



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:10 AM GMT

PDB ID : 2POH
Title : Structure of Phage P22 Tail Needle gp26
Authors : Olia, A.S.; Cingolani, G.
Deposited on : 2007-04-26
Resolution : 2.10 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

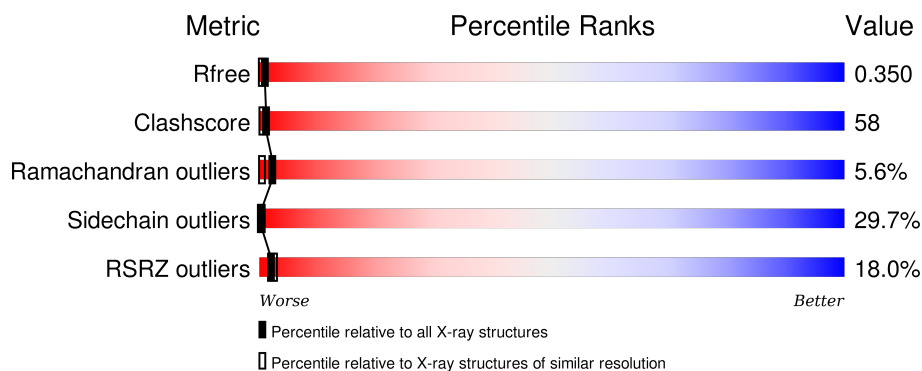
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	233	<div> <div>15%</div> <div>33%</div> <div>48%</div> <div>17%</div> <div>.</div> </div>
1	B	233	<div> <div>7%</div> <div>31%</div> <div>48%</div> <div>19%</div> <div>.</div> </div>
1	C	233	<div> <div>15%</div> <div>33%</div> <div>47%</div> <div>17%</div> <div>.</div> </div>
1	D	233	<div> <div>26%</div> <div>26%</div> <div>48%</div> <div>22%</div> <div>.</div> </div>
1	E	233	<div> <div>24%</div> <div>33%</div> <div>46%</div> <div>19%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	233	<div><div></div><div>21%</div><div>28%</div><div>48%</div><div>22%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11261 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 Head completion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	Se	0	0	0
			1738	1065	311	360	2			
1	B	233	Total	C	N	O	Se	0	0	0
			1738	1065	311	360	2			
1	C	233	Total	C	N	O	Se	0	0	0
			1738	1065	311	360	2			
1	D	233	Total	C	N	O	Se	0	0	0
			1715	1045	310	358	2			
1	E	233	Total	C	N	O	Se	0	0	0
			1712	1048	308	354	2			
1	F	233	Total	C	N	O	Se	0	0	0
			1734	1062	311	359	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
A	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
B	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
C	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
D	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
E	222	MSE	LEU	ENGINEERED	UNP Q8LTG5
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q8LTG5
F	222	MSE	LEU	ENGINEERED	UNP Q8LTG5

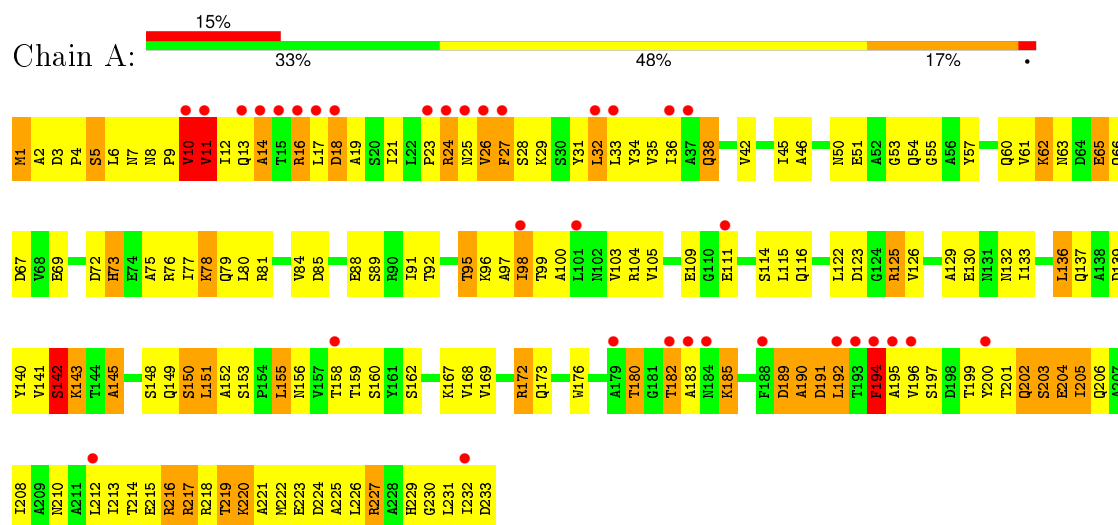
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	155	Total 155	O 155	0	0
2	B	167	Total 167	O 167	0	0
2	C	151	Total 151	O 151	0	0
2	D	124	Total 124	O 124	0	0
2	E	138	Total 138	O 138	0	0
2	F	151	Total 151	O 151	0	0

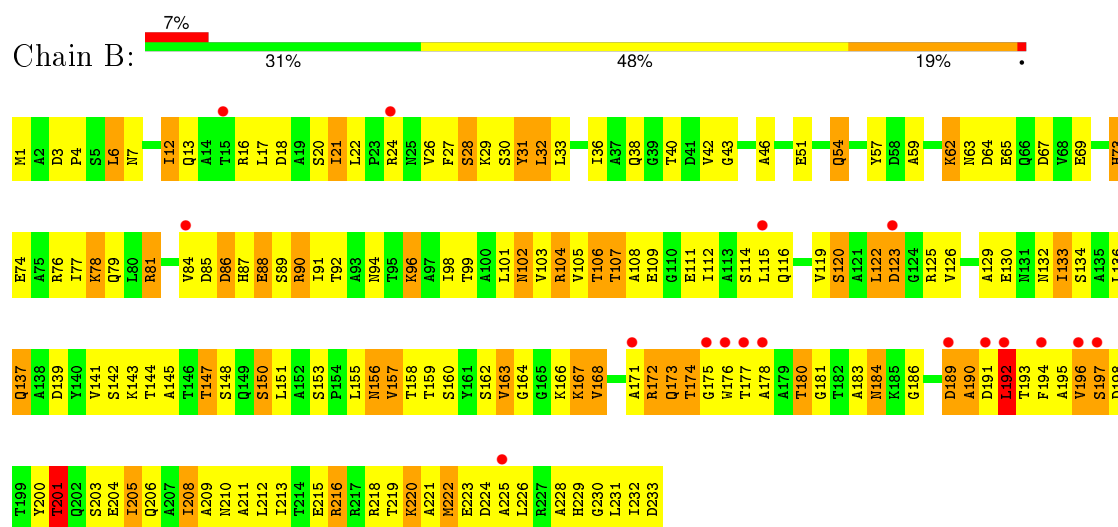
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Head completion protein

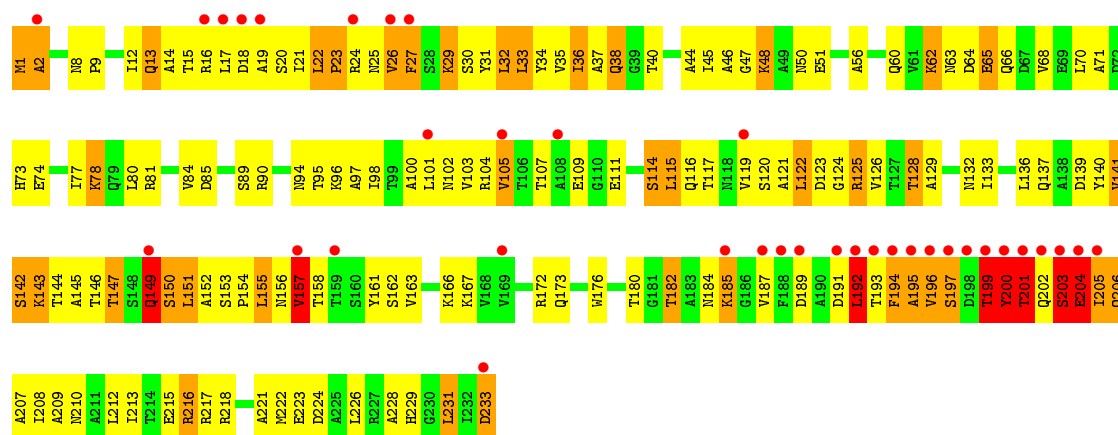


• Molecule 1: Head completion protein

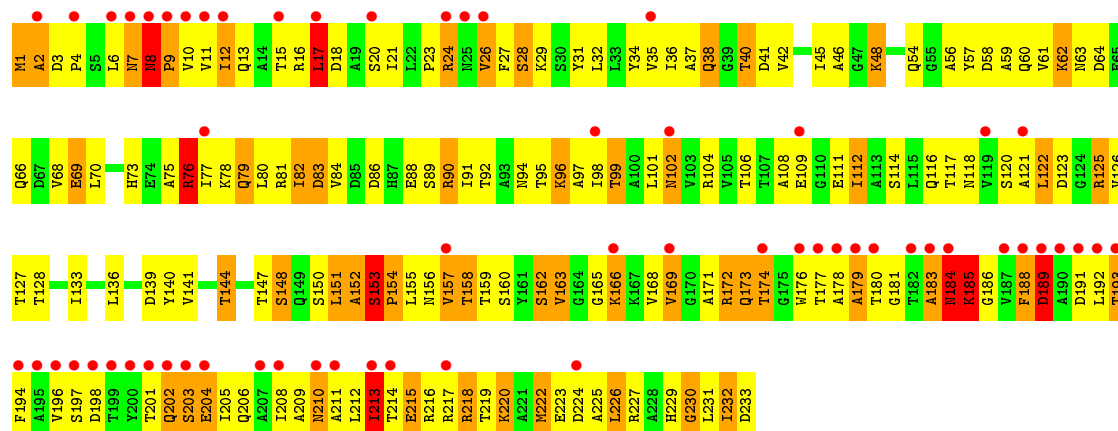


• Molecule 1: Head completion protein

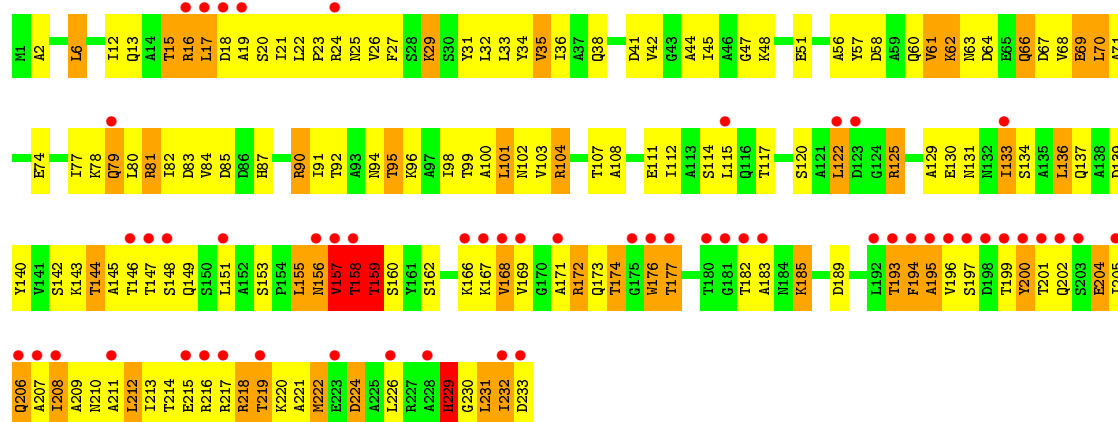




• Molecule 1: Head completion protein

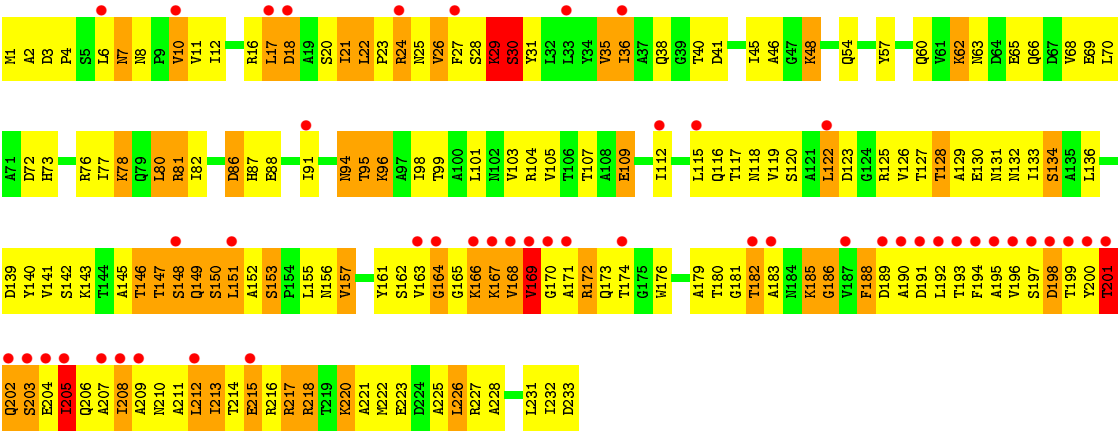


• Molecule 1: Head completion protein



• Molecule 1: Head completion protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.40 Å 114.03 Å 171.92 Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10 39.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.3 ((Not available)-2.10) 99.0 (39.21-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.00 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.167 , 0.232 0.304 , 0.350	Depositor DCC
R_{free} test set	4967 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.3	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 103960 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11261	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.38	0/1754	1.23	6/2384 (0.3%)
1	B	0.35	0/1754	1.03	2/2384 (0.1%)
1	C	0.46	1/1754 (0.1%)	1.09	7/2384 (0.3%)
1	D	0.33	0/1730	0.96	4/2347 (0.2%)
1	E	0.35	0/1728	0.99	5/2347 (0.2%)
1	F	0.34	0/1750	0.98	1/2377 (0.0%)
All	All	0.37	1/10470 (0.0%)	1.05	25/14223 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
1	D	0	7
1	E	0	3
1	F	0	2
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	GLN	CD-NE2	11.38	1.61	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	NE-CZ-NH2	22.31	131.46	120.30
1	A	172	ARG	NE-CZ-NH1	-21.44	109.58	120.30
1	A	172	ARG	CD-NE-CZ	13.99	143.18	123.60
1	E	229	HIS	O-C-N	-8.77	108.28	123.20
1	D	90	ARG	NE-CZ-NH1	8.40	124.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	TYR	CA-CB-CG	8.39	129.35	113.40
1	C	201	THR	CB-CA-C	-8.25	89.31	111.60
1	D	90	ARG	CD-NE-CZ	7.02	133.43	123.60
1	C	149	GLN	N-CA-CB	-6.73	98.49	110.60
1	C	149	GLN	CB-CG-CD	-6.56	94.54	111.60
1	B	189	ASP	CB-CG-OD1	6.10	123.79	118.30
1	E	159	THR	CA-CB-CG2	-5.95	104.07	112.40
1	E	125	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	D	1	MSE	CA-CB-CG	5.71	123.01	113.30
1	C	149	GLN	CA-CB-CG	5.67	125.88	113.40
1	A	217	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	C	199	THR	CA-C-N	5.64	129.60	117.20
1	E	104	ARG	CD-NE-CZ	5.55	131.37	123.60
1	A	194	PHE	CB-CG-CD2	-5.48	116.96	120.80
1	B	31	TYR	CB-CG-CD1	5.38	124.23	121.00
1	A	125	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	E	125	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	199	THR	CA-C-O	-5.05	109.50	120.10
1	D	191	ASP	CB-CG-OD2	5.02	122.81	118.30
1	F	166	LYS	CB-CG-CD	5.00	124.61	111.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	196	VAL	Peptide
1	C	199	THR	Peptide
1	C	203	SER	Peptide
1	D	1	MSE	Peptide
1	D	152	ALA	Peptide
1	D	153	SER	Peptide
1	D	188	PHE	Peptide
1	D	189	ASP	Peptide
1	D	2	ALA	Peptide
1	D	7	ASN	Peptide
1	E	156	ASN	Peptide
1	E	158	THR	Peptide
1	E	229	HIS	Mainchain
1	F	168	VAL	Peptide
1	F	169	VAL	Peptide

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	1738	0	1731	235	0
1	B	1738	0	1731	210	0
1	C	1738	0	1731	242	0
1	D	1715	0	1677	317	0
1	E	1712	0	1688	270	0
1	F	1734	0	1721	281	0
2	A	155	0	0	34	0
2	B	167	0	0	32	0
2	C	151	0	0	26	0
2	D	124	0	0	34	0
2	E	138	0	0	20	0
2	F	151	0	0	39	0
All	All	11261	0	10279	1200	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 58.

