	A	171	ASN
1	A	181	HIS
1	A	189	SER
1	A	194	TYR
1	A	196	TYR
1	A	203	PHE
1	A	216	THR
1	A	236	ASP
1	A	245	LEU
1	A	265	LEU
1	B	-5	ARG
1	B	-1	MET
1	B	10	THR
1	B	12	ASP
1	B	21	LEU
1	B	33	ARG
1	B	89	TRP
1	B	93	GLN
1	B	105	LEU
1	B	119	LEU
1	B	138	TYR
1	B	139	GLN
1	B	154	GLU
1	B	155	GLN

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Mol	Chain	Res	Type
1	B	171	ASN
1	B	189	SER
1	B	194	TYR
1	B	196	TYR
1	B	203	PHE
1	B	216	THR
1	B	240	THR
1	B	245	LEU
1	C	-1	MET
1	C	10	THR
1	C	12	ASP
1	C	21	LEU
1	C	89	TRP
1	C	93	GLN
1	C	105	LEU
1	C	119	LEU
1	C	138	TYR
1	C	139	GLN
1	C	154	GLU
1	C	155	GLN
1	C	171	ASN
1	C	181	HIS
1	C	189	SER
1	C	194	TYR
1	C	196	TYR
1	C	203	PHE
1	C	206	ASN
1	C	216	THR
1	C	239	MET
1	C	245	LEU
1	C	265	LEU
1	D	-1	MET
1	D	10	THR
1	D	12	ASP
1	D	21	LEU
1	D	33	ARG
1	D	89	TRP
1	D	93	GLN
1	D	105	LEU
1	D	119	LEU
1	D	138	TYR
1	D	139	GLN

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Mol	Chain	Res	Type
1	D	154	GLU
1	D	155	GLN
1	D	171	ASN
1	D	189	SER
1	D	194	TYR
1	D	196	TYR
1	D	203	PHE
1	D	206	ASN
1	D	216	THR
1	D	233	GLU
1	D	238	THR
1	D	245	LEU
1	D	265	LEU
1	E	-2	HIS
1	E	10	THR
1	E	12	ASP
1	E	21	LEU
1	E	33	ARG
1	E	68	SER
1	E	89	TRP
1	E	93	GLN
1	E	105	LEU
1	E	119	LEU
1	E	138	TYR
1	E	139	GLN
1	E	154	GLU
1	E	155	GLN
1	E	171	ASN
1	E	189	SER
1	E	194	TYR
1	E	196	TYR
1	E	203	PHE
1	E	216	THR
1	E	233	GLU
1	E	245	LEU
1	E	265	LEU
1	F	-1	MET
1	F	10	THR
1	F	12	ASP
1	F	21	LEU
1	F	33	ARG
1	F	89	TRP

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Mol	Chain	Res	Type
1	F	93	GLN
1	F	105	LEU
1	F	119	LEU
1	F	138	TYR
1	F	139	GLN
1	F	154	GLU
1	F	155	GLN
1	F	171	ASN
1	F	194	TYR
1	F	196	TYR
1	F	203	PHE
1	F	216	THR
1	F	233	GLU
1	F	245	LEU
1	F	265	LEU
1	G	-1	MET
1	G	10	THR
1	G	12	ASP
1	G	21	LEU
1	G	89	TRP
1	G	93	GLN
1	G	105	LEU
1	G	119	LEU
1	G	138	TYR
1	G	139	GLN
1	G	154	GLU
1	G	155	GLN
1	G	171	ASN
1	G	189	SER
1	G	194	TYR
1	G	196	TYR
1	G	203	PHE
1	G	216	THR
1	G	239	MET
1	G	241	HIS
1	G	245	LEU
1	G	265	LEU
1	H	-1	MET
1	H	10	THR
1	H	12	ASP
1	H	21	LEU
1	H	33	ARG

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Mol	Chain	Res	Type
1	H	89	TRP
1	H	93	GLN
1	H	105	LEU
1	H	119	LEU
1	H	138	TYR
1	H	139	GLN
1	H	143	GLU
1	H	154	GLU
1	H	155	GLN
1	H	171	ASN
1	H	194	TYR
1	H	196	TYR
1	H	203	PHE
1	H	216	THR
1	H	233	GLU
1	H	241	HIS
1	H	242	PRO
1	H	243	GLN
1	H	245	LEU
1	I	-5	ARG
1	I	-3	SER
1	I	-2	HIS
1	I	10	THR
1	I	12	ASP
1	I	21	LEU
1	I	89	TRP
1	I	93	GLN
1	I	105	LEU
1	I	119	LEU
1	I	138	TYR
1	I	139	GLN
1	I	154	GLU
1	I	155	GLN
1	I	171	ASN
1	I	189	SER
1	I	194	TYR
1	I	196	TYR
1	I	203	PHE
1	I	216	THR
1	I	245	LEU
1	I	265	LEU
1	J	2	ASP

