



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 09:10 AM EDT

PDB ID : 4I2V
Title : X-ray structure of the unliganded uridine phosphorylase from *Yersinia pseudotuberculosis* at 2.12Å resolution
Authors : Lashkov, A.A.; Balaev, V.V.; Prokofev, I.I.; Betzel, C.; Gabdoulkhakov, A.G.; Mikhailov, A.M.
Deposited on : 2012-11-23
Resolution : 2.12 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

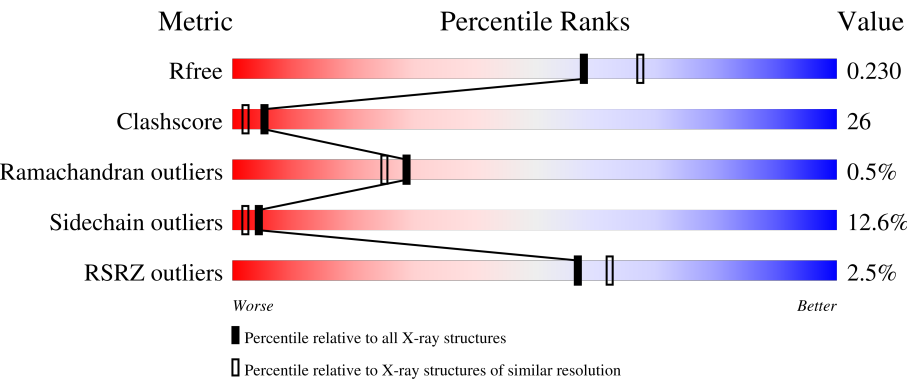
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.12 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	253	<div><div>2%</div><div>47%</div><div>46%</div><div>6%</div><div></div></div>
1	B	253	<div><div>2%</div><div>48%</div><div>41%</div><div>10%</div><div></div></div>
1	C	253	<div><div>2%</div><div>43%</div><div>47%</div><div>8%</div><div></div></div>
1	D	253	<div><div>2%</div><div>45%</div><div>47%</div><div>7%</div><div></div></div>
1	E	253	<div><div>4%</div><div>48%</div><div>43%</div><div>8%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	253	<div><div></div><div>3%</div><div>49%</div><div>45%</div><div>5%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11322 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	B	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	C	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	D	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	E	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			
1	F	250	Total	C	N	O	S	0	0	0
			1875	1173	330	360	12			

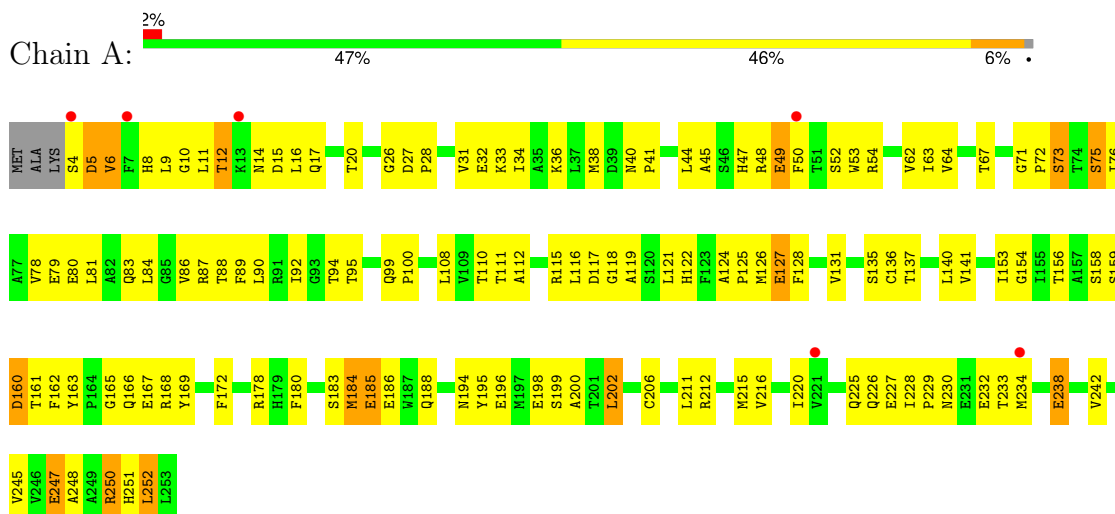
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	17	Total	O	0	0
			17	17		
2	C	13	Total	O	0	0
			13	13		
2	D	17	Total	O	0	0
			17	17		
2	E	4	Total	O	0	0
			4	4		
2	F	9	Total	O	0	0
			9	9		

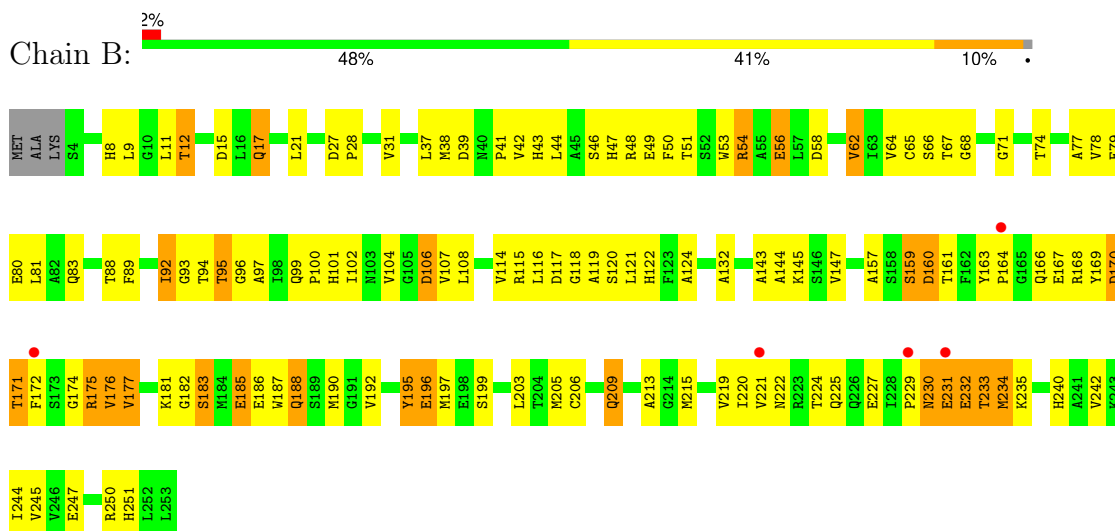
3 Residue-property plots [i](#)