All (1200) 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:D:222:MSE:SE	1:E:222:MSE:HE3	1.31	1.75
1:D:222:MSE:SE	1:E:222:MSE:CE	2.22	1.36
1:E:157:VAL:HG23	1:F:164:GLY:CA	1.54	1.35
1:D:153:SER:OG	1:E:158:THR:HB	1.36	1.25
1:E:157:VAL:CG2	1:E:158:THR:H	1.44	1.23
1:E:157:VAL:HG22	1:E:158:THR:N	1.43	1.21
1:F:168:VAL:O	1:F:169:VAL:HG23	1.40	1.19
1:E:156:ASN:ND2	1:E:157:VAL:HG12	1.59	1.14
1:D:172:ARG:HH11	1:D:172:ARG:HG2	1.14	1.12
1:E:157:VAL:HG23	1:F:164:GLY:HA2	1.13	1.11
1:B:189:ASP:HB3	1:B:192:LEU:HD12	1.11	1.10
1:D:163:VAL:HG22	1:F:171:ALA:HB2	1.19	1.10
1:D:152:ALA:HB2	2:D:293:HOH:O	1.49	1.09
1:E:231:LEU:HD13	1:F:168:VAL:HG22	1.30	1.07
1:D:150:SER:HB2	1:E:156:ASN:HD22	1.20	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASP:CB	1:B:192:LEU:HD12	1.87	1.05
1:D:8:ASN:H	1:D:9:PRO:CD	1.69	1.04
1:C:157:VAL:CG1	1:C:158:THR:H	1.70	1.03
1:E:157:VAL:CG2	1:F:164:GLY:HA2	1.88	1.03
1:D:189:ASP:OD1	1:E:216:ARG:HD2	1.56	1.02
1:D:106:THR:HG22	1:E:104:ARG:HH12	1.25	1.02
1:B:29:LYS:HE3	1:B:33:LEU:HD21	1.43	1.01
1:E:157:VAL:CG2	1:E:158:THR:N	2.12	1.01
1:D:8:ASN:H	1:D:9:PRO:HD3	1.25	1.00
1:F:17:LEU:HD13	1:F:36:ILE:HD12	1.37	1.00
1:E:157:VAL:CG2	1:F:164:GLY:CA	2.42	0.97
1:A:1:MSE:SE	1:A:2:ALA:N	2.48	0.97
1:F:176:TRP:HB2	1:F:233:ASP:HB3	1.48	0.96
1:B:189:ASP:HB3	1:B:192:LEU:CD1	1.96	0.95
1:D:188:PHE:CZ	1:E:216:ARG:HD3	2.03	0.94
1:F:169:VAL:HG12	1:F:170:GLY:H	1.33	0.93
1:B:62:LYS:HG3	1:C:1:MSE:HE2	1.51	0.93
1:C:157:VAL:HG13	1:C:158:THR:H	1.29	0.93
1:D:212:LEU:H	1:E:216:ARG:HH21	1.16	0.92
1:D:176:TRP:H	1:F:185:LYS:HD3	1.32	0.92
1:A:203:SER:HA	1:A:206:GLN:HE21	1.34	0.92
1:E:231:LEU:HD13	1:F:168:VAL:CG2	1.98	0.91
1:A:173:GLN:HE22	1:B:228:ALA:HB3	1.33	0.91
1:C:191:ASP:C	1:C:192:LEU:HD23	1.93	0.89
1:D:163:VAL:CG2	1:F:171:ALA:HB2	2.01	0.89
1:F:168:VAL:O	1:F:168:VAL:HG22	1.71	0.89
1:C:157:VAL:CG1	1:C:158:THR:N	2.30	0.89
1:F:202:GLN:HE21	1:F:203:SER:H	1.21	0.88
1:E:142:SER:H	1:E:149:GLN:HE22	1.22	0.88
1:D:4:PRO:HB2	2:D:248:HOH:O	1.72	0.87
1:F:183:ALA:HB1	1:F:221:ALA:HB2	1.56	0.87
1:A:226:LEU:HD22	1:A:231:LEU:HD12	1.57	0.85
1:E:168:VAL:HG12	1:E:168:VAL:O	1.74	0.85
1:D:174:THR:HA	1:D:233:ASP:HB2	1.57	0.85
1:B:192:LEU:HD23	1:B:193:THR:O	1.76	0.85
1:E:157:VAL:HG23	1:F:164:GLY:N	1.92	0.85
1:F:183:ALA:HB2	1:F:220:LYS:HE3	1.58	0.85
1:D:4:PRO:CG	1:D:64:ASP:OD2	2.25	0.85
1:A:183:ALA:HB2	1:A:220:LYS:HG3	1.59	0.85
1:D:91:ILE:HG12	1:E:91:ILE:HG12	1.57	0.84
1:D:3:ASP:N	1:D:4:PRO:HD3	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ARG:NH1	1:E:166:LYS:CE	2.42	0.83
1:C:157:VAL:HG12	1:C:158:THR:N	1.93	0.83
1:E:183:ALA:HB2	1:E:220:LYS:HB3	1.61	0.83
1:E:160:SER:CB	1:E:167:LYS:HE2	2.08	0.83
1:C:226:LEU:HD23	1:C:231:LEU:HD23	1.61	0.83
1:D:3:ASP:H	1:D:4:PRO:HD3	1.41	0.83
1:D:172:ARG:HH11	1:E:166:LYS:HG2	1.44	0.82
1:D:172:ARG:NH1	1:E:166:LYS:HE2	1.94	0.82
1:E:156:ASN:CG	1:E:157:VAL:N	2.33	0.82
1:D:226:LEU:HD12	1:F:222:MSE:HE3	1.59	0.82
1:E:157:VAL:CG2	1:F:164:GLY:O	2.28	0.81
1:B:31:TYR:HB2	1:C:21:ILE:HD12	1.61	0.81
1:D:172:ARG:NH1	1:D:172:ARG:HG2	1.91	0.81
1:E:205:ILE:HA	1:E:208:ILE:HD11	1.62	0.81
1:D:3:ASP:N	1:D:4:PRO:CD	2.43	0.81
1:D:176:TRP:HA	1:F:185:LYS:HG2	1.63	0.81
1:D:222:MSE:SE	1:E:226:LEU:HG	2.30	0.81
1:D:151:LEU:HB3	1:F:143:LYS:HA	1.61	0.81
1:E:160:SER:HB3	1:E:167:LYS:HE2	1.63	0.81
1:B:192:LEU:HD22	1:B:192:LEU:O	1.81	0.81
1:B:69:GLU:HG2	1:C:70:LEU:HD13	1.62	0.80
1:D:6:LEU:O	1:D:6:LEU:HG	1.82	0.80
1:A:105:VAL:O	1:A:109:GLU:HG3	1.83	0.79
1:D:172:ARG:HB3	1:E:168:VAL:CG2	2.12	0.79
1:B:106:THR:HA	1:B:109:GLU:OE2	1.83	0.79
1:A:150:SER:HB3	1:C:156:ASN:HD22	1.47	0.79
1:E:156:ASN:CG	1:E:157:VAL:H	1.85	0.79
1:F:212:LEU:O	1:F:216:ARG:HG2	1.83	0.79
1:F:87:HIS:O	1:F:91:ILE:HG22	1.83	0.79
1:D:215:GLU:O	1:D:219:THR:HG23	1.83	0.78
1:F:169:VAL:CG1	1:F:170:GLY:H	1.97	0.78
1:A:5:SER:HB2	2:C:344:HOH:O	1.84	0.78
1:D:8:ASN:N	1:D:9:PRO:CD	2.41	0.78
1:B:129:ALA:O	1:B:133:ILE:HG23	1.83	0.78
1:D:91:ILE:HG13	1:F:91:ILE:HD13	1.63	0.78
1:D:66:GLN:O	1:D:70:LEU:HD12	1.84	0.78
1:B:172:ARG:HB2	1:B:230:GLY:O	1.83	0.78
1:B:1:MSE:HG2	2:B:254:HOH:O	1.84	0.78
1:B:101:LEU:HD21	1:C:102:ASN:OD1	1.84	0.78
1:E:155:LEU:HB2	1:F:157:VAL:HG21	1.66	0.78
1:A:182:THR:HG23	2:A:345:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:THR:HG22	1:C:201:THR:O	1.83	0.78
1:E:157:VAL:HG21	1:F:164:GLY:O	1.84	0.78
1:E:206:GLN:O	1:E:209:ALA:HB3	1.84	0.77
1:E:226:LEU:HD12	1:E:232:ILE:HD11	1.66	0.77
1:B:163:VAL:HG12	1:B:168:VAL:HG21	1.64	0.77
1:F:62:LYS:O	1:F:66:GLN:HG3	1.84	0.77
1:A:216:ARG:NH2	1:B:192:LEU:HD11	1.99	0.77
1:C:1:MSE:HB2	1:C:64:ASP:OD1	1.84	0.77
1:A:142:SER:HA	1:C:139:ASP:O	1.85	0.77
1:F:130:GLU:HA	1:F:133:ILE:HD12	1.67	0.77
1:E:80:LEU:O	1:E:84:VAL:HG23	1.85	0.77
1:A:57:TYR:O	1:A:61:VAL:HG23	1.85	0.77
1:F:103:VAL:O	1:F:107:THR:HG23	1.85	0.77
1:F:151:LEU:HD21	1:F:155:LEU:HD12	1.66	0.77
1:E:209:ALA:O	1:E:213:ILE:HG13	1.84	0.76
1:C:103:VAL:O	1:C:107:THR:HG23	1.84	0.76
1:D:168:VAL:HG11	1:F:171:ALA:HA	1.67	0.76
1:D:172:ARG:NE	1:D:233:ASP:HA	2.00	0.76
1:A:192:LEU:H	1:A:192:LEU:HD22	1.49	0.76
1:E:208:ILE:O	1:E:212:LEU:HB2	1.85	0.76
1:E:21:ILE:HD12	1:F:31:TYR:HB2	1.66	0.76
1:D:108:ALA:O	1:D:112:ILE:HD12	1.86	0.76
1:F:29:LYS:HE3	1:F:29:LYS:H	1.51	0.76
1:A:1:MSE:SE	1:A:2:ALA:H	2.19	0.76
1:B:176:TRP:HB2	1:B:233:ASP:HB3	1.68	0.76
1:A:126:VAL:O	1:A:130:GLU:HG3	1.85	0.75
1:D:163:VAL:HG11	1:F:170:GLY:C	2.06	0.75
1:C:73:HIS:O	1:C:77:ILE:HG12	1.87	0.75
1:D:62:LYS:O	1:D:66:GLN:HG3	1.86	0.75
1:D:172:ARG:HG2	1:E:166:LYS:HG2	1.66	0.75
1:C:115:LEU:O	1:C:119:VAL:HG23	1.86	0.75
1:D:172:ARG:HB2	1:D:230:GLY:O	1.86	0.75
1:C:47:GLY:O	1:C:51:GLU:HG3	1.87	0.75
1:E:62:LYS:O	1:E:66:GLN:HG2	1.87	0.74
1:A:229:HIS:O	1:C:167:LYS:HE2	1.88	0.74
1:F:169:VAL:HG12	1:F:170:GLY:N	1.98	0.74
1:D:81:ARG:HD2	2:D:316:HOH:O	1.87	0.74
1:B:17:LEU:HD23	1:B:21:ILE:HD11	1.69	0.74
1:E:41:ASP:O	1:E:45:ILE:HG13	1.88	0.74
1:A:227:ARG:HD2	2:A:352:HOH:O	1.87	0.74
1:C:129:ALA:O	1:C:133:ILE:HG13	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:THR:HB	1:E:139:ASP:OD2	1.87	0.74
1:E:12:ILE:HD11	2:E:318:HOH:O	1.87	0.73
1:A:133:ILE:O	1:A:137:GLN:HG3	1.88	0.73
1:F:168:VAL:O	1:F:169:VAL:CG2	2.30	0.73
1:D:151:LEU:HB2	2:F:324:HOH:O	1.87	0.73
1:A:145:ALA:O	1:C:153:SER:HB3	1.88	0.73
1:E:91:ILE:HA	2:E:325:HOH:O	1.87	0.73
1:A:50:ASN:OD1	1:C:48:LYS:HD2	1.88	0.73
1:D:172:ARG:HE	1:D:233:ASP:HA	1.52	0.73
1:D:212:LEU:N	1:E:216:ARG:HH21	1.86	0.73
1:B:29:LYS:O	1:B:33:LEU:HG	1.89	0.73
1:F:94:ASN:O	1:F:98:ILE:HG13	1.89	0.73
1:A:148:SER:HB2	1:C:154:PRO:HB2	1.70	0.73
1:E:156:ASN:ND2	1:E:157:VAL:CG1	2.47	0.72
1:A:156:ASN:ND2	1:B:150:SER:HB3	2.04	0.72
1:E:108:ALA:O	1:E:112:ILE:HG13	1.89	0.72
1:B:1:MSE:HB3	1:B:64:ASP:OD1	1.89	0.72
1:D:162:SER:HB3	1:F:156:ASN:HB2	1.71	0.72
1:A:122:LEU:O	1:A:126:VAL:HG23	1.89	0.72
1:B:189:ASP:OD1	1:B:192:LEU:HB3	1.88	0.72
1:F:188:PHE:HZ	1:F:215:GLU:HA	1.54	0.72
1:B:125:ARG:HH21	1:C:126:VAL:HG12	1.52	0.72
1:D:23:PRO:HB2	1:D:26:VAL:HG11	1.72	0.72
1:D:189:ASP:OD2	1:E:216:ARG:HB3	1.90	0.72
1:A:206:GLN:HG2	1:B:196:VAL:HG11	1.71	0.72
1:C:94:ASN:O	1:C:98:ILE:HG23	1.90	0.72
1:D:189:ASP:CG	1:E:216:ARG:HD2	2.09	0.72
1:C:95:THR:O	1:C:98:ILE:HG13	1.89	0.72
1:C:18:ASP:O	1:C:22:LEU:HD22	1.90	0.72
1:B:104:ARG:NH1	1:C:105:VAL:HB	2.05	0.71
1:B:101:LEU:O	1:B:105:VAL:HG23	1.89	0.71
1:C:19:ALA:HA	1:C:22:LEU:HB2	1.72	0.71
1:D:172:ARG:NH1	1:E:166:LYS:HG2	2.04	0.71
1:D:156:ASN:HB2	1:F:150:SER:HA	1.71	0.71
1:C:124:GLY:O	1:C:128:THR:HG23	1.90	0.71
1:E:205:ILE:HG12	1:F:205:ILE:HG21	1.71	0.71
1:E:157:VAL:HG22	1:E:158:THR:H	0.60	0.71
1:C:145:ALA:HB3	2:C:326:HOH:O	1.89	0.71
1:A:26:VAL:HG21	1:C:26:VAL:HG21	1.71	0.71
1:A:223:GLU:O	1:A:227:ARG:HG2	1.90	0.71
1:D:77:ILE:HG23	1:E:80:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LEU:HD22	1:E:69:GLU:HG2	1.73	0.70
1:E:157:VAL:CG2	1:F:164:GLY:C	2.60	0.70
1:E:171:ALA:HB2	2:E:259:HOH:O	1.91	0.70
1:E:129:ALA:O	1:E:133:ILE:HG22	1.90	0.70
1:E:156:ASN:HD21	1:E:157:VAL:HG12	1.55	0.70
1:A:215:GLU:HG3	1:B:215:GLU:OE2	1.91	0.70
1:C:100:ALA:HB3	2:C:251:HOH:O	1.91	0.70
1:E:102:ASN:ND2	1:F:104:ARG:HH12	1.90	0.70
1:A:176:TRP:HB2	1:A:233:ASP:HB3	1.72	0.70
1:C:114:SER:HA	1:C:117:THR:OG1	1.91	0.70
1:A:202:GLN:O	1:A:206:GLN:HG3	1.90	0.70
1:D:172:ARG:HE	1:D:233:ASP:CA	2.05	0.70
1:E:215:GLU:HA	2:E:345:HOH:O	1.92	0.70
1:B:134:SER:HA	1:B:137:GLN:HE21	1.56	0.70
1:B:173:GLN:HE22	1:C:228:ALA:HB3	1.55	0.70
1:D:45:ILE:HD13	2:F:378:HOH:O	1.91	0.69
1:A:155:LEU:HB2	1:C:157:VAL:HG21	1.74	0.69
1:F:202:GLN:HE21	1:F:203:SER:N	1.91	0.69
1:B:104:ARG:HD3	1:C:109:GLU:OE2	1.92	0.69
1:E:82:ILE:HG23	2:E:348:HOH:O	1.89	0.69
1:C:8:ASN:HB2	2:C:346:HOH:O	1.91	0.69
1:A:220:LYS:HE3	1:A:224:ASP:OD1	1.93	0.69
1:D:46:ALA:HB2	1:E:45:ILE:HD13	1.73	0.69
1:D:121:ALA:O	1:D:125:ARG:HG3	1.93	0.69
1:D:83:ASP:O	1:D:86:ASP:HB3	1.92	0.69
1:C:194:PHE:HA	2:C:336:HOH:O	1.92	0.69
1:D:165:GLY:H	1:F:156:ASN:HD21	1.39	0.69
1:A:23:PRO:HB3	1:C:27:PHE:HB3	1.75	0.69
1:B:158:THR:OG1	1:C:152:ALA:HA	1.93	0.69
1:A:197:SER:HB2	1:A:199:THR:O	1.91	0.69
1:B:120:SER:HB2	2:F:331:HOH:O	1.92	0.69
1:D:226:LEU:HD22	1:D:231:LEU:HD12	1.74	0.69
1:D:4:PRO:HG3	1:D:64:ASP:OD2	1.92	0.69
1:E:157:VAL:HG23	1:F:164:GLY:C	2.13	0.69
1:A:215:GLU:OE2	1:C:215:GLU:HG3	1.93	0.69
1:C:121:ALA:HA	2:C:249:HOH:O	1.91	0.69
1:D:91:ILE:HG23	2:E:325:HOH:O	1.93	0.68
1:F:189:ASP:HB3	1:F:192:LEU:HB2	1.74	0.68
1:B:104:ARG:HH11	1:C:105:VAL:HB	1.58	0.68
1:C:191:ASP:HB3	2:C:345:HOH:O	1.92	0.68
1:B:87:HIS:O	1:B:91:ILE:HG13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:315:HOH:O	1:B:222:MSE:HE1	1.94	0.68
1:D:38:GLN:O	1:D:42:VAL:HG23	1.94	0.68
1:A:95:THR:HA	1:A:98:ILE:HG22	1.75	0.68
1:D:28:SER:HB3	2:D:279:HOH:O	1.93	0.68
1:D:172:ARG:HH11	1:D:172:ARG:CG	1.97	0.68
1:D:172:ARG:NH1	1:E:166:LYS:CG	2.57	0.68
1:E:185:LYS:HE3	1:F:176:TRP:NE1	2.09	0.68
1:F:45:ILE:HA	2:F:367:HOH:O	1.93	0.68
1:D:163:VAL:HG11	1:F:170:GLY:O	1.94	0.68
1:B:226:LEU:HD22	1:C:222:MSE:SE	2.44	0.67
1:A:156:ASN:HB3	1:B:150:SER:HA	1.76	0.67
1:B:134:SER:HA	1:B:137:GLN:NE2	2.08	0.67
1:B:225:ALA:HB3	2:B:317:HOH:O	1.92	0.67
1:D:185:LYS:HD2	1:E:176:TRP:HA	1.77	0.67
1:B:192:LEU:HD22	1:B:192:LEU:C	2.15	0.67
1:D:181:GLY:HA2	1:F:190:ALA:HB2	1.75	0.67
1:F:225:ALA:O	1:F:228:ALA:HB3	1.95	0.67
1:F:204:GLU:O	1:F:205:ILE:HB	1.94	0.67
1:E:155:LEU:HD23	1:E:156:ASN:H	1.60	0.67
1:A:220:LYS:HA	2:A:357:HOH:O	1.94	0.67
1:D:223:GLU:HA	1:F:222:MSE:HE2	1.75	0.67
1:B:216:ARG:O	1:B:219:THR:HB	1.95	0.67
1:A:99:THR:HA	2:A:346:HOH:O	1.95	0.67
1:D:61:VAL:HA	1:D:64:ASP:OD2	1.95	0.66
1:D:70:LEU:HD21	1:E:70:LEU:HD22	1.77	0.66
1:C:172:ARG:HD3	1:C:233:ASP:HA	1.77	0.66
1:E:189:ASP:OD2	1:F:180:THR:HG23	1.95	0.66
1:F:222:MSE:O	1:F:226:LEU:HB2	1.95	0.66
1:B:102:ASN:O	1:B:106:THR:HG22	1.94	0.66
1:B:173:GLN:NE2	1:C:228:ALA:HB3	2.10	0.66
1:D:125:ARG:HH21	1:F:126:VAL:HG12	1.61	0.66
2:E:336:HOH:O	1:F:167:LYS:HE3	1.96	0.66
1:D:150:SER:HB2	1:E:156:ASN:ND2	2.02	0.66
1:A:203:SER:HA	1:A:206:GLN:NE2	2.09	0.66
1:F:38:GLN:HG3	2:F:369:HOH:O	1.95	0.66
1:A:31:TYR:O	1:A:35:VAL:HG23	1.96	0.66
1:D:127:THR:HG22	1:E:125:ARG:HH22	1.59	0.66
2:A:342:HOH:O	1:B:77:ILE:HD13	1.96	0.66
1:A:143:LYS:HE2	1:C:149:GLN:HG2	1.78	0.66
1:A:153:SER:O	1:C:157:VAL:HG13	1.95	0.66
1:A:202:GLN:NE2	1:B:196:VAL:HG13	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:THR:O	1:D:120:SER:HB3	1.95	0.66
1:C:62:LYS:O	1:C:66:GLN:HG3	1.96	0.66
1:D:31:TYR:O	1:D:35:VAL:HG12	1.96	0.66
1:D:48:LYS:HG2	1:F:10:VAL:HB	1.78	0.66
1:D:24:ARG:O	1:D:26:VAL:HG12	1.96	0.65
1:F:169:VAL:CG1	1:F:170:GLY:N	2.53	0.65
1:D:157:VAL:HA	1:F:151:LEU:HD23	1.76	0.65
1:D:9:PRO:HD2	1:E:48:LYS:NZ	2.12	0.65
1:F:129:ALA:HB3	2:F:398:HOH:O	1.95	0.65
1:F:223:GLU:HG2	1:F:227:ARG:NH2	2.11	0.65
1:C:196:VAL:HG22	2:C:240:HOH:O	1.96	0.65
1:C:16:ARG:NH1	1:C:40:THR:HG22	2.11	0.65
1:A:212:LEU:HD21	2:B:333:HOH:O	1.96	0.65
1:B:156:ASN:HD22	1:B:157:VAL:H	1.45	0.65
1:A:6:LEU:HB3	1:A:57:TYR:HB2	1.79	0.65
1:F:168:VAL:O	1:F:168:VAL:CG2	2.45	0.65
1:E:200:TYR:HA	1:E:205:ILE:HD12	1.77	0.65
1:D:157:VAL:HA	2:F:366:HOH:O	1.97	0.65
1:A:160:SER:HB2	1:A:169:VAL:O	1.97	0.65
1:B:156:ASN:HD22	1:B:157:VAL:N	1.94	0.65
1:A:65:GLU:HG2	2:A:264:HOH:O	1.97	0.65
1:E:229:HIS:HD2	1:F:169:VAL:HG22	1.61	0.65
1:D:172:ARG:HH12	1:E:166:LYS:CE	2.09	0.65
1:A:54:GLN:HG2	2:A:340:HOH:O	1.95	0.65
1:C:212:LEU:HD13	1:C:216:ARG:HD3	1.79	0.65
1:E:2:ALA:HB3	2:E:352:HOH:O	1.97	0.64
1:E:102:ASN:HD21	1:F:104:ARG:HH12	1.44	0.64
1:D:141:VAL:HG13	1:F:141:VAL:HB	1.80	0.64
1:D:165:GLY:H	1:F:156:ASN:ND2	1.96	0.64
1:E:94:ASN:HB2	2:F:383:HOH:O	1.96	0.64
1:B:92:THR:O	1:B:96:LYS:HG2	1.97	0.64
1:A:173:GLN:NE2	1:B:228:ALA:HB3	2.10	0.64
1:E:231:LEU:HA	1:F:168:VAL:HG23	1.78	0.64
1:D:8:ASN:N	1:D:9:PRO:HD3	2.05	0.64
1:D:172:ARG:HH12	1:E:166:LYS:HE3	1.62	0.64
1:B:203:SER:HA	1:B:206:GLN:HG2	1.79	0.64
1:B:205:ILE:HG22	2:B:339:HOH:O	1.97	0.64
1:C:50:ASN:HB3	2:C:305:HOH:O	1.98	0.64