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Mol	Chain	Res	Type
1	J	10	THR
1	J	12	ASP
1	J	21	LEU
1	J	33	ARG
1	J	89	TRP
1	J	93	GLN
1	J	105	LEU
1	J	119	LEU
1	J	138	TYR
1	J	139	GLN
1	J	149	LEU
1	J	154	GLU
1	J	155	GLN
1	J	171	ASN
1	J	189	SER
1	J	194	TYR
1	J	196	TYR
1	J	203	PHE
1	J	206	ASN
1	J	216	THR
1	J	245	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	109	ASN
1	A	139	GLN
1	A	147	GLN
1	A	155	GLN
1	A	163	GLN
1	A	171	ASN
1	A	181	HIS
1	A	187	ASN
1	A	262	GLN
1	B	-2	HIS
1	B	93	GLN
1	B	109	ASN
1	B	139	GLN
1	B	155	GLN
1	B	163	GLN
1	B	171	ASN

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Mol	Chain	Res	Type
1	B	181	HIS
1	B	187	ASN
1	B	261	GLN
1	C	93	GLN
1	C	109	ASN
1	C	139	GLN
1	C	147	GLN
1	C	155	GLN
1	C	163	GLN
1	C	171	ASN
1	C	181	HIS
1	D	93	GLN
1	D	109	ASN
1	D	139	GLN
1	D	146	ASN
1	D	147	GLN
1	D	155	GLN
1	D	163	GLN
1	D	171	ASN
1	D	181	HIS
1	E	93	GLN
1	E	109	ASN
1	E	139	GLN
1	E	146	ASN
1	E	147	GLN
1	E	155	GLN
1	E	163	GLN
1	E	171	ASN
1	E	181	HIS
1	E	241	HIS
1	F	93	GLN
1	F	109	ASN
1	F	139	GLN
1	F	146	ASN
1	F	147	GLN
1	F	155	GLN
1	F	163	GLN
1	F	171	ASN
1	F	181	HIS
1	G	93	GLN
1	G	109	ASN
1	G	139	GLN