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

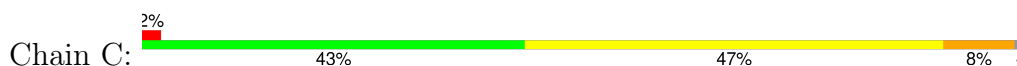
• Molecule 1: Uridine phosphorylase

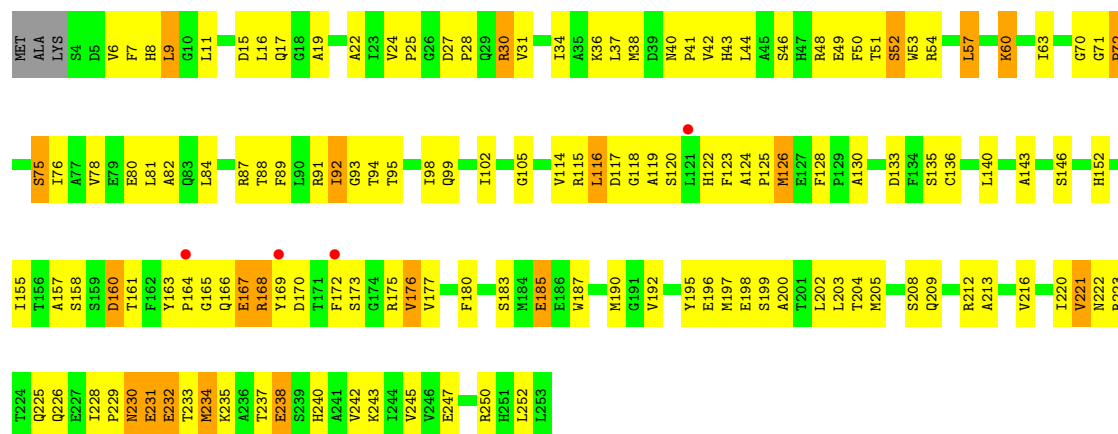


• Molecule 1: Uridine phosphorylase

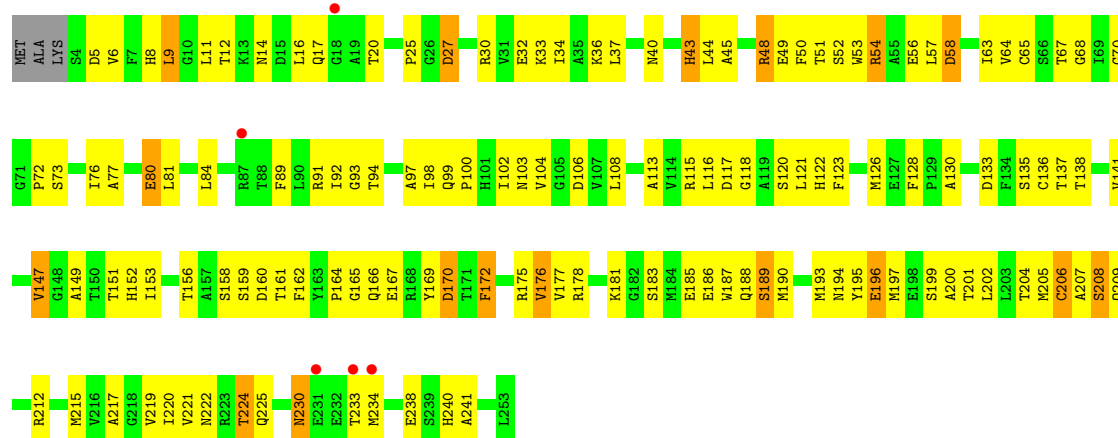
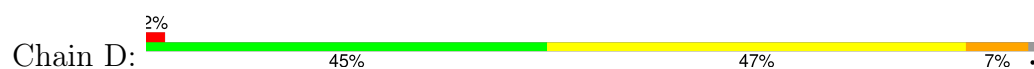


• Molecule 1: Uridine phosphorylase

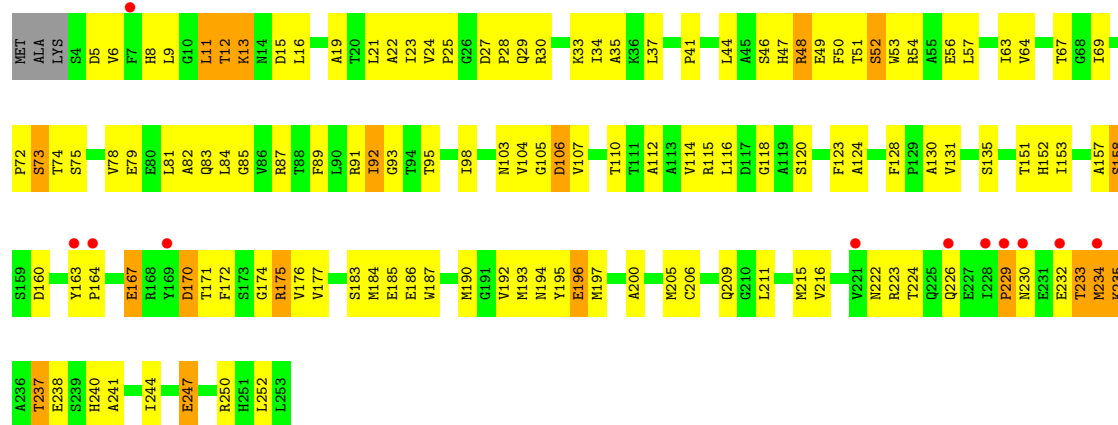




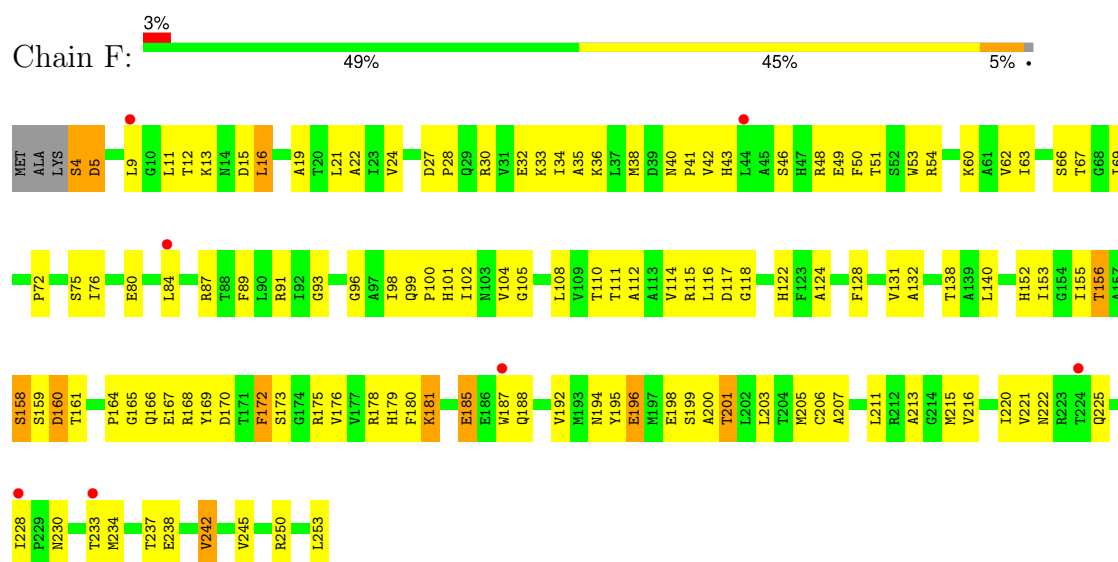
• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	156.68Å 156.68Å 48.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.61 – 2.12 29.61 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.61-2.12) 97.6 (29.61-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.200 , 0.242 0.203 , 0.230	Depositor DCC
R_{free} test set	3680 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 14.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.427 for -h,-k,l 0.075 for h,-h-k,-l 0.074 for -k,-h,-l	Xtriage
Reported twinning fraction	0.460 for -h,-k,l	Depositor
Outliers	0 of 73600 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11322	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	1/1908 (0.1%)	0.67	0/2590
1	B	0.45	0/1908	0.69	0/2590
1	C	0.43	0/1908	0.69	0/2590
1	D	0.44	0/1908	0.67	0/2590
1	E	0.41	0/1908	0.69	0/2590
1	F	0.43	0/1908	0.66	0/2590
All	All	0.44	1/11448 (0.0%)	0.68	0/15540