1:B:43:GLY:O	1:B:46:ALA:HB3	1.98	0.64
1:E:19:ALA:HA	1:E:22:LEU:HD12	1.79	0.64
1:A:69:GLU:HG3	2:B:320:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASP:H	1:A:60:GLN:NE2	1.95	0.63
2:A:350:HOH:O	1:C:45:ILE:HD13	1.98	0.63
1:D:179:ALA:HB1	2:F:380:HOH:O	1.97	0.63
1:F:163:VAL:HG23	2:F:306:HOH:O	1.99	0.63
1:E:215:GLU:HG3	2:E:345:HOH:O	1.99	0.63
1:E:200:TYR:HB2	1:F:200:TYR:CD1	2.34	0.63
1:C:122:LEU:O	1:C:126:VAL:HG23	1.99	0.63
1:D:102:ASN:HD22	1:E:101:LEU:HD21	1.64	0.63
1:A:23:PRO:HG3	1:C:27:PHE:HD2	1.63	0.63
1:A:189:ASP:HB2	1:C:180:THR:OG1	1.97	0.63
1:E:143:LYS:HE3	1:F:140:TYR:O	1.99	0.63
1:E:16:ARG:HG3	1:E:17:LEU:O	1.99	0.63
1:C:191:ASP:CA	1:C:192:LEU:HD23	2.29	0.62
1:E:58:ASP:O	1:E:61:VAL:HG13	1.99	0.62
1:E:87:HIS:O	1:E:91:ILE:HG13	1.99	0.62
1:E:57:TYR:O	1:E:61:VAL:HG12	1.99	0.62
1:F:35:VAL:HG12	1:F:36:ILE:HD13	1.81	0.62
1:E:130:GLU:O	1:E:133:ILE:HG23	1.99	0.62
1:E:144:THR:HB	1:F:139:ASP:OD1	1.99	0.62
1:E:208:ILE:HD13	1:E:208:ILE:H	1.63	0.62
1:D:116:GLN:HG3	1:E:115:LEU:HD11	1.81	0.62
1:C:149:GLN:NE2	2:C:326:HOH:O	2.32	0.62
1:A:78:LYS:HG3	2:A:292:HOH:O	1.99	0.62
1:E:231:LEU:CD1	1:F:168:VAL:HG22	2.20	0.62
1:C:199:THR:O	1:C:200:TYR:HB3	1.99	0.62
1:D:106:THR:O	1:D:109:GLU:HG2	1.99	0.62
1:E:98:ILE:HG23	1:F:101:LEU:HD11	1.81	0.62
1:C:128:THR:HG21	2:C:379:HOH:O	1.99	0.62
1:A:141:VAL:HB	1:C:141:VAL:HB	1.81	0.62
2:A:353:HOH:O	1:B:42:VAL:HG11	1.99	0.62
1:C:199:THR:HG23	1:C:200:TYR:H	1.65	0.61
1:E:61:VAL:HA	1:E:64:ASP:OD2	1.99	0.61
1:E:158:THR:HG22	1:E:159:THR:N	2.14	0.61
1:F:101:LEU:O	1:F:105:VAL:HG23	2.00	0.61
1:D:58:ASP:O	1:D:62:LYS:HG2	2.00	0.61
1:A:222:MSE:HA	1:A:222:MSE:HE3	1.82	0.61
1:C:32:LEU:O	1:C:36:ILE:HG13	2.01	0.61
1:A:156:ASN:HD22	1:B:150:SER:HB3	1.65	0.61
1:D:7:ASN:HA	2:D:255:HOH:O	2.00	0.61
1:D:45:ILE:HG22	1:E:45:ILE:HG21	1.82	0.61
1:D:96:LYS:HB3	2:D:307:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:HIS:HB3	1:E:231:LEU:HD22	1.83	0.61
1:E:168:VAL:O	1:E:168:VAL:CG1	2.47	0.61
1:B:195:ALA:O	1:B:204:GLU:HG3	2.01	0.61
1:F:29:LYS:HG2	1:F:29:LYS:O	2.01	0.61
1:D:76:ARG:HB3	1:F:77:ILE:HD13	1.83	0.61
1:D:177:THR:HB	1:F:186:GLY:O	1.99	0.61
1:E:158:THR:HG22	1:E:159:THR:H	1.64	0.61
1:A:212:LEU:HD13	1:A:216:ARG:HD3	1.82	0.61
1:B:157:VAL:HG22	1:C:153:SER:O	2.01	0.61
1:E:133:ILE:HD12	1:F:136:LEU:HD12	1.83	0.61
1:A:38:GLN:HG2	2:C:341:HOH:O	2.00	0.61
1:D:69:GLU:OE2	1:F:70:LEU:HD22	2.00	0.60
1:B:120:SER:O	1:B:123:ASP:HB2	2.00	0.60
1:D:36:ILE:HG23	2:D:257:HOH:O	2.00	0.60
1:D:231:LEU:HD23	1:E:168:VAL:HG13	1.82	0.60
1:B:201:THR:HB	1:B:204:GLU:HB2	1.82	0.60
1:F:200:TYR:CE1	1:F:205:ILE:HD13	2.37	0.60
1:A:223:GLU:HA	1:B:222:MSE:HE1	1.84	0.60
1:C:194:PHE:HA	2:C:303:HOH:O	2.00	0.60
1:D:181:GLY:HA3	2:D:297:HOH:O	2.01	0.60
1:A:212:LEU:HD11	2:B:333:HOH:O	2.00	0.60
1:D:41:ASP:OD2	1:F:12:ILE:HB	2.02	0.60
1:A:26:VAL:HG11	1:C:26:VAL:HG23	1.84	0.60
1:E:155:LEU:HD23	1:E:156:ASN:N	2.16	0.60
1:E:208:ILE:HG21	1:F:209:ALA:HB1	1.83	0.60
1:F:140:TYR:HB2	2:F:292:HOH:O	2.01	0.60
1:D:11:VAL:O	1:D:12:ILE:HB	2.02	0.60
1:D:99:THR:HA	1:D:102:ASN:OD1	2.02	0.60
1:E:220:LYS:HE2	1:E:224:ASP:OD1	2.02	0.60
1:E:67:ASP:HA	1:E:70:LEU:HB2	1.82	0.59
1:D:215:GLU:HG3	1:F:215:GLU:OE1	2.01	0.59
1:B:107:THR:HG23	2:B:349:HOH:O	2.02	0.59
1:E:15:THR:HA	2:E:266:HOH:O	2.03	0.59
1:B:189:ASP:CG	1:B:192:LEU:HD12	2.22	0.59
2:A:333:HOH:O	1:C:157:VAL:C	2.39	0.59
1:D:7:ASN:HB2	1:D:57:TYR:HB2	1.84	0.59
1:D:4:PRO:HG2	1:D:64:ASP:OD2	2.02	0.59
1:A:45:ILE:HD11	1:B:46:ALA:HB2	1.85	0.59
1:D:172:ARG:NH1	1:D:172:ARG:CG	2.61	0.59
1:B:192:LEU:N	1:B:192:LEU:HD13	2.18	0.59
1:D:34:TYR:CE2	1:D:38:GLN:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ILE:HA	1:E:80:LEU:HD12	1.83	0.59
1:A:141:VAL:HG23	1:B:141:VAL:HB	1.84	0.59
1:F:202:GLN:H	1:F:202:GLN:NE2	2.00	0.59
1:E:94:ASN:O	1:E:98:ILE:HG13	2.02	0.59
1:E:183:ALA:HB2	1:E:220:LYS:HD3	1.85	0.59
2:A:356:HOH:O	1:B:119:VAL:HG11	2.02	0.59
1:A:51:GLU:O	1:A:54:GLN:HB3	2.03	0.59
1:C:14:ALA:HB3	1:D:128:THR:OG1	2.03	0.59
1:C:141:VAL:HA	1:C:149:GLN:OE1	2.03	0.59
1:D:109:GLU:HB3	2:D:325:HOH:O	2.01	0.59
1:A:2:ALA:HA	1:A:60:GLN:HE21	1.68	0.59
1:A:201:THR:O	1:A:205:ILE:HG22	2.02	0.59
1:E:156:ASN:ND2	1:E:157:VAL:H	2.01	0.58
1:F:17:LEU:CD1	1:F:36:ILE:HA	2.33	0.58
1:A:216:ARG:NH2	1:B:192:LEU:CD1	2.66	0.58
1:B:212:LEU:O	1:B:215:GLU:HB3	2.03	0.58
1:F:91:ILE:O	1:F:95:THR:HG22	2.02	0.58
1:C:200:TYR:CE1	1:C:203:SER:HA	2.38	0.58
1:E:133:ILE:HD11	1:F:132:ASN:HB3	1.86	0.58
1:D:188:PHE:HE2	1:E:216:ARG:O	1.86	0.58
1:E:215:GLU:OE2	1:F:216:ARG:HB3	2.04	0.58
1:C:226:LEU:CD2	1:C:231:LEU:HD23	2.33	0.58
1:D:46:ALA:HB2	1:E:45:ILE:CD1	2.33	0.58
1:D:79:GLN:HA	1:D:82:ILE:HG22	1.86	0.58
1:F:72:ASP:O	1:F:76:ARG:HG3	2.04	0.58
1:A:1:MSE:C	1:A:1:MSE:SE	2.89	0.58
1:F:23:PRO:HB2	1:F:26:VAL:HG11	1.86	0.58
1:F:21:ILE:O	1:F:21:ILE:HG13	2.04	0.58
1:F:119:VAL:O	1:F:122:LEU:HB2	2.04	0.58
1:F:96:LYS:HD2	2:F:305:HOH:O	2.04	0.58
1:E:111:GLU:O	1:E:115:LEU:HD13	2.03	0.58
1:D:133:ILE:HD11	2:F:418:HOH:O	2.04	0.58
1:E:47:GLY:O	1:E:51:GLU:HG3	2.04	0.58
1:D:186:GLY:HA2	1:E:177:THR:OG1	2.04	0.57
1:A:216:ARG:HH21	1:B:192:LEU:CD1	2.17	0.57
1:D:173:GLN:HB3	2:F:345:HOH:O	2.03	0.57
1:D:157:VAL:O	1:D:158:THR:C	2.42	0.57
1:B:38:GLN:O	1:B:42:VAL:HG23	2.03	0.57
1:A:9:PRO:HB3	2:A:329:HOH:O	2.02	0.57
1:D:150:SER:CB	1:E:156:ASN:HD22	2.07	0.57
1:E:159:THR:HG21	2:E:303:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:GLU:OE2	1:E:215:GLU:HG2	2.04	0.57
1:C:192:LEU:N	1:C:192:LEU:HD23	2.19	0.57
1:D:56:ALA:O	1:D:60:GLN:HG3	2.04	0.57
1:C:31:TYR:O	1:C:35:VAL:HG22	2.04	0.57
1:C:13:GLN:O	1:C:13:GLN:HG3	2.04	0.57
1:D:60:GLN:O	1:D:64:ASP:OD2	2.22	0.57
1:C:184:ASN:HD22	1:C:218:ARG:HH11	1.53	0.57
1:B:31:TYR:CB	1:C:21:ILE:HD12	2.34	0.57
1:F:76:ARG:HD2	2:F:377:HOH:O	2.02	0.57
1:C:197:SER:HB2	1:C:200:TYR:HA	1.86	0.57
1:A:226:LEU:HD12	1:B:222:MSE:CE	2.34	0.57
1:A:192:LEU:HD13	1:A:192:LEU:N	2.20	0.57
1:E:79:GLN:HE21	1:E:79:GLN:N	2.02	0.57
1:E:153:SER:O	1:F:157:VAL:HG22	2.04	0.57
1:C:140:TYR:CZ	1:C:142:SER:HB2	2.40	0.57
1:D:17:LEU:HB3	2:D:257:HOH:O	2.04	0.57
1:A:226:LEU:HD12	1:B:222:MSE:HE3	1.85	0.57
1:D:181:GLY:HA2	1:F:190:ALA:CB	2.34	0.57
1:B:27:PHE:HB3	1:B:32:LEU:HD13	1.86	0.57
1:A:222:MSE:CA	1:A:222:MSE:HE3	2.35	0.56
1:A:17:LEU:HD13	1:C:34:TYR:CZ	2.40	0.56
1:D:153:SER:CB	1:D:154:PRO:CA	2.82	0.56
1:A:212:LEU:O	1:A:216:ARG:HG2	2.04	0.56
1:A:75:ALA:HA	1:A:78:LYS:CD	2.35	0.56
1:D:223:GLU:HA	1:F:222:MSE:CE	2.36	0.56
1:D:77:ILE:HG13	1:F:77:ILE:HD11	1.87	0.56
1:A:76:ARG:HB3	2:A:321:HOH:O	2.04	0.56
1:F:205:ILE:O	1:F:208:ILE:HD13	2.06	0.56
1:F:29:LYS:O	1:F:30:SER:HB2	2.05	0.56
1:D:79:GLN:HG2	1:D:82:ILE:HG21	1.87	0.56
2:B:313:HOH:O	1:C:13:GLN:HG2	2.06	0.56
1:F:77:ILE:O	1:F:80:LEU:HB2	2.06	0.56
1:D:147:THR:O	1:D:148:SER:HB2	2.05	0.56
1:F:171:ALA:O	1:F:172:ARG:C	2.43	0.56
1:D:179:ALA:HB2	1:F:218:ARG:NH2	2.21	0.56
1:A:79:GLN:HG3	1:B:81:ARG:HH22	1.71	0.56
1:C:218:ARG:O	1:C:221:ALA:HB3	2.06	0.56
1:F:40:THR:HG22	2:F:352:HOH:O	2.05	0.56
1:E:173:GLN:O	1:E:232:ILE:HG22	2.05	0.56
1:D:106:THR:HG22	1:E:104:ARG:NH1	2.08	0.56
1:C:56:ALA:O	1:C:60:GLN:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:ARG:HH11	1:F:24:ARG:HG3	1.71	0.56
1:B:162:SER:OG	1:B:167:LYS:HA	2.06	0.55
1:A:222:MSE:HE1	1:C:226:LEU:HD13	1.88	0.55
1:A:126:VAL:HG11	1:C:125:ARG:HD3	1.88	0.55
1:C:224:ASP:HB3	2:C:311:HOH:O	2.06	0.55
1:A:33:LEU:HD22	2:A:247:HOH:O	2.06	0.55
1:C:12:ILE:HD13	1:C:46:ALA:HB3	1.86	0.55
1:E:229:HIS:O	1:F:169:VAL:N	2.36	0.55
1:D:8:ASN:H	1:D:9:PRO:HD2	1.64	0.55
1:F:179:ALA:HB3	2:F:372:HOH:O	2.05	0.55
1:D:57:TYR:O	1:D:61:VAL:HG23	2.07	0.55
1:A:183:ALA:HB2	1:A:220:LYS:CG	2.33	0.55
1:E:133:ILE:O	1:E:137:GLN:HG3	2.05	0.55
1:B:18:ASP:OD2	1:B:20:SER:HB2	2.07	0.55
1:E:157:VAL:HB	1:F:164:GLY:O	2.07	0.55
1:D:162:SER:O	1:F:156:ASN:HA	2.06	0.55
1:A:148:SER:HA	1:C:154:PRO:HD2	1.89	0.55
1:A:62:LYS:O	1:A:66:GLN:HG3	2.06	0.55
1:A:111:GLU:HA	1:A:111:GLU:OE1	2.05	0.55
1:A:212:LEU:HD23	1:C:212:LEU:CD2	2.37	0.55
2:A:333:HOH:O	1:C:157:VAL:HA	2.07	0.55
1:D:45:ILE:HD11	1:F:46:ALA:HB2	1.88	0.55
1:F:45:ILE:HB	2:F:378:HOH:O	2.07	0.55
1:F:23:PRO:HB2	1:F:26:VAL:CG1	2.37	0.55
1:B:81:ARG:HA	1:B:84:VAL:HG22	1.89	0.55
1:A:125:ARG:NH2	1:B:126:VAL:HB	2.22	0.55
1:A:155:LEU:HD22	1:A:156:ASN:H	1.71	0.55
1:D:91:ILE:CG1	1:F:91:ILE:HD13	2.33	0.55
1:D:133:ILE:HG23	2:D:306:HOH:O	2.07	0.55
2:D:322:HOH:O	1:E:166:LYS:HB3	2.06	0.55
1:B:194:PHE:HZ	1:B:211:ALA:HB3	1.72	0.55
1:B:158:THR:O	1:B:159:THR:HB	2.07	0.55
1:D:196:VAL:HG21	1:E:206:GLN:HB3	1.89	0.55
1:D:17:LEU:HD12	1:D:36:ILE:HG23	1.89	0.55
1:D:202:GLN:HG3	1:F:198:ASP:HA	1.89	0.55
1:B:4:PRO:HA	1:B:57:TYR:CE2	2.42	0.55
1:B:62:LYS:HB3	1:B:62:LYS:NZ	2.22	0.54
1:F:129:ALA:HA	2:F:287:HOH:O	2.07	0.54
1:E:133:ILE:O	1:E:136:LEU:HB2	2.06	0.54
1:E:98:ILE:HG23	1:F:101:LEU:CD1	2.37	0.54
1:B:22:LEU:HD13	1:B:32:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HG	2:B:344:HOH:O	2.06	0.54
1:B:141:VAL:HG21	1:C:141:VAL:HG12	1.89	0.54
1:A:23:PRO:HB2	1:A:26:VAL:HG11	1.90	0.54
1:A:137:GLN:HG2	1:C:136:LEU:HD11	1.88	0.54
1:E:202:GLN:OE1	1:E:202:GLN:HA	2.08	0.54
1:D:168:VAL:HG23	1:D:169:VAL:HG23	1.89	0.54
1:E:208:ILE:HG21	1:F:209:ALA:CB	2.37	0.54
1:E:80:LEU:HD13	1:F:80:LEU:HD23	1.88	0.54
1:D:156:ASN:O	1:F:151:LEU:HB2	2.07	0.54
1:E:199:THR:HA	1:F:200:TYR:CZ	2.42	0.54
1:B:192:LEU:CD2	1:B:192:LEU:C	2.76	0.54
1:F:151:LEU:CD2	1:F:155:LEU:HD12	2.37	0.54
1:D:172:ARG:NH1	1:E:166:LYS:HE3	2.21	0.54
1:B:192:LEU:H	1:B:192:LEU:HD13	1.73	0.54
1:D:141:VAL:HA	2:D:256:HOH:O	2.08	0.54
1:A:183:ALA:HB1	1:A:221:ALA:HB2	1.89	0.54
1:A:222:MSE:CE	1:C:226:LEU:HD13	2.38	0.54
1:B:7:ASN:ND2	1:B:54:GLN:HA	2.23	0.54
1:E:98:ILE:CD1	1:F:94:ASN:HB2	2.38	0.54
1:D:206:GLN:O	1:D:210:ASN:HB2	2.08	0.54
2:D:234:HOH:O	1:F:78:LYS:HD2	2.07	0.54
1:C:173:GLN:HA	1:C:173:GLN:OE1	2.07	0.54
1:D:152:ALA:HB3	1:F:145:ALA:O	2.08	0.53
1:D:172:ARG:HB3	1:E:168:VAL:HG22	1.91	0.53
1:E:210:ASN:HA	1:E:213:ILE:HD12	1.90	0.53
1:A:213:ILE:HD12	1:A:214:THR:N	2.23	0.53
1:D:176:TRP:CE2	1:D:232:ILE:HG13	2.44	0.53
1:A:105:VAL:HG21	1:C:101:LEU:HD22	1.90	0.53
1:A:75:ALA:HA	1:A:78:LYS:HD2	1.90	0.53
1:D:223:GLU:HB2	2:D:300:HOH:O	2.08	0.53
1:C:97:ALA:HA	2:C:251:HOH:O	2.08	0.53
1:D:17:LEU:HD23	1:E:34:TYR:CZ	2.44	0.53
1:F:214:THR:HA	1:F:217:ARG:CD	2.39	0.53
1:E:199:THR:HG23	1:F:200:TYR:CE2	2.43	0.53
1:D:114:SER:O	1:D:117:THR:HB	2.08	0.53
1:C:65:GLU:HA	1:C:68:VAL:HG23	1.91	0.53
1:D:4:PRO:HD3	1:D:64:ASP:OD1	2.09	0.53
1:D:153:SER:H	1:E:158:THR:HG21	1.73	0.53
1:D:230:GLY:HA3	1:E:168:VAL:HA	1.89	0.53
1:D:46:ALA:HA	1:E:45:ILE:HG23	1.89	0.53
1:A:12:ILE:HD11	1:A:46:ALA:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:O	1:B:98:ILE:HG13	2.08	0.53
1:A:143:LYS:HA	1:C:151:LEU:HB3	1.90	0.53
1:E:22:LEU:HD21	1:E:35:VAL:HG21	1.90	0.53
1:A:38:GLN:HG3	2:A:353:HOH:O	2.09	0.53
1:F:214:THR:O	1:F:217:ARG:HB2	2.09	0.53
1:E:157:VAL:CB	1:F:164:GLY:O	2.57	0.53
1:C:176:TRP:HB2	1:C:233:ASP:OD1	2.09	0.53
1:E:142:SER:HB3	1:E:145:ALA:HB2	1.90	0.53
1:A:116:GLN:HG3	1:C:115:LEU:HD11	1.90	0.53
1:C:29:LYS:O	1:C:33:LEU:HG	2.09	0.53
1:A:150:SER:HB3	1:C:156:ASN:ND2	2.21	0.53
1:D:45:ILE:CD1	1:F:46:ALA:HB2	2.39	0.52
1:D:198:ASP:OD2	1:E:202:GLN:OE1	2.27	0.52
1:A:210:ASN:O	1:A:213:ILE:HG13	2.09	0.52
1:A:12:ILE:HD11	1:A:46:ALA:HB2	1.90	0.52
1:B:212:LEU:O	1:B:216:ARG:HG2	2.08	0.52
1:A:140:TYR:HE1	1:C:139:ASP:O	1.92	0.52
1:B:62:LYS:CG	1:C:1:MSE:HE2	2.34	0.52
1:B:73:HIS:O	1:B:77:ILE:HG13	2.10	0.52
1:C:89:SER:HB2	2:C:318:HOH:O	2.07	0.52
1:D:208:ILE:O	1:D:211:ALA:HB3	2.09	0.52
1:D:156:ASN:HB2	1:F:150:SER:CA	2.37	0.52
1:E:107:THR:HG22	1:E:111:GLU:OE2	2.08	0.52
1:B:1:MSE:HE3	2:B:234:HOH:O	2.08	0.52
1:A:27:PHE:HB3	2:A:338:HOH:O	2.08	0.52
1:D:155:LEU:O	1:E:162:SER:HB2	2.10	0.52
1:A:139:ASP:OD1	1:B:144:THR:HG23	2.09	0.52
1:E:183:ALA:CB	1:E:220:LYS:HB3	2.37	0.52
1:D:11:VAL:HG23	1:D:12:ILE:H	1.73	0.52
1:B:90:ARG:HG2	2:B:356:HOH:O	2.08	0.52
1:C:212:LEU:O	1:C:216:ARG:HG2	2.09	0.52
1:C:155:LEU:HD13	1:C:161:TYR:HE1	1.75	0.52
1:E:199:THR:HG23	1:F:200:TYR:CD2	2.45	0.52
1:F:29:LYS:N	1:F:29:LYS:HE3	2.20	0.52
1:B:201:THR:HB	1:B:204:GLU:CB	2.40	0.52
1:C:176:TRP:HB2	1:C:233:ASP:OD2	2.09	0.52
1:A:141:VAL:CG2	1:B:141:VAL:HB	2.39	0.52
1:C:149:GLN:O	1:C:150:SER:O	2.28	0.52
1:D:193:THR:CG2	1:D:208:ILE:HD13	2.40	0.52
1:A:137:GLN:HB3	2:A:309:HOH:O	2.09	0.52
1:B:86:ASP:OD2	1:B:87:HIS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:LYS:HG3	1:F:63:ASN:ND2	2.24	0.52
1:A:10:VAL:HG11	1:C:44:ALA:O	2.10	0.52
1:B:164:GLY:HA3	2:B:318:HOH:O	2.08	0.52
1:A:155:LEU:CD2	1:A:156:ASN:H	2.22	0.52
1:B:137:GLN:HB3	2:B:244:HOH:O	2.08	0.52
1:D:160:SER:HB2	1:D:169:VAL:O	2.11	0.52
1:A:23:PRO:O	1:A:26:VAL:HG13	2.09	0.52
1:B:159:THR:CG2	1:B:159:THR:O	2.58	0.51
1:A:223:GLU:HA	1:B:222:MSE:CE	2.39	0.51
1:E:69:GLU:O	1:E:69:GLU:HG3	2.10	0.51
1:B:3:ASP:O	1:B:6:LEU:HB2	2.09	0.51
1:D:80:LEU:HD21	1:F:81:ARG:HA	1.93	0.51