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Mol	Chain	Res	Type
1	G	146	ASN
1	G	147	GLN
1	G	155	GLN
1	G	163	GLN
1	G	171	ASN
1	G	181	HIS
1	H	93	GLN
1	H	109	ASN
1	H	139	GLN
1	H	146	ASN
1	H	147	GLN
1	H	155	GLN
1	H	163	GLN
1	H	171	ASN
1	H	181	HIS
1	I	-2	HIS
1	I	93	GLN
1	I	109	ASN
1	I	139	GLN
1	I	147	GLN
1	I	155	GLN
1	I	163	GLN
1	I	171	ASN
1	I	181	HIS
1	I	187	ASN
1	J	93	GLN
1	J	109	ASN
1	J	139	GLN
1	J	147	GLN
1	J	155	GLN
1	J	163	GLN
1	J	171	ASN
1	J	181	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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	264/339 (77%)	0.15	15 (5%) 27 24	12, 58, 138, 194	0
1	B	267/339 (78%)	0.20	12 (4%) 37 32	16, 49, 129, 200	0
1	C	262/339 (77%)	0.05	9 (3%) 49 43	18, 49, 119, 189	0
1	D	261/339 (76%)	0.27	23 (8%) 12 13	25, 61, 143, 200	0
1	E	262/339 (77%)	0.16	15 (5%) 27 24	23, 56, 122, 200	0
1	F	261/339 (76%)	0.34	20 (7%) 16 15	27, 73, 151, 189	0
1	G	262/339 (77%)	0.28	16 (6%) 25 22	21, 56, 130, 199	0
1	H	260/339 (76%)	0.38	19 (7%) 18 17	30, 75, 154, 200	0
1	I	264/339 (77%)	0.20	18 (6%) 20 19	19, 59, 134, 187	0
1	J	251/339 (74%)	0.76	40 (15%) 3 3	48, 99, 160, 200	0
All	All	2614/3390 (77%)	0.28	187 (7%) 18 17	12, 63, 145, 200	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	SER	6.9
1	J	52	ILE	5.9
1	D	227	THR	5.1
1	B	232	SER	5.1
1	H	193	ILE	4.9
1	J	101	ASP	4.8
1	D	193	ILE	4.8
1	H	232	SER	4.7
1	I	193	ILE	4.7
1	G	232	SER	4.6
1	J	44	ASP	4.6
1	B	266	VAL	4.6
1	A	216	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	H	261	GLN	4.5
1	A	154	GLU	4.4
1	F	266	VAL	4.4
1	J	45	THR	4.3
1	I	233	GLU	4.2
1	H	44	ASP	4.2
1	F	227	THR	4.2
1	G	266	VAL	4.1
1	H	223	TYR	4.1
1	G	154	GLU	4.1
1	B	220	ASN	4.1
1	G	265	LEU	4.0
1	A	227	THR	3.9
1	E	227	THR	3.9
1	J	34	LEU	3.8
1	B	204	GLY	3.8
1	F	221	TYR	3.8
1	G	221	TYR	3.8
1	H	264	GLY	3.8
1	G	227	THR	3.8
1	J	180	LYS	3.7
1	F	226	LYS	3.7
1	J	229	SER	3.7
1	H	221	TYR	3.6
1	I	194	TYR	3.6
1	D	226	LYS	3.5
1	E	226	LYS	3.5
1	F	207	ALA	3.5
1	A	225	THR	3.4
1	F	224	ASP	3.4
1	A	155	GLN	3.4
1	D	101	ASP	3.4
1	J	65	SER	3.4
1	J	43	SER	3.4
1	D	253	THR	3.4
1	B	221	TYR	3.4
1	D	196	TYR	3.4
1	G	220	ASN	3.3
1	J	33	ARG	3.3
1	J	196	TYR	3.3
1	H	101	ASP	3.3
1	C	231	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	194	TYR	3.3
1	B	43	SER	3.3
1	I	101	ASP	3.3
1	J	190	SER	3.3
1	J	218	PRO	3.2
1	I	232	SER	3.2
1	I	227	THR	3.2
1	C	193	ILE	3.2
1	G	231	ARG	3.2
1	E	195	SER	3.2
1	E	194	TYR	3.2
1	F	63	LEU	3.1
1	J	15	ALA	3.1
1	G	193	ILE	3.1
1	F	193	ILE	3.1
1	D	232	SER	3.1
1	C	101	ASP	3.1
1	D	204	GLY	3.0
1	J	94	TYR	3.0
1	E	224	ASP	3.0
1	J	193	ILE	3.0
1	B	101	ASP	3.0
1	A	215	GLN	3.0
1	A	231	ARG	2.9
1	E	231	ARG	2.9
1	F	233	GLU	2.9
1	A	195	SER	2.9
1	F	265	LEU	2.9
1	G	225	THR	2.9
1	I	153	SER	2.8
1	J	38	THR	2.8
1	G	226	LYS	2.7
1	B	225	THR	2.7
1	J	216	THR	2.7
1	E	172	SER	2.7
1	G	3	GLN	2.7
1	J	134	GLY	2.7
1	I	192	SER	2.7
1	I	7	THR	2.7
1	H	216	THR	2.7
1	B	44	ASP	2.7
1	J	73	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	155	GLN	2.6
1	I	225	THR	2.6
1	J	187	ASN	2.6
1	D	200	PHE	2.6
1	I	223	TYR	2.6
1	J	70	HIS	2.6
1	B	93	GLN	2.6
1	H	226	LYS	2.6
1	I	127	TRP	2.5
1	D	266	VAL	2.5
1	F	75	LYS	2.5
1	J	26	LYS	2.5
1	J	231	ARG	2.5
1	C	238	THR	2.5
1	F	230	VAL	2.5
1	C	227	THR	2.5
1	J	28	HIS	2.4
1	I	226	LYS	2.4
1	J	99	PHE	2.4
1	H	243	GLN	2.4
1	J	48	LYS	2.4
1	D	3	GLN	2.4
1	H	230	VAL	2.4
1	D	132	ASN	2.4
1	D	243	GLN	2.4
1	F	223	TYR	2.4
1	H	156	GLY	2.4
1	D	179	ARG	2.4
1	F	232	SER	2.4
1	I	44	ASP	2.3
1	E	225	THR	2.3
1	E	-2	HIS	2.3
1	H	194	TYR	2.3
1	G	223	TYR	2.3
1	J	74	MET	2.3
1	D	201	LYS	2.3
1	J	12	ASP	2.3
1	J	96	LYS	2.3
1	C	177	ASP	2.3
1	G	224	ASP	2.3
1	H	17	GLY	2.3
1	I	-1	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	211	HIS	2.3
1	J	77	PRO	2.2
1	J	250	ASP	2.2
1	B	261	GLN	2.2
1	J	87	HIS	2.2
1	F	229	SER	2.2
1	D	254	THR	2.2
1	D	104	THR	2.2
1	F	99	PHE	2.2
1	F	162	ASP	2.2
1	J	249	TRP	2.2
1	E	153	SER	2.2
1	J	35	ALA	2.2
1	H	260	LEU	2.2
1	J	230	VAL	2.2
1	E	228	LYS	2.2
1	E	150	HIS	2.2
1	D	192	SER	2.2
1	C	225	THR	2.1
1	F	92	THR	2.1
1	D	195	SER	2.1
1	F	194	TYR	2.1
1	D	194	TYR	2.1
1	G	178	ILE	2.1
1	A	187	ASN	2.1
1	D	224	ASP	2.1
1	A	226	LYS	2.1
1	H	48	LYS	2.1
1	I	195	SER	2.1
1	B	45	THR	2.1
1	H	3	GLN	2.1
1	I	202	ALA	2.1
1	E	240	THR	2.1
1	I	151	VAL	2.1
1	E	3	GLN	2.1
1	A	223	TYR	2.1
1	F	52	ILE	2.1
1	J	132	ASN	2.1
1	G	92	THR	2.0
1	E	201	LYS	2.0
1	A	74	MET	2.0
1	J	91	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	246	ASN	2.0
1	H	245	LEU	2.0
1	J	153	SER	2.0
1	A	220	ASN	2.0
1	A	162	ASP	2.0
1	D	223	TYR	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.