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	B	0	1
1	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	CYS	CB-SG	-5.05	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	232	GLU	Peptide
1	E	232	GLU	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	1875	0	1869	117	0
1	B	1875	0	1869	104	0
1	C	1875	0	1869	113	0
1	D	1875	0	1869	119	0
1	E	1875	0	1869	97	0
1	F	1875	0	1869	94	0
2	A	12	0	0	1	0
2	B	17	0	0	0	0
2	C	13	0	0	1	0
2	D	17	0	0	4	0
2	E	4	0	0	0	0
2	F	9	0	0	1	0
All	All	11322	0	11214	595	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 26.

All (595) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:HB3	1:B:164:PRO:HB2	1.43	1.00
1:F:16:LEU:HG	1:F:63:ILE:HG13	1.48	0.93
1:D:49:GLU:HG2	1:D:68:GLY:HA2	1.55	0.88
1:E:167:GLU:HG3	1:E:183:SER:HB2	1.54	0.87
1:E:164:PRO:HB2	1:F:122:HIS:HB3	1.57	0.85
1:A:8:HIS:CD2	1:A:50:PHE:HE2	1.95	0.83
1:E:175:ARG:HH21	1:E:177:VAL:HA	1.44	0.82
1:C:72:PRO:HG2	1:D:72:PRO:HD2	1.62	0.80
1:C:115:ARG:HH21	1:C:120:SER:HB2	1.46	0.79
1:C:49:GLU:HG3	1:D:49:GLU:HB2	1.64	0.79
1:C:187:TRP:HB3	1:C:192:VAL:HB	1.65	0.79
1:A:8:HIS:HD2	1:A:50:PHE:HE2	1.32	0.78
1:C:94:THR:HB	1:C:220:ILE:HD13	1.64	0.78
1:A:8:HIS:CD2	1:A:50:PHE:CE2	2.70	0.78
1:A:8:HIS:HB3	1:A:50:PHE:CD2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:SER:HA	1:C:202:LEU:HB3	1.67	0.76
1:C:175:ARG:NH2	1:D:123:PHE:O	2.20	0.75
1:A:8:HIS:HB3	1:A:50:PHE:CE2	2.22	0.75
1:D:65:CYS:HB3	1:D:81:LEU:HD11	1.68	0.74
1:B:102:ILE:O	1:B:222:ASN:ND2	2.21	0.74
1:E:16:LEU:HB3	1:E:19:ALA:HB3	1.70	0.73
1:B:99:GLN:HB3	1:B:101:HIS:CE1	2.23	0.73
1:B:99:GLN:NE2	1:B:188:GLN:O	2.21	0.73
1:A:99:GLN:NE2	1:A:188:GLN:O	2.22	0.72
1:A:185:GLU:HA	1:A:188:GLN:HB2	1.70	0.72
1:C:71:GLY:O	1:C:75:SER:N	2.23	0.72
1:F:196:GLU:OE2	1:F:199:SER:N	2.22	0.72
1:A:115:ARG:NH1	1:A:128:PHE:O	2.24	0.70
1:C:16:LEU:HD22	1:C:63:ILE:HG13	1.74	0.70
1:B:43:HIS:NE2	1:B:46:SER:OG	2.25	0.70
1:D:5:ASP:H	1:D:12:THR:HG22	1.58	0.69
1:D:222:ASN:HB3	1:D:225:GLN:HB2	1.74	0.69
1:C:17:GLN:HB3	1:C:54:ARG:HH12	1.57	0.69
1:B:183:SER:HA	1:B:186:GLU:HB3	1.73	0.68
1:C:164:PRO:HB2	1:D:122:HIS:HB3	1.75	0.68
1:A:115:ARG:NH2	1:A:124:ALA:O	2.25	0.68
1:A:183:SER:HA	1:A:186:GLU:HB2	1.75	0.68
1:E:114:VAL:HB	1:E:157:ALA:HA	1.76	0.68
1:D:97:ALA:O	1:D:222:ASN:ND2	2.27	0.67
1:E:44:LEU:HD21	1:E:54:ARG:HB2	1.76	0.67
1:F:102:ILE:HG21	1:F:108:LEU:HD21	1.75	0.67
1:F:89:PHE:HE2	1:F:211:LEU:HD13	1.60	0.67
1:E:34:ILE:HB	1:E:64:VAL:HG11	1.77	0.67
1:E:6:VAL:HG21	1:E:9:LEU:HB2	1.75	0.67
1:B:247:GLU:OE2	1:B:251:HIS:NE2	2.24	0.66
1:E:41:PRO:HB2	1:E:53:TRP:HZ3	1.60	0.66
1:E:205:MET:O	1:E:209:GLN:NE2	2.26	0.66
1:B:118:GLY:N	1:B:160:ASP:OD2	2.28	0.66
1:C:118:GLY:H	1:C:160:ASP:HB2	1.61	0.66
1:A:12:THR:H	1:A:15:ASP:HB3	1.61	0.65
1:E:110:THR:HB	1:E:215:MET:HB3	1.78	0.65
1:F:155:ILE:HG22	1:F:192:VAL:HG22	1.79	0.65
1:A:198:GLU:OE1	1:A:198:GLU:N	2.30	0.65
1:B:175:ARG:HH12	1:B:177:VAL:HA	1.62	0.65
1:E:46:SER:HA	1:E:51:THR:HA	1.77	0.65
1:C:187:TRP:HA	1:C:190:MET:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LEU:HA	1:C:84:LEU:HD12	1.79	0.64
1:D:147:VAL:HG12	1:D:149:ALA:H	1.63	0.64
1:E:209:GLN:HB3	1:F:172:PHE:CE2	2.33	0.64
1:A:166:GLN:OE1	1:A:168:ARG:NH2	2.31	0.64
1:A:16:LEU:HD23	1:A:63:ILE:HG13	1.80	0.63
1:C:115:ARG:NH1	1:C:128:PHE:O	2.30	0.63
1:D:6:VAL:HG22	1:D:11:LEU:H	1.62	0.63
1:F:140:LEU:HD22	1:F:216:VAL:HB	1.80	0.63
1:B:97:ALA:HB1	1:B:102:ILE:HB	1.81	0.63
1:F:161:THR:HB	1:F:164:PRO:HD2	1.80	0.63
1:A:6:VAL:HG21	1:A:84:LEU:HD11	1.79	0.63
1:A:72:PRO:HB3	1:B:197:MET:HE1	1.80	0.63
1:C:99:GLN:NE2	1:C:192:VAL:O	2.30	0.63