1:C:194:PHE:O	1:C:195:ALA:HB2	2.11	0.51
1:E:6:LEU:CD2	1:E:56:ALA:HB3	2.41	0.51
1:A:195:ALA:O	1:A:204:GLU:HG2	2.11	0.51
1:D:168:VAL:CG1	1:F:171:ALA:HA	2.40	0.51
1:A:149:GLN:O	1:C:155:LEU:HD23	2.09	0.51
2:D:234:HOH:O	1:F:78:LYS:HE3	2.11	0.51
1:C:80:LEU:O	1:C:84:VAL:HG23	2.09	0.51
1:B:209:ALA:HB2	1:C:208:ILE:HG12	1.92	0.51
1:F:223:GLU:HG2	1:F:227:ARG:HH22	1.73	0.51
1:D:126:VAL:HG12	1:E:125:ARG:NH2	2.24	0.51
1:B:4:PRO:HA	1:B:57:TYR:HE2	1.75	0.51
1:A:55:GLY:HA2	2:B:246:HOH:O	2.10	0.51
1:F:147:THR:O	1:F:149:GLN:HG3	2.10	0.51
1:B:139:ASP:OD1	1:C:144:THR:HG23	2.10	0.51
1:B:203:SER:HA	1:B:206:GLN:CG	2.40	0.51
1:C:182:THR:O	1:C:217:ARG:HG2	2.11	0.51
1:A:202:GLN:HA	1:A:205:ILE:HG23	1.93	0.51
1:B:105:VAL:O	1:B:109:GLU:HG3	2.10	0.51
1:B:112:ILE:O	1:B:116:GLN:HG3	2.11	0.51
1:D:81:ARG:HA	1:D:84:VAL:HG12	1.91	0.51
1:D:11:VAL:HG23	1:D:12:ILE:N	2.25	0.51
1:B:28:SER:OG	1:B:30:SER:HB2	2.11	0.51
2:D:292:HOH:O	1:F:133:ILE:HD13	2.10	0.51
1:E:231:LEU:CD1	1:F:168:VAL:CG2	2.83	0.51
1:A:212:LEU:CD1	1:A:216:ARG:HD3	2.39	0.51
1:C:216:ARG:HH11	1:C:216:ARG:HG3	1.76	0.51
1:B:160:SER:HB3	1:B:167:LYS:HE2	1.92	0.51
1:A:173:GLN:HG2	1:B:229:HIS:HE2	1.76	0.51
1:A:148:SER:CA	1:C:154:PRO:HD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HB	1:B:190:ALA:HB2	1.93	0.51
1:F:206:GLN:O	1:F:210:ASN:HB2	2.11	0.51
1:F:17:LEU:O	1:F:18:ASP:HB2	2.10	0.51
1:A:173:GLN:HG2	1:B:229:HIS:NE2	2.26	0.51
1:F:101:LEU:HG	2:F:278:HOH:O	2.11	0.51
1:F:94:ASN:HD22	1:F:94:ASN:H	1.59	0.51
1:D:125:ARG:HH21	1:F:126:VAL:CG1	2.22	0.51
1:D:111:GLU:OE1	1:F:112:ILE:HG21	2.10	0.51
1:D:156:ASN:HB2	1:F:150:SER:HB3	1.93	0.50
1:C:184:ASN:ND2	1:C:218:ARG:HH11	2.09	0.50
1:F:213:ILE:O	1:F:217:ARG:HG3	2.11	0.50
1:A:12:ILE:HG22	1:A:12:ILE:O	2.11	0.50
1:F:109:GLU:O	1:F:112:ILE:HB	2.11	0.50
1:D:168:VAL:HG11	1:F:170:GLY:O	2.10	0.50
1:B:172:ARG:O	1:B:231:LEU:O	2.29	0.50
1:D:156:ASN:HB2	1:F:150:SER:CB	2.42	0.50
1:E:204:GLU:O	1:E:207:ALA:HB3	2.11	0.50
1:E:200:TYR:HA	1:E:205:ILE:CD1	2.40	0.50
1:E:212:LEU:HD22	1:E:212:LEU:O	2.12	0.50
1:E:173:GLN:HB2	1:E:232:ILE:CG2	2.41	0.50
1:C:23:PRO:HG2	1:C:27:PHE:CZ	2.46	0.50
1:A:17:LEU:O	1:A:18:ASP:OD2	2.30	0.50
1:D:159:THR:O	1:D:160:SER:HB3	2.12	0.50
1:F:129:ALA:O	1:F:133:ILE:HG13	2.10	0.50
1:B:125:ARG:NH2	1:C:126:VAL:HG12	2.23	0.50
1:D:31:TYR:HB2	1:F:21:ILE:O	2.12	0.50
1:F:116:GLN:O	1:F:119:VAL:HG12	2.11	0.50
1:F:94:ASN:H	1:F:94:ASN:ND2	2.09	0.50
1:A:45:ILE:HG22	1:C:45:ILE:HG21	1.93	0.50
1:A:149:GLN:HE21	1:B:143:LYS:HE2	1.76	0.50
1:C:101:LEU:O	1:C:105:VAL:HG23	2.12	0.50
1:D:45:ILE:HD11	1:F:12:ILE:HG21	1.94	0.50
1:C:65:GLU:HG2	2:C:352:HOH:O	2.12	0.50
1:B:32:LEU:O	1:B:36:ILE:HG12	2.11	0.50
1:A:143:LYS:CE	1:C:149:GLN:HG2	2.41	0.50
1:E:15:THR:OG1	1:E:15:THR:O	2.29	0.50
1:C:204:GLU:O	1:C:206:GLN:HG2	2.11	0.50
1:E:231:LEU:HA	1:F:168:VAL:CG2	2.41	0.50
1:D:98:ILE:HG13	1:D:99:THR:H	1.77	0.50
1:D:79:GLN:HG2	1:D:82:ILE:CG2	2.41	0.50
1:E:81:ARG:HG2	2:F:323:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:GLN:O	1:E:233:ASP:OD2	2.30	0.49
1:C:90:ARG:O	1:C:94:ASN:OD1	2.30	0.49
1:C:193:THR:O	1:C:194:PHE:O	2.30	0.49
1:E:197:SER:HA	1:F:206:GLN:NE2	2.27	0.49
1:A:11:VAL:HG22	1:A:11:VAL:O	2.10	0.49
1:D:204:GLU:OE2	1:D:204:GLU:O	2.29	0.49
1:B:194:PHE:CD2	1:B:208:ILE:HG22	2.47	0.49
1:E:101:LEU:HD23	2:E:281:HOH:O	2.11	0.49
1:C:1:MSE:SE	1:C:60:GLN:HB3	2.61	0.49
1:A:205:ILE:HD13	1:B:205:ILE:HD11	1.93	0.49
1:A:206:GLN:CG	1:B:196:VAL:HG11	2.41	0.49
1:B:177:THR:O	1:B:223:GLU:OE1	2.30	0.49
1:B:223:GLU:HA	1:C:222:MSE:SE	2.62	0.49
1:A:95:THR:HB	1:C:94:ASN:HD21	1.76	0.49
2:A:378:HOH:O	1:C:40:THR:HB	2.12	0.49
1:A:130:GLU:HB3	2:A:371:HOH:O	2.11	0.49
1:A:148:SER:HB2	1:C:154:PRO:CB	2.39	0.49
1:F:7:ASN:OD1	1:F:54:GLN:OE1	2.30	0.49
1:D:9:PRO:HD2	1:E:48:LYS:CE	2.43	0.49
1:A:23:PRO:HB2	1:A:26:VAL:CG1	2.43	0.49
1:A:73:HIS:HA	2:A:342:HOH:O	2.13	0.49
1:B:190:ALA:O	1:B:191:ASP:OD1	2.30	0.49
1:D:229:HIS:CE1	1:E:231:LEU:HD12	2.48	0.49
1:B:194:PHE:CE2	1:B:208:ILE:HA	2.47	0.49
1:D:121:ALA:HB1	2:D:318:HOH:O	2.11	0.49
2:A:333:HOH:O	1:C:157:VAL:CA	2.60	0.49
1:F:179:ALA:CB	1:F:220:LYS:HB2	2.43	0.49
1:E:91:ILE:O	1:E:91:ILE:HG22	2.12	0.49
1:B:103:VAL:HA	1:B:106:THR:HG22	1.94	0.49
1:D:58:ASP:O	1:D:62:LYS:HE2	2.12	0.49
1:B:172:ARG:O	1:B:232:ILE:HA	2.12	0.49
1:D:157:VAL:CA	1:F:151:LEU:HD23	2.42	0.49
1:E:194:PHE:HB3	2:E:305:HOH:O	2.12	0.49
2:D:344:HOH:O	1:F:171:ALA:CB	2.60	0.49
1:B:197:SER:OG	1:B:204:GLU:OE1	2.30	0.49
1:C:172:ARG:HD3	1:C:233:ASP:CA	2.41	0.49
1:C:140:TYR:O	1:C:141:VAL:O	2.30	0.49
2:B:339:HOH:O	1:C:196:VAL:HG12	2.12	0.49
1:F:116:GLN:HA	1:F:119:VAL:HG12	1.95	0.49
1:D:172:ARG:HE	1:D:233:ASP:N	2.11	0.49
1:F:62:LYS:HD2	1:F:66:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:O	1:A:67:ASP:OD2	2.30	0.49
1:D:73:HIS:O	1:D:77:ILE:HG13	2.13	0.48
1:F:91:ILE:HA	1:F:94:ASN:HD21	1.77	0.48
1:E:60:GLN:O	1:E:64:ASP:OD2	2.30	0.48
1:D:157:VAL:O	1:D:158:THR:O	2.30	0.48
1:B:151:LEU:HD23	2:B:329:HOH:O	2.13	0.48
1:C:78:LYS:HG2	2:C:283:HOH:O	2.12	0.48
1:B:223:GLU:HB2	1:C:222:MSE:HE1	1.93	0.48
1:A:225:ALA:O	1:A:229:HIS:HD2	1.96	0.48
1:D:70:LEU:HD21	1:E:70:LEU:CD2	2.40	0.48
1:A:126:VAL:HG11	1:C:125:ARG:HG3	1.95	0.48
1:A:116:GLN:HB2	1:A:116:GLN:HE21	1.40	0.48
1:C:132:ASN:O	1:C:136:LEU:HD13	2.12	0.48
1:D:77:ILE:CG1	1:F:77:ILE:HD11	2.44	0.48
1:E:183:ALA:HB1	1:E:221:ALA:N	2.29	0.48
1:A:150:SER:HA	1:C:156:ASN:O	2.12	0.48
1:D:212:LEU:O	1:D:213:ILE:HD13	2.13	0.48
1:F:200:TYR:O	1:F:201:THR:O	2.29	0.48
1:E:91:ILE:HA	2:F:383:HOH:O	2.13	0.48
1:F:189:ASP:CB	1:F:192:LEU:HB2	2.41	0.48
1:A:97:ALA:O	1:A:100:ALA:HB3	2.13	0.48
1:B:141:VAL:CG2	1:C:141:VAL:HG12	2.44	0.48
1:A:205:ILE:O	1:A:208:ILE:HB	2.14	0.48
1:A:129:ALA:O	1:A:133:ILE:HB	2.13	0.48
1:D:201:THR:HG22	1:D:203:SER:OG	2.13	0.48
1:F:11:VAL:HA	2:F:334:HOH:O	2.14	0.48
1:D:152:ALA:HB3	1:F:146:THR:HA	1.96	0.48
1:F:215:GLU:HG3	1:F:216:ARG:N	2.29	0.48
1:A:223:GLU:HG2	2:A:315:HOH:O	2.14	0.48
1:B:104:ARG:HG3	2:B:393:HOH:O	2.13	0.48
1:D:58:ASP:C	1:D:62:LYS:HE2	2.34	0.48
1:F:62:LYS:HD2	1:F:66:GLN:HE21	1.78	0.48
1:F:130:GLU:HG3	2:F:398:HOH:O	2.14	0.48
1:A:98:ILE:CD1	1:C:97:ALA:HB1	2.44	0.48
1:C:9:PRO:HA	1:C:50:ASN:OD1	2.13	0.48
1:C:74:GLU:HG3	1:C:78:LYS:HD3	1.95	0.48
1:E:199:THR:HA	1:F:200:TYR:CE2	2.49	0.47
1:E:229:HIS:NE2	1:F:231:LEU:HB3	2.29	0.47
1:D:95:THR:O	1:D:98:ILE:HG13	2.14	0.47
1:B:157:VAL:HG21	1:C:155:LEU:HB2	1.96	0.47
1:B:159:THR:O	1:B:160:SER:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ILE:HG22	1:D:216:ARG:HD3	1.97	0.47
1:D:189:ASP:OD2	1:E:216:ARG:HD2	2.15	0.47
1:C:192:LEU:N	1:C:192:LEU:CD2	2.77	0.47
1:E:19:ALA:O	1:E:22:LEU:HB2	2.15	0.47
1:D:163:VAL:HG13	1:F:171:ALA:HA	1.96	0.47
1:B:59:ALA:HA	1:C:1:MSE:HE1	1.96	0.47
1:C:184:ASN:O	1:C:185:LYS:HD2	2.14	0.47
1:A:172:ARG:HG3	1:A:230:GLY:O	2.14	0.47
1:D:183:ALA:HB1	1:D:217:ARG:HB3	1.97	0.47
1:F:2:ALA:O	1:F:4:PRO:HD3	2.14	0.47
1:D:222:MSE:O	1:D:222:MSE:CE	2.62	0.47
1:D:225:ALA:HB2	1:E:176:TRP:CZ2	2.50	0.47
1:A:212:LEU:HD23	1:C:212:LEU:HD21	1.97	0.47
1:F:17:LEU:HD12	1:F:17:LEU:O	2.15	0.47
1:E:60:GLN:HA	1:E:63:ASN:HB2	1.97	0.47
1:A:75:ALA:O	1:A:78:LYS:HG2	2.15	0.47
1:B:76:ARG:HH22	1:C:74:GLU:CD	2.17	0.47
1:B:142:SER:HB3	1:B:145:ALA:HB2	1.96	0.47
1:D:185:LYS:O	1:E:177:THR:OG1	2.29	0.47
1:D:222:MSE:SE	1:E:222:MSE:HE1	2.48	0.47
1:B:212:LEU:HB2	2:B:344:HOH:O	2.15	0.47
1:A:143:LYS:HD3	1:C:139:ASP:HA	1.97	0.47
1:E:215:GLU:O	1:E:219:THR:OG1	2.29	0.47
1:F:200:TYR:HE2	1:F:202:GLN:HB3	1.79	0.47
1:D:90:ARG:HB3	1:F:91:ILE:HD11	1.96	0.47
1:D:62:LYS:HE3	1:F:60:GLN:HG2	1.96	0.47
1:D:101:LEU:HD23	2:D:309:HOH:O	2.13	0.47
1:B:153:SER:HB2	1:C:147:THR:O	2.14	0.47
2:D:344:HOH:O	1:F:171:ALA:HB2	2.14	0.47
1:F:151:LEU:HD23	2:F:366:HOH:O	2.15	0.47
1:F:117:THR:O	1:F:120:SER:OG	2.30	0.47
1:D:118:ASN:ND2	2:D:311:HOH:O	2.47	0.47
1:A:62:LYS:HE2	1:A:62:LYS:HB2	1.48	0.47
1:F:54:GLN:HG3	2:F:330:HOH:O	2.14	0.47
1:E:193:THR:N	2:E:338:HOH:O	2.48	0.47
1:F:171:ALA:O	1:F:172:ARG:O	2.32	0.47
1:D:162:SER:N	1:F:155:LEU:O	2.48	0.47
1:E:156:ASN:HD21	1:E:157:VAL:CG1	2.18	0.46
1:E:160:SER:HB2	1:E:167:LYS:HE2	1.93	0.46
1:D:91:ILE:CG1	1:E:91:ILE:HG12	2.37	0.46
1:B:174:THR:HB	1:B:175:GLY:H	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:HG11	1:C:26:VAL:CG2	2.45	0.46
1:B:96:LYS:HB2	2:B:278:HOH:O	2.14	0.46
1:D:220:LYS:HE3	1:D:224:ASP:OD1	2.14	0.46
1:F:173:GLN:HA	1:F:173:GLN:OE1	2.15	0.46
1:A:80:LEU:O	1:A:84:VAL:HG23	2.15	0.46
1:B:111:GLU:CD	1:C:116:GLN:HE22	2.18	0.46
1:E:209:ALA:HA	1:E:212:LEU:HB3	1.98	0.46
1:D:59:ALA:HA	1:D:62:LYS:CG	2.45	0.46
1:A:77:ILE:HD11	1:C:77:ILE:HD11	1.96	0.46
1:D:202:GLN:NE2	1:D:202:GLN:O	2.48	0.46
1:C:74:GLU:HG3	1:C:78:LYS:CD	2.44	0.46
1:D:9:PRO:HD2	1:E:48:LYS:HE2	1.97	0.46
1:D:9:PRO:HD2	1:E:48:LYS:HZ3	1.78	0.46
1:B:7:ASN:HD22	1:B:54:GLN:HB3	1.80	0.46
1:D:183:ALA:O	1:D:217:ARG:NH2	2.48	0.46
1:A:151:LEU:O	1:B:143:LYS:O	2.33	0.46
1:D:34:TYR:CZ	1:F:17:LEU:HG	2.50	0.46
1:A:167:LYS:HE2	1:B:229:HIS:O	2.16	0.46
1:A:105:VAL:HG12	1:C:104:ARG:NH2	2.31	0.46
1:F:155:LEU:HB2	2:F:366:HOH:O	2.14	0.46
1:E:133:ILE:CD1	1:F:132:ASN:HB3	2.45	0.46
1:A:14:ALA:HB2	1:C:37:ALA:HB1	1.96	0.46
1:D:133:ILE:HA	2:D:306:HOH:O	2.14	0.46
1:F:214:THR:HA	1:F:217:ARG:HD3	1.96	0.46
1:C:191:ASP:HB2	1:C:192:LEU:HD23	1.96	0.46
1:B:105:VAL:O	1:B:108:ALA:HB3	2.15	0.46
1:F:211:ALA:HA	2:F:361:HOH:O	2.16	0.46
1:E:26:VAL:HG13	1:E:27:PHE:CD1	2.51	0.46
1:D:185:LYS:HD2	1:E:176:TRP:CA	2.44	0.46
1:B:166:LYS:O	1:B:168:VAL:HG22	2.16	0.46
1:D:70:LEU:HD22	1:E:69:GLU:CG	2.45	0.46
1:E:205:ILE:HG12	1:F:205:ILE:CG2	2.42	0.46
1:D:97:ALA:HB1	1:F:98:ILE:HG21	1.98	0.46
1:B:172:ARG:HG3	1:B:172:ARG:O	2.16	0.46
1:A:34:TYR:CZ	1:B:17:LEU:HG	2.51	0.46
1:A:96:LYS:HG2	2:A:248:HOH:O	2.15	0.46
1:D:106:THR:HA	1:D:109:GLU:CD	2.36	0.46
1:F:176:TRP:HZ3	1:F:223:GLU:OE2	1.97	0.46
1:C:8:ASN:HD22	1:C:9:PRO:HD2	1.80	0.46
1:A:92:THR:HG22	1:A:96:LYS:HD2	1.98	0.46
1:D:176:TRP:H	1:F:185:LYS:CD	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD22	1:A:231:LEU:CD1	2.38	0.46
1:C:122:LEU:HA	1:C:125:ARG:HG2	1.97	0.46
1:A:10:VAL:HG22	1:C:48:LYS:HD2	1.97	0.46
1:D:80:LEU:HG	1:F:81:ARG:HH21	1.81	0.46
1:E:189:ASP:HA	1:F:180:THR:CG2	2.46	0.46
1:D:8:ASN:N	1:D:9:PRO:HD2	2.26	0.45
1:A:140:TYR:CE1	1:A:142:SER:HB2	2.51	0.45
1:C:139:ASP:OD1	1:C:139:ASP:N	2.49	0.45
1:C:140:TYR:OH	1:C:142:SER:HB2	2.16	0.45
1:F:3:ASP:O	1:F:6:LEU:HG	2.16	0.45
1:A:32:LEU:N	2:A:338:HOH:O	2.49	0.45
1:D:171:ALA:O	1:D:173:GLN:NE2	2.49	0.45
1:E:94:ASN:ND2	2:E:325:HOH:O	2.50	0.45
1:E:66:GLN:NE2	1:F:66:GLN:OE1	2.49	0.45
1:B:1:MSE:N	2:B:288:HOH:O	2.48	0.45
1:A:125:ARG:NH1	1:B:130:GLU:OE2	2.50	0.45
1:D:220:LYS:O	1:D:224:ASP:N	2.50	0.45
1:A:212:LEU:HD12	1:B:194:PHE:HE1	1.81	0.45
1:B:162:SER:HA	1:B:168:VAL:CG2	2.46	0.45
1:F:94:ASN:HD22	1:F:94:ASN:N	2.13	0.45
1:E:183:ALA:HB2	1:E:220:LYS:CD	2.46	0.45
1:D:63:ASN:O	1:D:66:GLN:N	2.50	0.45
1:A:95:THR:CG2	1:C:94:ASN:HD21	2.30	0.45
1:E:130:GLU:OE1	1:F:125:ARG:NH2	2.49	0.45
1:A:213:ILE:O	1:A:217:ARG:HG3	2.17	0.45
1:A:195:ALA:HB2	2:A:374:HOH:O	2.15	0.45
1:A:24:ARG:HE	1:A:24:ARG:HB3	1.49	0.45
1:D:20:SER:N	2:D:291:HOH:O	2.49	0.45
1:C:216:ARG:NH1	2:C:236:HOH:O	2.49	0.45
1:A:1:MSE:HE3	1:A:2:ALA:O	2.16	0.45
1:F:227:ARG:HD3	1:F:233:ASP:O	2.16	0.45
1:C:1:MSE:HB3	1:C:2:ALA:H	1.55	0.45
1:E:209:ALA:O	1:E:213:ILE:N	2.49	0.45
1:E:145:ALA:O	1:F:153:SER:HB3	2.16	0.45
1:C:22:LEU:O	1:C:23:PRO:O	2.34	0.45
1:A:17:LEU:HD13	1:C:34:TYR:CE1	2.51	0.45
1:F:24:ARG:NH1	1:F:25:ASN:OD1	2.50	0.45
1:F:182:THR:O	1:F:217:ARG:NH1	2.50	0.45
1:E:81:ARG:NH1	1:E:85:ASP:OD2	2.49	0.45
1:A:172:ARG:NH2	1:C:166:LYS:HG2	2.31	0.45
1:B:183:ALA:HB2	1:B:220:LYS:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ILE:HG22	1:C:137:GLN:NE2	2.31	0.45
1:A:95:THR:CB	1:C:94:ASN:HD21	2.29	0.45
1:C:114:SER:HB2	2:C:347:HOH:O	2.17	0.45
1:A:156:ASN:ND2	2:A:322:HOH:O	2.50	0.45
1:D:102:ASN:O	1:D:106:THR:HG23	2.16	0.45
1:F:17:LEU:HD13	1:F:36:ILE:HA	1.98	0.45
1:D:173:GLN:NE2	2:D:330:HOH:O	2.50	0.45
1:A:105:VAL:HG21	1:C:101:LEU:CD2	2.46	0.45
1:C:29:LYS:HG2	1:C:30:SER:N	2.31	0.45
1:A:78:LYS:HB3	1:A:78:LYS:HE3	1.29	0.45
1:A:194:PHE:HB3	1:A:195:ALA:H	1.55	0.45
1:C:213:ILE:CG2	1:C:217:ARG:HD2	2.47	0.45
1:A:92:THR:O	1:A:96:LYS:HD2	2.16	0.45
1:D:18:ASP:O	1:D:21:ILE:HG12	2.17	0.45
1:B:163:VAL:CG1	1:B:168:VAL:HG21	2.41	0.45
1:D:213:ILE:N	1:D:216:ARG:HD3	2.30	0.45
1:C:199:THR:HG23	1:C:200:TYR:N	2.29	0.45
1:D:76:ARG:NH1	2:D:315:HOH:O	2.50	0.45
1:D:63:ASN:OD1	1:E:66:GLN:NE2	2.49	0.45
1:A:73:HIS:HE1	1:B:74:GLU:HG2	1.81	0.45
1:D:17:LEU:HD23	1:E:34:TYR:CE1	2.52	0.45
1:D:197:SER:OG	1:D:198:ASP:N	2.50	0.45
1:F:168:VAL:C	1:F:169:VAL:HG23	2.28	0.45
1:E:95:THR:HA	2:F:364:HOH:O	2.17	0.45
1:C:22:LEU:HD12	1:C:22:LEU:HA	1.81	0.45
1:F:24:ARG:NH1	1:F:24:ARG:HG3	2.31	0.45
1:A:125:ARG:HD2	1:B:130:GLU:OE1	2.17	0.45
1:D:88:GLU:OE2	1:E:90:ARG:NH1	2.50	0.45
1:D:153:SER:H	1:E:158:THR:CG2	2.30	0.45
1:A:151:LEU:O	1:A:152:ALA:HB3	2.17	0.45