1:B:115:ARG:NH2	1:B:124:ALA:O	2.31	0.62
1:B:115:ARG:NH2	1:B:120:SER:O	2.33	0.62
1:E:41:PRO:HB2	1:E:53:TRP:CZ3	2.35	0.62
1:F:238:GLU:O	1:F:242:VAL:HB	1.99	0.62
1:E:171:THR:HG23	1:E:174:GLY:H	1.64	0.62
1:A:118:GLY:N	1:A:160:ASP:OD2	2.31	0.62
1:F:30:ARG:HG3	1:F:33:LYS:HD3	1.81	0.62
1:A:26:GLY:O	1:B:48:ARG:NH2	2.33	0.62
1:E:57:LEU:HD13	1:E:250:ARG:HB3	1.82	0.61
1:A:8:HIS:CB	1:A:50:PHE:CE2	2.84	0.61
1:D:196:GLU:OE2	1:D:199:SER:N	2.31	0.61
1:B:170:ASP:N	1:B:170:ASP:OD1	2.34	0.61
1:C:187:TRP:O	1:C:190:MET:N	2.34	0.61
1:D:141:VAL:HG22	1:D:153:ILE:HG12	1.82	0.61
1:B:119:ALA:N	1:B:160:ASP:OD2	2.34	0.60
1:A:9:LEU:HD12	1:A:84:LEU:HD12	1.82	0.60
1:B:21:LEU:HG	1:B:88:THR:HB	1.83	0.60
1:D:25:PRO:HB3	1:D:92:ILE:HG23	1.83	0.60
1:A:158:SER:HA	1:A:196:GLU:O	2.02	0.60
1:C:163:TYR:HB2	1:C:164:PRO:HD3	1.84	0.60
1:B:163:TYR:HB2	1:B:164:PRO:HD3	1.84	0.60
1:E:72:PRO:HG2	1:F:72:PRO:HD2	1.83	0.60
1:C:168:ARG:HD3	1:C:223:ARG:HH12	1.67	0.60
1:C:72:PRO:HG2	1:D:72:PRO:CD	2.32	0.59
1:F:32:GLU:HG2	1:F:36:LYS:HE2	1.84	0.59
1:A:72:PRO:HG3	1:B:160:ASP:O	2.02	0.59
1:C:91:ARG:HB2	1:C:202:LEU:HD21	1.84	0.59
1:D:115:ARG:HH21	1:D:120:SER:HB2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ILE:HG13	1:F:48:ARG:HD2	1.84	0.59
1:E:118:GLY:N	1:E:160:ASP:OD2	2.30	0.59
1:A:247:GLU:HB2	1:A:250:ARG:HH21	1.67	0.59
1:B:159:SER:HB3	1:B:166:GLN:HG2	1.84	0.59
1:B:205:MET:O	1:B:209:GLN:HB2	2.02	0.59
1:E:209:GLN:HG2	1:F:173:SER:HB3	1.84	0.59
1:E:247:GLU:O	1:E:250:ARG:HG2	2.03	0.59
1:D:104:VAL:HA	1:D:219:VAL:HG12	1.85	0.59
1:E:92:ILE:HD13	1:E:93:GLY:N	2.18	0.59
1:A:33:LYS:NZ	1:A:238:GLU:OE1	2.30	0.58
1:B:17:GLN:OE1	1:B:54:ARG:NH1	2.36	0.58
1:C:44:LEU:HB2	1:C:52:SER:HB2	1.85	0.58
1:D:178:ARG:HA	1:D:181:LYS:HE3	1.85	0.58
1:C:76:ILE:HD11	1:D:162:PHE:HB2	1.84	0.58
1:D:118:GLY:O	1:D:122:HIS:ND1	2.35	0.58
1:F:158:SER:HA	1:F:196:GLU:O	2.03	0.58
1:B:166:GLN:HA	1:B:195:TYR:CE1	2.39	0.57
1:A:28:PRO:HD2	1:B:48:ARG:HG2	1.86	0.57
1:E:187:TRP:O	1:E:192:VAL:N	2.37	0.57
1:E:95:THR:HG21	1:E:194:ASN:HD22	1.70	0.57
1:D:44:LEU:HD11	1:D:54:ARG:HB2	1.85	0.56
1:D:166:GLN:NE2	1:D:197:MET:HG2	2.20	0.56
1:B:79:GLU:O	1:B:83:GLN:HB2	2.05	0.56
1:E:27:ASP:OD1	1:E:27:ASP:N	2.38	0.56
1:F:5:ASP:N	1:F:5:ASP:OD1	2.37	0.56
1:C:99:GLN:O	1:C:222:ASN:ND2	2.36	0.56
1:E:186:GLU:O	1:E:190:MET:N	2.38	0.56
1:B:67:THR:HG22	1:B:77:ALA:HB3	1.87	0.56
1:C:72:PRO:HD2	1:D:72:PRO:HG2	1.87	0.56
1:F:111:THR:HG23	1:F:153:ILE:HG22	1.88	0.56
1:D:121:LEU:HD21	1:D:126:MET:HB2	1.87	0.56
1:A:122:HIS:ND1	1:B:161:THR:OG1	2.23	0.56
1:A:156:THR:OG1	1:A:194:ASN:OD1	2.21	0.56
1:E:13:LYS:HG2	1:E:84:LEU:HA	1.86	0.56
1:F:13:LYS:HA	1:F:84:LEU:HD22	1.87	0.56
1:E:49:GLU:OE2	1:F:69:ILE:N	2.37	0.56
1:E:115:ARG:NH2	1:E:124:ALA:O	2.25	0.56
1:D:233:THR:HG23	1:D:234:MET:H	1.70	0.56
1:A:45:ALA:HB1	1:A:47:HIS:CD2	2.41	0.56
1:A:115:ARG:HH21	1:A:121:LEU:HA	1.69	0.56
1:C:124:ALA:HB1	1:C:128:PHE:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:GLY:HA2	1:E:237:THR:HB	1.86	0.56
1:E:91:ARG:HG2	1:E:215:MET:SD	2.46	0.55
1:A:111:THR:HG23	1:A:153:ILE:HG22	1.89	0.55
1:B:114:VAL:HB	1:B:157:ALA:HA	1.88	0.55
1:C:221:VAL:HG23	1:C:229:PRO:HD3	1.89	0.55
1:A:80:GLU:HA	1:A:83:GLN:HB2	1.88	0.55
1:B:199:SER:HB3	1:B:215:MET:SD	2.46	0.55
1:A:49:GLU:HB2	1:B:49:GLU:HG3	1.88	0.55
1:A:95:THR:HG21	1:A:108:LEU:HD12	1.87	0.55
1:A:12:THR:HG23	1:A:15:ASP:HB2	1.89	0.55
1:A:206:CYS:HB3	1:A:211:LEU:O	2.06	0.55
1:B:118:GLY:HA2	1:B:121:LEU:HG	1.88	0.55
1:C:157:ALA:O	1:C:195:TYR:HA	2.07	0.55
1:A:8:HIS:CG	1:A:50:PHE:CE2	2.95	0.54
1:F:98:ILE:O	1:F:188:GLN:HG2	2.08	0.54