1:D:109:GLU:OE1	1:E:104:ARG:NH1	2.50	0.45
1:D:98:ILE:O	1:D:102:ASN:ND2	2.50	0.45
1:D:208:ILE:O	1:D:211:ALA:O	2.35	0.45
1:A:189:ASP:OD1	1:A:190:ALA:N	2.50	0.45
2:A:234:HOH:O	1:C:63:ASN:ND2	2.49	0.45
1:F:148:SER:O	1:F:149:GLN:HB2	2.17	0.45
1:F:128:THR:HA	1:F:131:ASN:HB2	1.98	0.45
1:B:180:THR:OG1	1:C:189:ASP:OD1	2.33	0.45
1:A:85:ASP:N	1:A:85:ASP:OD1	2.50	0.45
1:A:219:THR:HG21	1:B:215:GLU:OE2	2.17	0.45
1:A:185:LYS:HE2	1:C:176:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:VAL:O	1:F:87:HIS:HE1	2.00	0.45
1:A:217:ARG:NH2	1:B:191:ASP:OD2	2.50	0.45
1:F:172:ARG:HA	1:F:231:LEU:O	2.17	0.44
1:A:3:ASP:OD1	1:A:4:PRO:HD2	2.17	0.44
1:E:95:THR:HG22	1:E:96:LYS:N	2.32	0.44
1:C:8:ASN:HD22	1:C:9:PRO:CD	2.30	0.44
1:B:74:GLU:O	1:B:78:LYS:HB2	2.17	0.44
1:A:189:ASP:C	1:A:191:ASP:H	2.19	0.44
1:F:206:GLN:O	1:F:210:ASN:N	2.50	0.44
1:B:12:ILE:HD13	2:B:258:HOH:O	2.17	0.44
1:F:48:LYS:HB2	1:F:48:LYS:HE3	1.78	0.44
1:D:222:MSE:O	1:D:222:MSE:HE2	2.18	0.44
1:A:140:TYR:CZ	1:A:142:SER:HB2	2.51	0.44
1:A:202:GLN:HA	1:A:205:ILE:CG2	2.47	0.44
1:F:194:PHE:CG	1:F:208:ILE:HG22	2.52	0.44
1:D:162:SER:HB3	1:F:156:ASN:CB	2.43	0.44
1:C:176:TRP:HB2	1:C:233:ASP:CG	2.38	0.44
1:B:223:GLU:CB	1:C:222:MSE:HE1	2.48	0.44
1:A:220:LYS:HE3	1:A:224:ASP:CG	2.38	0.44
1:D:94:ASN:ND2	1:F:91:ILE:HD12	2.32	0.44
1:B:133:ILE:HG13	1:B:134:SER:N	2.33	0.44
1:F:151:LEU:O	1:F:152:ALA:HB3	2.18	0.44
1:F:46:ALA:N	2:F:378:HOH:O	2.50	0.44
1:F:76:ARG:NE	2:F:395:HOH:O	2.50	0.44
1:E:92:THR:HG22	2:E:301:HOH:O	2.16	0.44
1:E:38:GLN:O	1:E:42:VAL:HG23	2.18	0.44
1:D:230:GLY:HA3	1:E:167:LYS:O	2.18	0.44
1:D:216:ARG:HG2	1:F:215:GLU:HB2	1.99	0.44
1:D:4:PRO:HD3	1:D:64:ASP:CG	2.38	0.44
1:D:136:LEU:HB3	1:E:136:LEU:HD11	2.00	0.44
1:F:123:ASP:O	1:F:127:THR:OG1	2.30	0.44
1:E:100:ALA:HA	2:E:283:HOH:O	2.18	0.44
1:E:172:ARG:HG3	1:E:230:GLY:O	2.17	0.44
1:F:91:ILE:O	1:F:94:ASN:ND2	2.50	0.44
1:B:115:LEU:HD22	1:C:119:VAL:HG21	1.98	0.44
1:F:119:VAL:HB	2:F:358:HOH:O	2.16	0.44
1:C:185:LYS:HA	1:C:185:LYS:NZ	2.33	0.44
1:B:36:ILE:N	1:B:36:ILE:HD13	2.32	0.44
1:C:216:ARG:HG2	1:C:216:ARG:H	1.59	0.44
1:C:149:GLN:HB2	1:C:149:GLN:HE21	1.50	0.44
1:D:95:THR:HA	1:D:98:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:234:HOH:O	1:F:78:LYS:HA	2.18	0.44
1:B:90:ARG:NH2	2:B:356:HOH:O	2.50	0.44
1:B:76:ARG:HD2	2:B:289:HOH:O	2.16	0.44
1:C:96:LYS:HD3	2:C:371:HOH:O	2.18	0.44
1:B:184:ASN:OD1	1:B:186:GLY:N	2.50	0.44
1:E:29:LYS:HG3	1:E:29:LYS:O	2.16	0.44
1:E:157:VAL:HG23	1:F:164:GLY:H	1.78	0.44
1:A:141:VAL:O	1:A:149:GLN:NE2	2.50	0.44
1:D:173:GLN:HB2	1:D:232:ILE:HD12	1.99	0.44
1:B:115:LEU:CD2	1:C:119:VAL:HG21	2.48	0.44
1:D:26:VAL:O	1:F:23:PRO:HG3	2.18	0.44
1:C:37:ALA:HA	1:C:40:THR:OG1	2.18	0.44
1:E:23:PRO:HB2	1:E:26:VAL:CG1	2.48	0.44
1:F:127:THR:O	1:F:131:ASN:OD1	2.35	0.44
1:D:185:LYS:O	1:D:185:LYS:HG3	2.17	0.44
1:D:226:LEU:CD1	1:F:222:MSE:HE3	2.38	0.44
1:A:185:LYS:HA	1:A:218:ARG:NH1	2.33	0.44
1:B:108:ALA:O	1:B:112:ILE:HD12	2.18	0.44
1:B:231:LEU:O	1:C:229:HIS:HE1	2.01	0.44
1:B:147:THR:HA	2:B:328:HOH:O	2.18	0.44
2:E:314:HOH:O	1:F:181:GLY:HA2	2.18	0.44
1:C:157:VAL:HG13	1:C:158:THR:N	2.08	0.44
1:D:176:TRP:CA	1:F:185:LYS:HG2	2.42	0.44
1:F:6:LEU:HD12	1:F:57:TYR:HA	1.99	0.44
1:E:194:PHE:O	1:E:195:ALA:HB2	2.16	0.44
1:D:176:TRP:N	1:F:185:LYS:HD3	2.16	0.43
1:B:174:THR:HA	1:B:233:ASP:HB2	1.99	0.43
1:A:212:LEU:HD23	1:C:212:LEU:HD23	1.98	0.43
1:D:79:GLN:O	1:D:82:ILE:HG23	2.18	0.43
1:B:178:ALA:HA	1:B:223:GLU:OE1	2.19	0.43
1:F:6:LEU:HD11	1:F:60:GLN:OE1	2.18	0.43
1:A:159:THR:O	1:A:160:SER:HB3	2.18	0.43
1:E:78:LYS:HG3	1:F:76:ARG:HH12	1.82	0.43
1:C:81:ARG:HD3	1:C:85:ASP:OD1	2.17	0.43
1:B:171:ALA:O	1:C:229:HIS:NE2	2.50	0.43
1:F:41:ASP:O	1:F:45:ILE:HD12	2.19	0.43
1:D:80:LEU:O	1:D:83:ASP:HB2	2.18	0.43
1:D:31:TYR:CE2	1:F:22:LEU:HD23	2.53	0.43
1:D:147:THR:HG22	1:D:148:SER:N	2.33	0.43
1:C:71:ALA:HB2	2:C:256:HOH:O	2.18	0.43
1:D:203:SER:O	1:D:206:GLN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ASP:HA	1:E:122:LEU:HD11	2.01	0.43
1:E:32:LEU:O	1:E:36:ILE:HG12	2.18	0.43
1:A:215:GLU:O	1:A:218:ARG:HB3	2.19	0.43
1:D:90:ARG:NH2	1:F:88:GLU:OE2	2.50	0.43
1:F:94:ASN:HB3	2:F:364:HOH:O	2.18	0.43
1:D:59:ALA:HA	1:D:62:LYS:CE	2.49	0.43
1:E:140:TYR:CE1	1:F:136:LEU:HD21	2.53	0.43
1:A:100:ALA:O	1:A:103:VAL:HG22	2.18	0.43
1:B:132:ASN:ND2	2:B:245:HOH:O	2.50	0.43
1:D:152:ALA:HA	1:E:158:THR:OG1	2.19	0.43
1:F:174:THR:HA	1:F:233:ASP:HB2	2.01	0.43
1:D:117:THR:HG22	1:D:118:ASN:N	2.33	0.43
1:D:48:LYS:HD3	1:D:48:LYS:HA	1.46	0.43
1:C:37:ALA:O	1:C:40:THR:N	2.51	0.43
1:C:204:GLU:O	1:C:205:ILE:HG22	2.18	0.43
1:B:186:GLY:O	1:B:218:ARG:NH1	2.51	0.43
1:D:150:SER:HB2	1:E:156:ASN:HB3	2.00	0.43
1:A:215:GLU:OE1	1:A:215:GLU:HA	2.18	0.43
1:D:189:ASP:OD2	1:E:216:ARG:CB	2.65	0.43
1:F:188:PHE:CZ	1:F:215:GLU:HA	2.43	0.43
1:B:222:MSE:HB3	1:C:222:MSE:HE3	1.99	0.43
1:A:222:MSE:O	1:A:225:ALA:HB3	2.19	0.43
1:A:21:ILE:HD12	1:C:31:TYR:HD1	1.84	0.43
1:C:22:LEU:HD23	1:C:32:LEU:HD11	2.01	0.43
1:C:143:LYS:HB2	1:C:143:LYS:HE3	1.52	0.43
1:E:167:LYS:O	1:E:168:VAL:HG23	2.18	0.43
1:F:227:ARG:HD3	1:F:233:ASP:C	2.39	0.43
1:E:218:ARG:HH21	1:F:179:ALA:HB2	1.83	0.43
1:A:6:LEU:HD22	1:A:53:GLY:HA2	2.00	0.43
1:F:155:LEU:HD23	1:F:156:ASN:N	2.34	0.43
1:E:31:TYR:O	1:E:35:VAL:HG13	2.19	0.43
1:F:207:ALA:HA	1:F:210:ASN:HB2	2.01	0.43
1:E:23:PRO:HA	2:E:253:HOH:O	2.18	0.43
1:D:122:LEU:HD12	1:D:122:LEU:HA	1.81	0.43
1:F:201:THR:HG22	1:F:203:SER:HB3	2.00	0.42
1:D:91:ILE:HA	1:D:94:ASN:HB2	2.01	0.42
1:D:29:LYS:HA	1:D:32:LEU:HD12	2.00	0.42
1:F:118:ASN:O	1:F:122:LEU:HD22	2.19	0.42
1:C:218:ARG:NH1	1:C:218:ARG:HG3	2.34	0.42
1:E:172:ARG:HG3	1:E:232:ILE:HA	2.02	0.42
1:D:174:THR:HA	1:D:233:ASP:CB	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:LYS:HB3	2:F:389:HOH:O	2.18	0.42
2:D:327:HOH:O	1:F:143:LYS:NZ	2.49	0.42
1:D:213:ILE:CA	1:D:216:ARG:HD3	2.49	0.42
1:C:191:ASP:HB2	1:C:192:LEU:CD2	2.49	0.42
1:A:26:VAL:HG21	1:C:26:VAL:CG2	2.45	0.42
1:D:48:LYS:HG2	1:F:10:VAL:CB	2.48	0.42
1:A:111:GLU:O	1:A:114:SER:HB2	2.19	0.42
1:F:226:LEU:HB3	1:F:232:ILE:HG12	2.01	0.42
1:B:223:GLU:O	1:B:223:GLU:HG3	2.20	0.42
1:E:63:ASN:OD1	1:E:66:GLN:NE2	2.52	0.42
1:B:1:MSE:HE2	1:B:64:ASP:CG	2.39	0.42
1:E:82:ILE:HA	1:E:82:ILE:HD13	1.84	0.42
1:D:68:VAL:HG13	1:D:69:GLU:H	1.83	0.42
1:C:205:ILE:HA	2:C:234:HOH:O	2.19	0.42
1:E:91:ILE:HG23	2:F:383:HOH:O	2.19	0.42
1:D:63:ASN:O	1:D:66:GLN:HB2	2.20	0.42
1:D:162:SER:O	1:F:161:TYR:OH	2.30	0.42
1:A:98:ILE:HG21	2:C:290:HOH:O	2.19	0.42
1:B:32:LEU:HA	1:B:32:LEU:HD12	1.78	0.42
1:C:207:ALA:HB3	2:C:234:HOH:O	2.18	0.42
1:B:194:PHE:O	1:B:195:ALA:HB3	2.19	0.42
1:A:88:GLU:OE2	1:C:90:ARG:NH1	2.50	0.42
1:C:29:LYS:O	1:C:32:LEU:HB3	2.19	0.42
1:B:81:ARG:O	1:B:84:VAL:HG22	2.19	0.42
1:D:92:THR:HA	2:D:277:HOH:O	2.18	0.42
1:B:213:ILE:HG12	1:C:192:LEU:HB3	2.01	0.42
1:D:208:ILE:O	1:D:211:ALA:N	2.52	0.42
1:F:179:ALA:HB3	1:F:220:LYS:HB2	2.00	0.42
1:E:70:LEU:HD13	1:E:70:LEU:HA	1.83	0.42
1:C:35:VAL:HG23	1:C:36:ILE:N	2.34	0.42
1:E:102:ASN:HB2	2:E:358:HOH:O	2.19	0.42
1:B:96:LYS:HZ2	1:B:96:LYS:N	2.17	0.42
1:A:75:ALA:HA	1:A:78:LYS:CG	2.49	0.42
1:B:220:LYS:O	1:B:224:ASP:OD2	2.38	0.42
1:D:75:ALA:HB2	2:D:265:HOH:O	2.20	0.42
1:B:16:ARG:NE	2:B:290:HOH:O	2.52	0.42
1:A:95:THR:HG22	1:C:94:ASN:HD21	1.85	0.42
1:C:26:VAL:HG13	1:C:27:PHE:N	2.34	0.42
1:F:86:ASP:HB2	2:F:424:HOH:O	2.19	0.42
1:A:89:SER:HB3	2:A:305:HOH:O	2.19	0.42
1:D:184:ASN:O	1:D:185:LYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD12	1:B:194:PHE:CE1	2.55	0.42
1:A:218:ARG:NH2	1:C:223:GLU:OE2	2.51	0.42
1:E:99:THR:O	1:E:103:VAL:HG23	2.20	0.42
1:A:29:LYS:HD2	1:A:29:LYS:HA	1.74	0.42
1:D:173:GLN:HG3	2:F:345:HOH:O	2.20	0.42
1:F:81:ARG:HE	1:F:81:ARG:HB2	1.67	0.42
1:B:122:LEU:O	1:B:126:VAL:HG23	2.20	0.42
1:D:188:PHE:CE2	1:E:216:ARG:HB3	2.54	0.42
1:D:193:THR:HB	1:D:208:ILE:HD13	2.02	0.42
1:B:84:VAL:HG23	1:B:85:ASP:N	2.35	0.42
1:B:76:ARG:NH1	2:B:237:HOH:O	2.50	0.42
1:B:181:GLY:O	1:B:220:LYS:HE2	2.19	0.42
1:A:81:ARG:O	1:A:85:ASP:OD1	2.37	0.42
1:E:229:HIS:CD2	1:F:231:LEU:HD22	2.54	0.41
1:D:8:ASN:OD1	1:D:54:GLN:OE1	2.38	0.41
1:A:202:GLN:O	1:A:205:ILE:HG23	2.20	0.41
1:E:189:ASP:HA	1:F:180:THR:HG22	2.02	0.41
1:A:62:LYS:HG2	1:B:63:ASN:CG	2.41	0.41
1:A:194:PHE:CE2	1:C:209:ALA:HB3	2.55	0.41
1:C:111:GLU:O	1:C:115:LEU:HD13	2.20	0.41
1:C:13:GLN:HB2	1:C:13:GLN:HE21	1.60	0.41
1:E:197:SER:H	1:F:206:GLN:HE22	1.67	0.41
1:A:92:THR:HG23	2:A:324:HOH:O	2.19	0.41
1:D:154:PRO:CA	1:E:160:SER:O	2.67	0.41
1:C:212:LEU:CD1	1:C:216:ARG:HD3	2.49	0.41
1:D:98:ILE:HG13	1:D:99:THR:N	2.36	0.41
1:A:115:LEU:HD21	2:B:350:HOH:O	2.20	0.41
1:E:66:GLN:O	1:E:70:LEU:HD23	2.21	0.41
1:C:35:VAL:HG23	1:C:36:ILE:H	1.85	0.41
1:D:27:PHE:HB2	1:D:32:LEU:HD21	2.02	0.41
1:A:66:GLN:NE2	2:A:234:HOH:O	2.50	0.41
1:D:183:ALA:HB1	1:D:217:ARG:O	2.21	0.41
1:D:218:ARG:HD2	1:D:218:ARG:HA	1.29	0.41
1:E:156:ASN:HA	1:F:162:SER:HB2	2.02	0.41
1:A:91:ILE:HG13	1:B:91:ILE:HD13	2.02	0.41
1:B:7:ASN:ND2	2:B:304:HOH:O	2.53	0.41
1:E:151:LEU:HD23	1:E:153:SER:HB3	2.03	0.41
1:B:157:VAL:HG22	1:B:158:THR:H	1.86	0.41
1:F:35:VAL:HG12	1:F:36:ILE:N	2.35	0.41
1:A:115:LEU:HD21	1:B:116:GLN:HG2	2.02	0.41
1:A:148:SER:HB2	1:C:154:PRO:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HA	1:A:98:ILE:CG2	2.49	0.41
1:C:35:VAL:O	1:C:38:GLN:HB2	2.20	0.41
1:C:12:ILE:HD13	1:C:46:ALA:CB	2.50	0.41
1:B:183:ALA:HB1	1:B:221:ALA:HA	2.02	0.41
1:F:115:LEU:HD23	1:F:115:LEU:HA	1.90	0.41
1:C:141:VAL:HG13	1:C:149:GLN:OE1	2.20	0.41
1:C:17:LEU:HB3	1:C:18:ASP:H	1.57	0.41
1:C:8:ASN:HA	1:C:9:PRO:HD3	1.85	0.41
1:D:125:ARG:HB3	1:D:125:ARG:HE	1.65	0.41
1:D:116:GLN:CG	1:E:115:LEU:HD11	2.49	0.41
1:E:194:PHE:HE1	1:E:211:ALA:HB3	1.85	0.41
1:B:220:LYS:HG3	1:B:224:ASP:OD2	2.20	0.41
1:E:147:THR:HG23	1:E:147:THR:O	2.20	0.41
1:D:229:HIS:NE2	1:E:172:ARG:HA	2.35	0.41
1:D:90:ARG:HG2	2:D:269:HOH:O	2.20	0.41
1:F:213:ILE:HG22	1:F:214:THR:N	2.36	0.41
1:D:139:ASP:OD1	1:F:142:SER:OG	2.33	0.41
1:D:37:ALA:HA	1:D:40:THR:HG23	2.03	0.41
1:E:174:THR:HA	1:E:233:ASP:OD1	2.19	0.41
1:A:140:TYR:CD1	1:C:140:TYR:HA	2.55	0.41
1:B:159:THR:O	1:B:160:SER:CB	2.69	0.41
1:D:91:ILE:CD1	1:F:91:ILE:HD13	2.50	0.41
1:D:165:GLY:C	1:D:166:LYS:HZ3	2.24	0.41
1:D:32:LEU:HA	1:D:35:VAL:CG1	2.51	0.41
1:D:220:LYS:HE3	1:D:224:ASP:CG	2.41	0.41
1:D:188:PHE:CE1	1:E:216:ARG:HD3	2.52	0.41
1:F:194:PHE:CD2	1:F:208:ILE:HG22	2.56	0.41
1:D:81:ARG:HA	1:D:84:VAL:CG1	2.51	0.41
1:A:136:LEU:HD12	1:C:136:LEU:HD23	2.03	0.41
1:D:127:THR:HG22	1:E:125:ARG:NH2	2.30	0.41
1:B:92:THR:HB	2:B:327:HOH:O	2.20	0.41
1:B:183:ALA:HB2	1:B:220:LYS:HG3	2.03	0.41
1:B:183:ALA:HB1	1:B:221:ALA:CA	2.51	0.41
1:F:131:ASN:O	1:F:134:SER:HB2	2.21	0.41
1:F:69:GLU:O	1:F:73:HIS:ND1	2.54	0.41
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.83	0.41
1:F:6:LEU:CD1	1:F:57:TYR:HA	2.51	0.41
1:D:45:ILE:HG21	2:F:378:HOH:O	2.21	0.41
1:C:194:PHE:O	1:C:195:ALA:CB	2.69	0.41
1:B:206:GLN:O	1:B:210:ASN:HB2	2.21	0.41
1:E:74:GLU:OE2	1:E:78:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD13	1:A:32:LEU:HA	1.90	0.41
1:C:217:ARG:NH2	2:C:320:HOH:O	2.54	0.41
1:E:68:VAL:O	1:E:71:ALA:HB3	2.20	0.41
1:D:150:SER:O	1:F:143:LYS:HB3	2.21	0.40
1:A:151:LEU:N	2:A:333:HOH:O	2.50	0.40
1:D:216:ARG:HG2	1:F:215:GLU:OE1	2.20	0.40
1:E:142:SER:OG	1:E:145:ALA:N	2.54	0.40
1:A:126:VAL:HG11	1:C:125:ARG:CD	2.51	0.40
1:A:98:ILE:HD11	1:C:97:ALA:HB1	2.03	0.40
1:D:118:ASN:ND2	2:D:304:HOH:O	2.49	0.40
1:C:185:LYS:HA	1:C:185:LYS:CE	2.47	0.40
1:E:79:GLN:HE21	1:E:79:GLN:CA	2.33	0.40
1:B:81:ARG:HH11	1:B:84:VAL:HG21	1.85	0.40
1:F:73:HIS:HD2	2:F:276:HOH:O	2.04	0.40
1:A:23:PRO:CB	1:C:27:PHE:HB3	2.49	0.40
1:B:88:GLU:HA	2:B:326:HOH:O	2.22	0.40
1:B:215:GLU:HB2	2:B:333:HOH:O	2.21	0.40
1:E:41:ASP:O	1:E:44:ALA:HB3	2.21	0.40
1:D:29:LYS:N	2:D:254:HOH:O	2.54	0.40
1:C:16:ARG:HH11	1:C:40:THR:HG22	1.83	0.40
1:A:72:ASP:OD1	1:A:76:ARG:NH1	2.54	0.40
1:E:176:TRP:CE2	1:E:232:ILE:HG21	2.56	0.40
1:C:196:VAL:HB	1:C:197:SER:CA	2.49	0.40
1:D:208:ILE:HD12	1:E:209:ALA:HB2	2.03	0.40
1:B:103:VAL:HA	1:B:106:THR:CG2	2.51	0.40
1:E:63:ASN:HA	1:E:66:GLN:HE21	1.86	0.40
1:A:7:ASN:HB2	1:A:57:TYR:CD1	2.55	0.40
1:A:23:PRO:C	1:A:26:VAL:HG13	2.42	0.40
1:C:62:LYS:HE3	1:C:65:GLU:OE2	2.21	0.40
1:D:140:TYR:HB3	2:D:263:HOH:O	2.20	0.40
1:E:131:ASN:HA	1:E:131:ASN:HD22	1.63	0.40
1:D:216:ARG:O	1:D:219:THR:OG1	2.40	0.40
1:C:200:TYR:HE1	1:C:203:SER:HA	1.85	0.40
1:D:209:ALA:O	1:D:211:ALA:O	2.39	0.40
1:D:196:VAL:HG11	1:E:206:GLN:NE2	2.36	0.40
1:B:203:SER:HA	1:B:206:GLN:CD	2.42	0.40
1:A:36:ILE:HD13	1:A:36:ILE:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	231/233 (99%)	199 (86%)	19 (8%)	13 (6%)	2	0
1	B	231/233 (99%)	211 (91%)	14 (6%)	6 (3%)	7	2
1	C	231/233 (99%)	199 (86%)	18 (8%)	14 (6%)	2	0
1	D	231/233 (99%)	176 (76%)	36 (16%)	19 (8%)	1	0
1	E	231/233 (99%)	204 (88%)	17 (7%)	10 (4%)	3	1
1	F	231/233 (99%)	200 (87%)	16 (7%)	15 (6%)	1	0
All	All	1386/1398 (99%)	1189 (86%)	120 (9%)	77 (6%)	2	0