1:B:247:GLU:O	1:B:250:ARG:HB3	2.08	0.54
1:C:118:GLY:HA3	1:D:118:GLY:HA3	1.88	0.54
1:C:242:VAL:HA	1:C:245:VAL:HG12	1.90	0.54
1:E:92:ILE:HG12	1:E:216:VAL:HG13	1.89	0.54
1:F:30:ARG:NH2	1:F:93:GLY:HA2	2.22	0.54
1:D:48:ARG:NH1	2:D:301:HOH:O	2.41	0.54
1:A:80:GLU:O	1:A:84:LEU:N	2.41	0.54
1:A:160:ASP:H	1:B:122:HIS:HE1	1.56	0.54
1:C:205:MET:O	1:C:209:GLN:HB2	2.07	0.54
1:A:33:LYS:NZ	1:A:238:GLU:HB3	2.23	0.53
1:B:74:THR:O	1:B:78:VAL:HG23	2.07	0.53
1:C:6:VAL:HG21	1:C:9:LEU:HB3	1.89	0.53
1:A:225:GLN:HG2	1:A:226:GLN:H	1.73	0.53
1:C:199:SER:O	1:C:203:LEU:N	2.22	0.53
1:D:158:SER:HA	1:D:196:GLU:O	2.08	0.53
1:B:12:THR:O	1:B:15:ASP:HB2	2.07	0.53
1:C:115:ARG:HB2	1:C:126:MET:SD	2.47	0.53
1:D:27:ASP:HB2	1:D:30:ARG:HG3	1.91	0.53
1:F:206:CYS:O	1:F:211:LEU:N	2.34	0.53
1:C:198:GLU:OE2	1:C:198:GLU:N	2.40	0.53
1:D:67:THR:OG1	1:D:91:ARG:NH1	2.42	0.53
1:A:48:ARG:HG3	1:B:28:PRO:HD2	1.91	0.53
1:B:132:ALA:HA	1:B:203:LEU:HD22	1.90	0.53
1:D:16:LEU:HD13	1:D:84:LEU:HD13	1.91	0.53
1:A:16:LEU:HD11	1:A:84:LEU:HD13	1.89	0.53
1:A:116:LEU:HB2	1:A:159:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:OG1	1:A:212:ARG:NH2	2.40	0.53
1:A:122:HIS:HB3	1:B:164:PRO:CB	2.26	0.53
1:E:206:CYS:HA	1:E:211:LEU:HD12	1.90	0.53
1:C:140:LEU:HD22	1:C:216:VAL:HB	1.90	0.52
1:F:233:THR:HG23	1:F:234:MET:H	1.74	0.52
1:C:28:PRO:HB3	1:C:51:THR:OG1	2.09	0.52
1:F:41:PRO:HB2	1:F:53:TRP:HZ3	1.74	0.52
1:E:112:ALA:HA	1:E:131:VAL:HA	1.90	0.52
1:A:112:ALA:HB2	1:A:131:VAL:HG23	1.91	0.52
1:D:8:HIS:CD2	1:D:76:ILE:HD13	2.43	0.52
1:C:16:LEU:HB3	1:C:19:ALA:HB3	1.91	0.52
1:F:4:SER:O	1:F:4:SER:OG	2.24	0.52
1:C:161:THR:CG2	1:C:164:PRO:HD2	2.40	0.52
1:D:30:ARG:NH1	1:D:94:THR:OG1	2.43	0.52
1:B:41:PRO:HB2	1:B:53:TRP:CZ3	2.45	0.52
1:F:67:THR:OG1	1:F:91:ARG:NH1	2.35	0.52
1:F:124:ALA:HB1	1:F:128:PHE:HB3	1.92	0.52
1:F:196:GLU:OE2	1:F:198:GLU:N	2.43	0.52
1:B:185:GLU:HA	1:B:188:GLN:HB3	1.90	0.52
1:C:114:VAL:HB	1:C:157:ALA:HA	1.92	0.52
1:D:92:ILE:HD11	1:D:241:ALA:HB1	1.91	0.52
1:D:97:ALA:HA	1:D:194:ASN:HA	1.92	0.52
1:D:115:ARG:HE	1:D:120:SER:HB2	1.73	0.52
1:B:67:THR:HB	1:B:74:THR:HA	1.91	0.51
1:D:98:ILE:N	1:D:193:MET:O	2.39	0.51
1:B:116:LEU:HD21	1:B:187:TRP:HZ2	1.76	0.51
1:F:99:GLN:OE1	1:F:100:PRO:HD2	2.10	0.51
1:C:115:ARG:NH1	1:C:125:PRO:O	2.42	0.51
1:F:222:ASN:HB3	1:F:225:GLN:HB2	1.91	0.51
1:C:44:LEU:HD11	1:C:63:ILE:HD12	1.92	0.51
1:D:204:THR:O	1:D:208:SER:OG	2.27	0.51
1:E:29:GLN:O	1:E:33:LYS:HE2	2.10	0.51
1:F:76:ILE:O	1:F:80:GLU:HB2	2.09	0.51
1:A:33:LYS:HZ1	1:A:238:GLU:HB3	1.76	0.51
1:C:204:THR:O	1:C:208:SER:OG	2.28	0.51
1:D:108:LEU:HD22	1:D:152:HIS:HB2	1.93	0.51
1:C:230:ASN:OD1	1:C:230:ASN:N	2.44	0.51
1:D:117:ASP:HB2	1:D:160:ASP:OD1	2.11	0.51
1:D:147:VAL:HG12	1:D:149:ALA:N	2.25	0.51
1:C:167:GLU:HG2	1:C:176:VAL:HG11	1.91	0.51
1:A:41:PRO:HB2	1:A:53:TRP:CZ3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:LEU:HG	1:D:63:ILE:HG13	1.91	0.51
1:D:185:GLU:HA	1:D:188:GLN:OE1	2.11	0.50
1:E:11:LEU:HD13	1:E:84:LEU:HD11	1.92	0.50
1:F:35:ALA:HA	1:F:38:MET:HE3	1.92	0.50
1:C:122:HIS:HB3	1:D:164:PRO:HG2	1.92	0.50
1:D:158:SER:HB2	1:D:196:GLU:OE2	2.12	0.50
1:E:9:LEU:HD11	1:E:81:LEU:HG	1.94	0.50
1:C:43:HIS:HB2	1:C:53:TRP:CE2	2.46	0.50
1:B:169:TYR:OH	1:B:181:LYS:HG3	2.12	0.50
1:E:234:MET:SD	1:E:234:MET:N	2.84	0.50
1:A:117:ASP:HA	1:A:160:ASP:HB2	1.94	0.50
1:A:162:PHE:O	1:A:166:GLN:HB2	2.11	0.50
1:C:114:VAL:HG12	1:C:116:LEU:HG	1.93	0.50
1:F:99:GLN:HG2	1:F:192:VAL:O	2.11	0.50
1:A:38:MET:O	1:A:41:PRO:HG3	2.12	0.50
1:C:27:ASP:OD1	1:C:30:ARG:HB2	2.11	0.50
1:A:115:ARG:CZ	1:A:126:MET:HA	2.42	0.50
1:A:230:ASN:ND2	1:A:232:GLU:HB2	2.27	0.50