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	190	ALA
1	A	191	ASP
1	A	194	PHE
1	A	200	TYR
1	C	23	PRO
1	C	150	SER
1	C	187	VAL
1	C	192	LEU
1	C	194	PHE
1	C	195	ALA
1	C	200	TYR
1	C	201	THR
1	C	204	GLU
1	C	205	ILE
1	D	2	ALA
1	D	8	ASN
1	D	9	PRO
1	D	26	VAL
1	D	148	SER

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Mol	Chain	Res	Type
1	D	154	PRO
1	D	158	THR
1	D	183	ALA
1	D	185	LYS
1	E	18	ASP
1	E	157	VAL
1	E	158	THR
1	E	168	VAL
1	E	169	VAL
1	E	195	ALA
1	F	7	ASN
1	F	18	ASP
1	F	148	SER
1	F	169	VAL
1	F	172	ARG
1	F	186	GLY
1	F	195	ALA
1	F	205	ILE
1	A	11	VAL
1	A	145	ALA
1	B	198	ASP
1	D	10	VAL
1	D	17	LEU
1	D	184	ASN
1	E	176	TRP
1	F	30	SER
1	F	149	GLN
1	F	201	THR
1	A	14	ALA
1	A	16	ARG
1	A	142	SER
1	B	173	GLN
1	B	192	LEU
1	B	200	TYR
1	C	141	VAL
1	E	204	GLU
1	F	29	LYS
1	A	10	VAL
1	A	13	GLN
1	A	19	ALA
1	B	201	THR
1	D	76	ARG