1:B:49:GLU:HG2	1:B:68:GLY:HA2	1.94	0.50
1:B:97:ALA:HB3	1:B:222:ASN:HD22	1.77	0.50
1:A:161:THR:OG1	1:B:122:HIS:ND1	2.27	0.49
1:B:187:TRP:HB3	1:B:192:VAL:HB	1.94	0.49
1:F:110:THR:HG21	1:F:156:THR:HB	1.94	0.49
1:D:166:GLN:HE21	1:D:197:MET:HG2	1.77	0.49
1:E:24:VAL:O	1:E:91:ARG:HD2	2.12	0.49
1:E:163:TYR:HB2	1:E:164:PRO:HD3	1.93	0.49
1:A:4:SER:HB2	1:A:10:GLY:HA2	1.94	0.49
1:D:11:LEU:HD21	1:D:44:LEU:HB3	1.94	0.49
1:F:43:HIS:HB2	1:F:53:TRP:CE2	2.47	0.49
1:C:11:LEU:HD21	1:C:52:SER:OG	2.13	0.49
1:C:78:VAL:O	1:C:82:ALA:N	2.36	0.49
1:C:173:SER:HB2	1:D:209:GLN:OE1	2.12	0.49
1:E:92:ILE:HD13	1:E:93:GLY:H	1.76	0.49
1:F:98:ILE:HD12	1:F:188:GLN:HG3	1.93	0.49
1:E:106:ASP:HB3	1:E:152:HIS:NE2	2.28	0.49
1:F:42:VAL:O	1:F:54:ARG:N	2.41	0.49
1:B:50:PHE:CE1	1:B:77:ALA:HB2	2.48	0.49
1:D:89:PHE:N	1:D:212:ARG:O	2.43	0.49
1:E:157:ALA:N	1:E:194:ASN:O	2.45	0.49
1:E:197:MET:CE	1:F:72:PRO:HB3	2.42	0.49
1:C:31:VAL:HG12	1:C:53:TRP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:CB	1:B:164:PRO:HB2	2.30	0.49
1:B:49:GLU:HG2	1:B:68:GLY:CA	2.41	0.49
1:D:68:GLY:HA3	1:D:73:SER:OG	2.13	0.49
1:F:36:LYS:NZ	2:F:308:HOH:O	2.45	0.49
1:A:87:ARG:HA	1:A:211:LEU:HD22	1.94	0.49
1:A:158:SER:HB3	1:A:200:ALA:HB2	1.95	0.49
1:D:196:GLU:CD	1:D:199:SER:H	2.16	0.49
1:F:30:ARG:HH22	1:F:93:GLY:HA2	1.76	0.49
1:A:6:VAL:HG11	1:A:80:GLU:HB3	1.94	0.48
1:A:199:SER:O	1:A:202:LEU:N	2.46	0.48
1:A:71:GLY:O	1:A:75:SER:N	2.34	0.48
1:B:114:VAL:HG12	1:B:116:LEU:HG	1.94	0.48
1:A:12:THR:H	1:A:15:ASP:CB	2.24	0.48
1:E:67:THR:HG1	1:E:91:ARG:HH12	1.60	0.48
1:D:9:LEU:HB2	1:D:11:LEU:HD12	1.94	0.48
1:B:164:PRO:HA	1:B:176:VAL:HG22	1.94	0.48
1:E:187:TRP:HB3	1:E:192:VAL:HB	1.95	0.48
1:A:75:SER:O	1:A:79:GLU:N	2.29	0.48
1:A:125:PRO:O	1:A:127:GLU:N	2.40	0.48
1:D:33:LYS:HZ2	1:D:238:GLU:HG2	1.79	0.48
1:F:132:ALA:HA	1:F:203:LEU:HD22	1.95	0.48
1:B:41:PRO:HB2	1:B:53:TRP:HZ3	1.78	0.48
1:E:104:VAL:HG11	1:E:229:PRO:HB3	1.96	0.48
1:E:230:ASN:OD1	1:E:230:ASN:N	2.46	0.48
1:F:115:ARG:NH1	1:F:128:PHE:O	2.45	0.48
1:A:158:SER:HB2	1:A:196:GLU:OE2	2.14	0.48
1:D:32:GLU:O	1:D:36:LYS:HG3	2.13	0.48
1:E:103:ASN:HB2	1:E:106:ASP:OD1	2.13	0.48
1:F:49:GLU:O	1:F:66:SER:OG	2.32	0.48
1:F:206:CYS:HB3	1:F:211:LEU:O	2.13	0.48
1:A:78:VAL:HG13	1:A:89:PHE:CZ	2.49	0.48
1:B:240:HIS:O	1:B:244:ILE:HD12	2.13	0.48
1:C:88:THR:OG1	1:C:212:ARG:NH2	2.46	0.48
1:C:240:HIS:O	1:C:243:LYS:HB3	2.14	0.48
1:D:54:ARG:NH2	1:D:56:GLU:HG3	2.29	0.48
1:D:186:GLU:O	1:D:190:MET:HG3	2.13	0.48
1:E:41:PRO:HA	1:E:54:ARG:O	2.13	0.48
1:E:72:PRO:HD2	1:F:72:PRO:HG2	1.96	0.48
1:B:224:THR:OG1	1:B:225:GLN:N	2.46	0.47
1:B:41:PRO:HA	1:B:54:ARG:O	2.14	0.47
1:E:75:SER:HB2	1:E:123:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ALA:O	1:E:195:TYR:HA	2.14	0.47
1:D:48:ARG:N	1:D:48:ARG:HD3	2.29	0.47
1:F:96:GLY:O	1:F:194:ASN:HB2	2.14	0.47
1:A:6:VAL:HG23	1:A:11:LEU:H	1.79	0.47
1:B:230:ASN:OD1	1:B:230:ASN:N	2.47	0.47
1:C:25:PRO:HG3	1:C:34:ILE:HD12	1.96	0.47
1:C:158:SER:HA	1:C:196:GLU:O	2.15	0.47
1:E:28:PRO:HB3	1:E:51:THR:HB	1.95	0.47
1:C:98:ILE:HG21	1:C:195:TYR:CE2	2.50	0.47
1:F:40:ASN:N	1:F:41:PRO:HD3	2.30	0.47
1:A:67:THR:O	1:A:73:SER:HB2	2.14	0.47
1:D:115:ARG:HG2	1:D:200:ALA:HB1	1.96	0.47
1:D:199:SER:HB3	1:D:215:MET:SD	2.55	0.47
1:E:8:HIS:HB3	1:E:50:PHE:HE2	1.80	0.47
1:E:16:LEU:HB3	1:E:19:ALA:CB	2.39	0.47
1:F:60:LYS:HB2	1:F:253:LEU:HD13	1.96	0.47
1:F:233:THR:HG23	1:F:234:MET:N	2.29	0.47
1:C:95:THR:O	1:C:220:ILE:HG12	2.15	0.47
1:A:248:ALA:O	1:A:252:LEU:HD12	2.15	0.47
1:C:28:PRO:HA	1:C:51:THR:HB	1.97	0.47
1:E:79:GLU:O	1:E:82:ALA:HB3	2.14	0.47
1:E:115:ARG:NH1	1:E:128:PHE:O	2.47	0.47