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Mol	Chain	Res	Type
1	D	157	VAL
1	D	178	ALA
1	D	213	ILE
1	D	230	GLY
1	F	164	GLY
1	B	190	ALA
1	C	2	ALA
1	D	179	ALA
1	E	20	SER
1	E	200	TYR
1	D	12	ILE
1	F	165	GLY
1	F	26	VAL
1	C	26	VAL
1	C	157	VAL

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	184/182 (101%)	136 (74%)	48 (26%)	0	0
1	B	184/182 (101%)	127 (69%)	57 (31%)	0	0
1	C	184/182 (101%)	136 (74%)	48 (26%)	0	0
1	D	177/182 (97%)	121 (68%)	56 (32%)	0	0
1	E	178/182 (98%)	124 (70%)	54 (30%)	0	0
1	F	183/182 (100%)	122 (67%)	61 (33%)	0	0
All	All	1090/1092 (100%)	766 (70%)	324 (30%)	0	0

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	5	SER
1	A	8	ASN

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Mol	Chain	Res	Type
1	A	10	VAL
1	A	11	VAL
1	A	16	ARG
1	A	24	ARG
1	A	25	ASN
1	A	26	VAL
1	A	27	PHE
1	A	28	SER
1	A	32	LEU
1	A	38	GLN
1	A	42	VAL
1	A	62	LYS
1	A	65	GLU
1	A	73	HIS
1	A	78	LYS
1	A	95	THR
1	A	98	ILE
1	A	104	ARG
1	A	123	ASP
1	A	132	ASN
1	A	136	LEU
1	A	142	SER
1	A	143	LYS
1	A	150	SER
1	A	151	LEU
1	A	155	LEU
1	A	158	THR
1	A	162	SER
1	A	168	VAL
1	A	180	THR
1	A	182	THR
1	A	185	LYS
1	A	189	ASP
1	A	192	LEU
1	A	194	PHE
1	A	196	VAL
1	A	202	GLN
1	A	203	SER
1	A	204	GLU
1	A	205	ILE
1	A	216	ARG
1	A	219	THR