1:F:99:GLN:HB3	1:F:101:HIS:CE1	2.50	0.47
1:B:167:GLU:OE2	1:B:183:SER:N	2.48	0.46
1:B:231:GLU:H	1:B:231:GLU:HG3	1.37	0.46
1:C:7:PHE:CD2	1:D:162:PHE:HE2	2.33	0.46
1:C:116:LEU:HD21	1:C:187:TRP:CZ2	2.50	0.46
1:C:116:LEU:HD12	1:C:157:ALA:HB1	1.96	0.46
1:D:30:ARG:O	1:D:34:ILE:HG12	2.15	0.46
1:A:17:GLN:HG3	1:A:54:ARG:NH1	2.31	0.46
1:C:60:LYS:HE3	1:C:60:LYS:H	1.79	0.46
1:C:234:MET:HA	2:C:312:HOH:O	2.15	0.46
1:B:163:TYR:HA	1:B:168:ARG:HB2	1.97	0.46
1:B:196:GLU:OE2	1:B:199:SER:OG	2.23	0.46
1:C:228:ILE:HG22	1:C:229:PRO:O	2.15	0.46
1:F:112:ALA:HA	1:F:131:VAL:HA	1.98	0.46
1:B:233:THR:HG23	1:B:234:MET:N	2.30	0.46
1:C:119:ALA:O	1:C:122:HIS:HB2	2.15	0.46
1:B:230:ASN:ND2	1:B:232:GLU:O	2.48	0.46
1:D:91:ARG:NH2	2:D:302:HOH:O	2.48	0.46
1:E:57:LEU:HD23	1:E:57:LEU:HA	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:LEU:HD23	1:F:19:ALA:N	2.31	0.46
1:A:167:GLU:HG2	1:A:169:TYR:CE2	2.51	0.46
1:B:186:GLU:HG3	1:B:190:MET:HE3	1.97	0.46
1:F:9:LEU:HD11	1:F:80:GLU:HB3	1.98	0.46
1:A:14:ASN:O	1:A:17:GLN:HG2	2.15	0.46
1:C:38:MET:SD	1:C:57:LEU:HG	2.56	0.46
1:C:72:PRO:HB3	1:D:70:GLY:HA3	1.98	0.46
1:E:30:ARG:HG2	1:E:34:ILE:HD11	1.97	0.46
1:C:15:ASP:HB3	1:C:44:LEU:HD22	1.98	0.46
1:E:120:SER:HB3	1:E:200:ALA:O	2.16	0.46
1:F:116:LEU:HB2	1:F:159:SER:HA	1.98	0.46
1:A:78:VAL:HG13	1:A:89:PHE:CE2	2.51	0.45
1:B:15:ASP:O	1:B:54:ARG:NH1	2.48	0.45
1:C:36:LYS:HA	1:C:41:PRO:HG3	1.97	0.45
1:F:54:ARG:HA	1:F:63:ILE:HD13	1.98	0.45
1:C:168:ARG:NH1	1:C:170:ASP:OD2	2.49	0.45
1:E:241:ALA:HA	1:E:244:ILE:HD12	1.98	0.45
1:F:104:VAL:HG13	1:F:220:ILE:HA	1.98	0.45
1:A:90:LEU:HD11	1:A:252:LEU:HD13	1.97	0.45
1:B:171:THR:HG23	1:B:174:GLY:H	1.81	0.45
1:F:122:HIS:N	1:F:122:HIS:CD2	2.84	0.45
1:F:167:GLU:HG2	1:F:169:TYR:CE2	2.51	0.45
1:F:168:ARG:HH11	1:F:168:ARG:HB3	1.82	0.45
1:C:222:ASN:HB3	1:C:225:GLN:HB2	1.99	0.45
1:D:6:VAL:CG2	1:D:11:LEU:H	2.27	0.45
1:D:156:THR:HG23	1:D:194:ASN:ND2	2.32	0.45
1:A:41:PRO:HA	1:A:54:ARG:O	2.16	0.45
1:A:75:SER:OG	1:A:76:ILE:N	2.48	0.45
1:A:163:TYR:CD1	1:A:168:ARG:HD2	2.52	0.45
1:B:38:MET:SD	1:B:62:VAL:HG11	2.57	0.45
1:C:247:GLU:O	1:C:250:ARG:HG2	2.16	0.45
1:D:233:THR:HA	2:D:310:HOH:O	2.16	0.45
1:A:117:ASP:HB2	1:A:119:ALA:H	1.81	0.45
1:F:12:THR:OG1	1:F:15:ASP:OD1	2.34	0.45
1:F:46:SER:HA	1:F:51:THR:HA	1.98	0.45
1:E:79:GLU:O	1:E:83:GLN:HG3	2.17	0.45
1:E:158:SER:HA	1:E:196:GLU:O	2.16	0.45
1:F:16:LEU:HD22	1:F:84:LEU:O	2.17	0.45
1:B:92:ILE:HD13	1:B:93:GLY:N	2.31	0.45
1:A:140:LEU:HD22	1:A:216:VAL:HB	1.99	0.45
1:C:70:GLY:HA2	1:C:197:MET:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:THR:HG22	1:D:205:MET:SD	2.57	0.45
1:D:202:LEU:O	1:D:206:CYS:HB2	2.16	0.45
1:E:49:GLU:OE2	1:F:49:GLU:HG3	2.17	0.45
1:E:107:VAL:HB	1:E:151:THR:HG23	1.99	0.45
1:A:14:ASN:C	1:A:17:GLN:H	2.19	0.44
1:B:107:VAL:O	1:B:108:LEU:HD23	2.16	0.44
1:B:233:THR:HG23	1:B:235:LYS:H	1.81	0.44
1:D:169:TYR:CE1	1:D:176:VAL:HB	2.52	0.44
1:D:183:SER:O	1:D:187:TRP:NE1	2.50	0.44
1:F:89:PHE:O	1:F:213:ALA:HA	2.17	0.44
1:F:99:GLN:HA	1:F:100:PRO:HD2	1.83	0.44
1:B:167:GLU:OE1	1:B:182:GLY:N	2.31	0.44
1:C:40:ASN:O	1:C:42:VAL:HG23	2.18	0.44
1:C:183:SER:O	1:C:187:TRP:NE1	2.51	0.44
1:C:196:GLU:CD	1:C:199:SER:H	2.20	0.44
1:E:104:VAL:HG11	1:E:229:PRO:CB	2.47	0.44
1:F:201:THR:O	1:F:205:MET:HG2	2.17	0.44
1:A:76:ILE:HA	1:B:163:TYR:HE2	1.83	0.44
1:B:65:CYS:HB3	1:B:81:LEU:HD11	1.99	0.44
1:B:116:LEU:HD21	1:B:187:TRP:CZ2	2.51	0.44
1:C:235:LYS:HA	1:C:238:GLU:HB3	1.99	0.44
1:F:179:HIS:HD2	1:F:180:PHE:CE1	2.35	0.44
1:A:28:PRO:HD3	1:A:49:GLU:OE2	2.18	0.44
1:D:137:THR:O	1:D:141:VAL:HG23	2.17	0.44
1:E:98:ILE:HG22	1:E:223:ARG:HD3	1.98	0.44