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Mol	Chain	Res	Type
1	A	220	LYS
1	A	227	ARG
1	A	232	ILE
1	B	6	LEU
1	B	12	ILE
1	B	13	GLN
1	B	21	ILE
1	B	24	ARG
1	B	26	VAL
1	B	28	SER
1	B	32	LEU
1	B	40	THR
1	B	51	GLU
1	B	54	GLN
1	B	62	LYS
1	B	65	GLU
1	B	67	ASP
1	B	73	HIS
1	B	78	LYS
1	B	79	GLN
1	B	81	ARG
1	B	86	ASP
1	B	88	GLU
1	B	89	SER
1	B	90	ARG
1	B	96	LYS
1	B	99	THR
1	B	102	ASN
1	B	104	ARG
1	B	106	THR
1	B	107	THR
1	B	114	SER
1	B	120	SER
1	B	122	LEU
1	B	123	ASP
1	B	133	ILE
1	B	136	LEU
1	B	137	GLN
1	B	147	THR
1	B	148	SER
1	B	150	SER
1	B	155	LEU

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Mol	Chain	Res	Type
1	B	156	ASN
1	B	157	VAL
1	B	163	VAL
1	B	167	LYS
1	B	168	VAL
1	B	172	ARG
1	B	174	THR
1	B	180	THR
1	B	184	ASN
1	B	192	LEU
1	B	196	VAL
1	B	197	SER
1	B	201	THR
1	B	205	ILE
1	B	208	ILE
1	B	216	ARG
1	B	220	LYS
1	B	222	MSE
1	C	1	MSE
1	C	13	GLN
1	C	15	THR
1	C	20	SER
1	C	22	LEU
1	C	24	ARG
1	C	25	ASN
1	C	27	PHE
1	C	29	LYS
1	C	32	LEU
1	C	33	LEU
1	C	36	ILE
1	C	38	GLN
1	C	48	LYS
1	C	62	LYS
1	C	65	GLU
1	C	78	LYS
1	C	105	VAL
1	C	114	SER
1	C	115	LEU
1	C	120	SER
1	C	122	LEU
1	C	123	ASP
1	C	125	ARG

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Mol	Chain	Res	Type
1	C	128	THR
1	C	142	SER
1	C	143	LYS
1	C	146	THR
1	C	147	THR
1	C	149	GLN
1	C	151	LEU
1	C	155	LEU
1	C	157	VAL
1	C	162	SER
1	C	163	VAL
1	C	182	THR
1	C	185	LYS
1	C	192	LEU
1	C	197	SER
1	C	200	TYR
1	C	202	GLN
1	C	203	SER
1	C	204	GLU
1	C	206	GLN
1	C	210	ASN
1	C	216	ARG
1	C	231	LEU
1	C	233	ASP
1	D	8	ASN
1	D	13	GLN
1	D	15	THR
1	D	16	ARG
1	D	17	LEU
1	D	24	ARG
1	D	28	SER
1	D	38	GLN
1	D	40	THR
1	D	48	LYS
1	D	62	LYS
1	D	69	GLU
1	D	76	ARG
1	D	78	LYS
1	D	79	GLN
1	D	82	ILE
1	D	83	ASP
1	D	89	SER

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Mol	Chain	Res	Type
1	D	96	LYS
1	D	99	THR
1	D	102	ASN
1	D	104	ARG
1	D	112	ILE
1	D	122	LEU
1	D	125	ARG
1	D	144	THR
1	D	151	LEU
1	D	153	SER
1	D	162	SER
1	D	163	VAL
1	D	166	LYS
1	D	169	VAL
1	D	172	ARG
1	D	173	GLN
1	D	174	THR
1	D	180	THR
1	D	184	ASN
1	D	185	LYS
1	D	189	ASP
1	D	192	LEU
1	D	193	THR
1	D	194	PHE
1	D	202	GLN
1	D	203	SER
1	D	204	GLU
1	D	205	ILE
1	D	210	ASN
1	D	213	ILE
1	D	214	THR
1	D	215	GLU
1	D	218	ARG
1	D	220	LYS
1	D	222	MSE
1	D	226	LEU
1	D	227	ARG
1	D	232	ILE
1	E	6	LEU
1	E	13	GLN
1	E	15	THR
1	E	16	ARG

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Mol	Chain	Res	Type
1	E	17	LEU
1	E	24	ARG
1	E	25	ASN
1	E	29	LYS
1	E	33	LEU
1	E	35	VAL
1	E	61	VAL
1	E	62	LYS
1	E	66	GLN
1	E	69	GLU
1	E	70	LEU
1	E	79	GLN
1	E	81	ARG
1	E	83	ASP
1	E	90	ARG
1	E	95	THR
1	E	101	LEU
1	E	114	SER
1	E	117	THR
1	E	120	SER
1	E	122	LEU
1	E	133	ILE
1	E	134	SER
1	E	136	LEU
1	E	144	THR
1	E	146	THR
1	E	148	SER
1	E	155	LEU
1	E	157	VAL
1	E	159	THR
1	E	172	ARG
1	E	174	THR
1	E	177	THR
1	E	182	THR
1	E	185	LYS
1	E	193	THR
1	E	194	PHE
1	E	196	VAL
1	E	201	THR
1	E	206	GLN
1	E	208	ILE
1	E	212	LEU

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Mol	Chain	Res	Type
1	E	214	THR
1	E	217	ARG
1	E	218	ARG
1	E	219	THR
1	E	222	MSE
1	E	224	ASP
1	E	231	LEU
1	E	232	ILE
1	F	1	MSE
1	F	8	ASN
1	F	10	VAL
1	F	16	ARG
1	F	17	LEU
1	F	20	SER
1	F	21	ILE
1	F	22	LEU
1	F	24	ARG
1	F	27	PHE
1	F	28	SER
1	F	29	LYS
1	F	30	SER
1	F	35	VAL
1	F	36	ILE
1	F	48	LYS
1	F	62	LYS
1	F	65	GLU
1	F	68	VAL
1	F	78	LYS
1	F	80	LEU
1	F	81	ARG
1	F	82	ILE
1	F	86	ASP
1	F	94	ASN
1	F	95	THR
1	F	96	LYS
1	F	99	THR
1	F	109	GLU
1	F	122	LEU
1	F	128	THR
1	F	134	SER
1	F	146	THR
1	F	147	THR

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Mol	Chain	Res	Type
1	F	150	SER
1	F	151	LEU
1	F	153	SER
1	F	157	VAL
1	F	166	LYS
1	F	167	LYS
1	F	182	THR
1	F	185	LYS
1	F	188	PHE
1	F	191	ASP
1	F	193	THR
1	F	196	VAL
1	F	197	SER
1	F	198	ASP
1	F	199	THR
1	F	201	THR
1	F	202	GLN
1	F	203	SER
1	F	205	ILE
1	F	208	ILE
1	F	212	LEU
1	F	213	ILE
1	F	215	GLU
1	F	217	ARG
1	F	218	ARG
1	F	220	LYS
1	F	226	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	8	ASN
1	A	38	GLN
1	A	60	GLN
1	A	66	GLN
1	A	73	HIS
1	A	94	ASN
1	A	149	GLN
1	A	156	ASN
1	A	202	GLN
1	A	206	GLN

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Mol	Chain	Res	Type
1	A	210	ASN
1	B	7	ASN
1	B	8	ASN
1	B	38	GLN
1	B	87	HIS
1	B	132	ASN
1	B	137	GLN
1	B	206	GLN
1	C	8	ASN
1	C	13	GLN
1	C	60	GLN
1	C	79	GLN
1	C	94	ASN
1	C	116	GLN
1	C	137	GLN
1	C	184	ASN
1	C	210	ASN
1	D	38	GLN
1	D	118	ASN
1	D	132	ASN
1	D	173	GLN
1	D	206	GLN
1	D	210	ASN
1	E	25	ASN
1	E	50	ASN
1	E	54	GLN
1	E	66	GLN
1	E	79	GLN
1	E	87	HIS
1	E	102	ASN
1	E	118	ASN
1	E	131	ASN
1	E	149	GLN
1	E	156	ASN
1	E	229	HIS
1	F	8	ASN
1	F	54	GLN
1	F	63	ASN
1	F	66	GLN
1	F	73	HIS
1	F	87	HIS
1	F	94	ASN

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Mol	Chain	Res	Type
1	F	102	ASN
1	F	131	ASN
1	F	156	ASN
1	F	202	GLN
1	F	206	GLN
1	F	210	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	231/233 (99%)	1.04	34 (14%) 3 5	2, 14, 36, 48	0
1	B	231/233 (99%)	0.87	17 (7%) 17 24	2, 16, 29, 38	0
1	C	231/233 (99%)	1.41	36 (15%) 3 4	3, 15, 55, 75	0
1	D	231/233 (99%)	1.71	60 (25%) 1 1	5, 21, 56, 75	0
1	E	231/233 (99%)	1.44	55 (23%) 1 1	4, 18, 59, 77	0
1	F	231/233 (99%)	1.41	48 (20%) 1 1	3, 17, 43, 56	0
All	All	1386/1398 (99%)	1.31	250 (18%) 2 2	2, 17, 48, 77	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	THR	12.2
1	F	194	PHE	11.5
1	D	196	VAL	11.4
1	D	195	ALA	11.1
1	D	178	ALA	11.1
1	C	202	GLN	10.7
1	C	195	ALA	10.4
1	E	192	LEU	9.2
1	E	202	GLN	8.9
1	D	199	THR	8.4
1	C	192	LEU	8.4
1	D	197	SER	8.3
1	C	198	ASP	7.5
1	E	205	ILE	7.3
1	E	208	ILE	7.1
1	E	147	THR	7.0
1	D	200	TYR	6.9
1	F	196	VAL	6.8
1	F	190	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	D	202	GLN	6.5
1	C	194	PHE	6.4
1	D	192	LEU	6.4
1	D	194	PHE	6.2
1	F	170	GLY	6.2
1	D	211	ALA	6.2
1	C	199	THR	6.2
1	C	201	THR	6.1
1	D	213	ILE	6.0
1	D	201	THR	5.9
1	F	195	ALA	5.8
1	D	157	VAL	5.8
1	E	193	THR	5.8
1	E	203	SER	5.7
1	E	196	VAL	5.7
1	F	200	TYR	5.7
1	F	193	THR	5.7
1	E	201	THR	5.6
1	E	157	VAL	5.6
1	D	11	VAL	5.6
1	F	203	SER	5.6
1	D	188	PHE	5.5
1	E	175	GLY	5.4
1	C	200	TYR	5.4
1	F	199	THR	5.4
1	C	197	SER	5.3
1	D	180	THR	5.3
1	C	18	ASP	5.1
1	F	208	ILE	5.1
1	D	10	VAL	5.1
1	D	208	ILE	5.0
1	C	19	ALA	5.0
1	A	182	THR	5.0
1	F	164	GLY	5.0
1	F	167	LYS	5.0
1	F	183	ALA	4.9
1	A	183	ALA	4.9
1	B	189	ASP	4.9
1	F	205	ILE	4.8
1	D	15	THR	4.7
1	C	189	ASP	4.6
1	A	194	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	11	VAL	4.6
1	F	151	LEU	4.5
1	D	179	ALA	4.5
1	E	183	ALA	4.4
1	E	17	LEU	4.3
1	D	184	ASN	4.3
1	E	198	ASP	4.2
1	E	197	SER	4.2
1	A	192	LEU	4.1
1	F	18	ASP	4.1
1	F	204	GLU	4.1
1	D	189	ASP	4.0
1	C	187	VAL	4.0
1	C	205	ILE	4.0
1	C	149	GLN	4.0
1	E	158	THR	4.0
1	C	26	VAL	4.0
1	B	194	PHE	3.9
1	A	25	ASN	3.9
1	D	193	THR	3.9
1	C	196	VAL	3.9
1	E	233	ASP	3.9
1	A	195	ALA	3.8
1	D	198	ASP	3.8
1	E	181	GLY	3.8
1	D	204	GLU	3.8
1	F	169	VAL	3.7
1	C	203	SER	3.7
1	D	203	SER	3.7
1	B	192	LEU	3.7
1	E	176	TRP	3.7
1	A	101	LEU	3.7
1	F	209	ALA	3.7
1	B	175	GLY	3.6
1	F	91	ILE	3.6
1	F	166	LYS	3.6
1	E	207	ALA	3.6
1	A	15	THR	3.5
1	D	190	ALA	3.5
1	F	168	VAL	3.5
1	D	25	ASN	3.5
1	A	32	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	9	PRO	3.4
1	F	202	GLN	3.4
1	E	200	TYR	3.4
1	E	215	GLU	3.4
1	F	207	ALA	3.4
1	E	219	THR	3.4
1	A	23	PRO	3.3
1	E	167	LYS	3.3
1	E	156	ASN	3.3
1	A	36	ILE	3.3
1	D	20	SER	3.3
1	D	174	THR	3.3
1	E	195	ALA	3.2
1	D	191	ASP	3.2
1	D	98	ILE	3.2
1	D	210	ASN	3.2
1	D	187	VAL	3.2
1	C	17	LEU	3.2
1	A	179	ALA	3.2
1	D	224	ASP	3.2
1	A	200	TYR	3.2
1	A	196	VAL	3.2
1	E	168	VAL	3.2
1	F	17	LEU	3.2
1	D	177	THR	3.1
1	A	24	ARG	3.1
1	F	212	LEU	3.1
1	C	204	GLU	3.1
1	E	133	ILE	3.1
1	D	2	ALA	3.1
1	D	6	LEU	3.1
1	D	183	ALA	3.1
1	F	122	LEU	3.0
1	E	182	THR	3.0
1	B	24	ARG	3.0
1	B	196	VAL	3.0
1	D	102	ASN	3.0
1	F	191	ASP	3.0
1	B	177	THR	3.0
1	D	8	ASN	3.0
1	F	174	THR	3.0
1	E	206	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	24	ARG	3.0
1	E	226	LEU	3.0
1	E	18	ASP	2.9
1	A	33	LEU	2.9
1	C	233	ASP	2.9
1	E	16	ARG	2.9
1	C	191	ASP	2.9
1	A	18	ASP	2.9
1	E	24	ARG	2.8
1	F	24	ARG	2.8
1	B	176	TRP	2.8
1	A	193	THR	2.8
1	A	17	LEU	2.8
1	F	148	SER	2.8
1	C	16	ARG	2.8
1	A	98	ILE	2.8
1	E	146	THR	2.8
1	C	101	LEU	2.7
1	E	177	THR	2.7
1	F	192	LEU	2.7
1	C	157	VAL	2.7
1	D	182	THR	2.7
1	F	6	LEU	2.7
1	F	115	LEU	2.7
1	D	26	VAL	2.7
1	D	176	TRP	2.7
1	F	163	VAL	2.6
1	E	148	SER	2.6
1	B	178	ALA	2.6
1	D	4	PRO	2.6
1	F	197	SER	2.6
1	F	201	THR	2.6
1	B	197	SER	2.6
1	D	214	THR	2.6
1	F	171	ALA	2.5
1	A	27	PHE	2.5
1	A	111	GLU	2.5
1	D	7	ASN	2.5
1	E	151	LEU	2.5
1	B	84	VAL	2.5
1	C	119	VAL	2.5
1	D	12	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	223	GLU	2.5
1	F	36	ILE	2.5
1	A	212	LEU	2.5
1	E	115	LEU	2.5
1	D	217	ARG	2.5
1	E	217	ARG	2.4
1	D	35	VAL	2.4
1	E	169	VAL	2.4
1	B	123	ASP	2.4
1	A	184	ASN	2.4
1	E	123	ASP	2.4
1	D	77	ILE	2.4
1	E	79	GLN	2.4
1	D	119	VAL	2.4
1	B	15	THR	2.4
1	D	121	ALA	2.4
1	E	171	ALA	2.4
1	E	166	LYS	2.4
1	A	13	GLN	2.4
1	D	24	ARG	2.3
1	D	109	GLU	2.3
1	F	112	ILE	2.3
1	F	182	THR	2.3
1	E	216	ARG	2.3
1	A	37	ALA	2.3
1	C	2	ALA	2.3
1	E	211	ALA	2.3
1	E	228	ALA	2.3
1	C	105	VAL	2.2
1	E	199	THR	2.2
1	A	14	ALA	2.2
1	B	171	ALA	2.2
1	F	215	GLU	2.2
1	F	27	PHE	2.2
1	F	198	ASP	2.2
1	E	232	ILE	2.2
1	D	17	LEU	2.2
1	E	194	PHE	2.2
1	D	207	ALA	2.2
1	E	19	ALA	2.2
1	A	188	PHE	2.2
1	A	26	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	2.1
1	C	27	PHE	2.1
1	C	169	VAL	2.1
1	E	180	THR	2.1
1	E	122	LEU	2.1
1	B	191	ASP	2.1
1	D	166	LYS	2.1
1	A	158	THR	2.1
1	C	159	THR	2.1
1	F	33	LEU	2.1
1	A	16	ARG	2.1
1	B	225	ALA	2.1
1	C	108	ALA	2.1
1	A	10	VAL	2.1
1	D	169	VAL	2.1
1	F	189	ASP	2.1
1	C	188	PHE	2.0
1	F	187	VAL	2.0
1	F	10	VAL	2.0
1	A	232	ILE	2.0
1	C	185	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.