1:E:163:TYR:HB3	1:E:171:THR:HB	2.00	0.44
1:F:28:PRO:HD3	1:F:49:GLU:OE2	2.17	0.44
1:F:158:SER:HB2	1:F:200:ALA:HB2	1.98	0.44
1:C:128:PHE:CZ	1:C:208:SER:HB3	2.52	0.44
1:D:186:GLU:O	1:D:189:SER:OG	2.35	0.44
1:E:116:LEU:HD12	1:E:195:TYR:HE1	1.82	0.44
1:E:222:ASN:OD1	1:E:224:THR:OG1	2.29	0.44
1:F:102:ILE:HG23	1:F:152:HIS:CD2	2.52	0.44
1:A:88:THR:HG21	1:A:252:LEU:HD22	1.99	0.44
1:C:114:VAL:HG23	1:C:155:ILE:HG22	2.00	0.44
1:D:115:ARG:NH1	1:D:128:PHE:O	2.50	0.44
1:A:83:GLN:HG2	1:B:172:PHE:CG	2.53	0.44
1:D:91:ARG:HG3	1:D:92:ILE:N	2.33	0.44
1:D:117:ASP:HB2	1:D:160:ASP:CG	2.37	0.44
1:D:230:ASN:O	1:D:233:THR:HG22	2.18	0.44
1:E:22:ALA:HB3	1:E:89:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:O	1:A:141:VAL:HG23	2.18	0.44
1:C:160:ASP:O	1:D:72:PRO:HG3	2.18	0.44
1:C:187:TRP:HB3	1:C:192:VAL:CB	2.43	0.44
1:D:6:VAL:HG22	1:D:11:LEU:O	2.18	0.44
1:B:81:LEU:HD13	1:B:89:PHE:HE1	1.83	0.43
1:B:104:VAL:HG11	1:B:229:PRO:HB3	2.00	0.43
1:C:133:ASP:HB3	1:C:136:CYS:HB2	2.00	0.43
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.79	0.43
1:E:69:ILE:HD12	1:F:50:PHE:HE1	1.81	0.43
1:F:87:ARG:H	1:F:87:ARG:HG2	1.62	0.43
1:A:81:LEU:HB3	1:A:86:VAL:HG21	2.00	0.43
1:A:122:HIS:CE1	1:B:161:THR:HG1	2.25	0.43
1:C:87:ARG:HD3	1:C:87:ARG:HA	1.79	0.43
1:C:209:GLN:HB3	1:D:172:PHE:CZ	2.53	0.43
1:D:97:ALA:HB3	1:D:222:ASN:HD22	1.83	0.43
1:A:8:HIS:CE1	1:A:76:ILE:HD13	2.53	0.43
1:B:144:ALA:HA	1:B:244:ILE:HG12	1.99	0.43
1:C:72:PRO:HG3	1:D:160:ASP:O	2.18	0.43
1:D:116:LEU:HB2	1:D:159:SER:HB3	2.01	0.43
1:E:205:MET:O	1:E:209:GLN:HB2	2.17	0.43
1:A:166:GLN:HG2	1:A:195:TYR:CD1	2.53	0.43
1:A:184:MET:O	1:A:188:GLN:HG3	2.18	0.43
1:C:102:ILE:HG12	1:C:152:HIS:CE1	2.53	0.43
1:D:40:ASN:HB3	1:D:54:ARG:HH22	1.84	0.43
1:A:242:VAL:O	1:A:245:VAL:HG12	2.18	0.43
1:B:11:LEU:HD21	1:B:44:LEU:HB3	2.00	0.43
1:B:100:PRO:O	1:B:225:GLN:NE2	2.51	0.43
1:B:169:TYR:CE2	1:B:176:VAL:HB	2.53	0.43
1:D:201:THR:O	1:D:205:MET:HG2	2.18	0.43
1:E:23:ILE:HG22	1:E:25:PRO:HD3	1.99	0.43
1:C:158:SER:OG	1:C:196:GLU:OE2	2.23	0.43
1:C:231:GLU:HG3	1:C:232:GLU:N	2.34	0.43
1:D:11:LEU:HD11	1:D:52:SER:OG	2.19	0.43
1:E:30:ARG:O	1:E:34:ILE:HG13	2.19	0.43
1:F:166:GLN:HA	1:F:195:TYR:CZ	2.52	0.43
1:A:34:ILE:CD1	1:A:92:ILE:HG21	2.49	0.43
1:D:43:HIS:HB2	1:D:53:TRP:CE2	2.54	0.43
1:D:170:ASP:OD1	1:D:170:ASP:N	2.50	0.43
1:E:233:THR:HG22	1:E:234:MET:HE3	2.00	0.43
1:A:6:VAL:CG2	1:A:11:LEU:H	2.32	0.43
1:A:94:THR:HB	1:A:220:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:THR:HB	1:B:220:ILE:HG23	2.00	0.43
1:B:206:CYS:SG	1:B:213:ALA:HB2	2.59	0.43
1:D:44:LEU:HD23	1:D:44:LEU:HA	1.91	0.43
1:D:91:ARG:HG2	1:D:215:MET:HG3	2.01	0.43
1:F:21:LEU:HD23	1:F:22:ALA:N	2.34	0.43
1:F:196:GLU:HG2	1:F:215:MET:HE1	2.01	0.43
1:F:230:ASN:O	1:F:233:THR:HG22	2.18	0.43
1:A:20:THR:O	1:A:87:ARG:N	2.50	0.43
1:A:32:GLU:O	1:A:36:LYS:HG3	2.18	0.43
1:A:87:ARG:O	1:A:211:LEU:HB3	2.18	0.43
1:A:228:ILE:HA	1:A:229:PRO:HD3	1.90	0.43
1:E:235:LYS:O	1:E:238:GLU:HB3	2.19	0.43
1:B:51:THR:N	1:B:66:SER:OG	2.50	0.43
1:C:123:PHE:O	1:D:175:ARG:NH2	2.48	0.43
1:D:133:ASP:HB3	1:D:136:CYS:HB2	2.01	0.43
1:E:234:MET:HA	1:E:237:THR:HG23	2.00	0.43
1:B:95:THR:O	1:B:220:ILE:HG12	2.18	0.42
1:C:70:GLY:HA3	1:D:72:PRO:HB2	2.01	0.42
1:C:118:GLY:N	1:C:160:ASP:HB2	2.32	0.42
1:A:233:THR:HG23	1:A:234:MET:H	1.83	0.42
1:B:44:LEU:HD11	1:B:54:ARG:HB2	2.01	0.42
1:C:89:PHE:O	1:C:213:ALA:HA	2.19	0.42
1:D:103:ASN:O	1:D:106:ASP:HB2	2.19	0.42
1:D:115:ARG:NH2	1:D:120:SER:O	2.52	0.42
1:E:44:LEU:HD12	1:E:52:SER:HB2	2.00	0.42
1:E:170:ASP:OD1	1:E:170:ASP:N	2.52	0.42
1:A:156:THR:HG21	1:A:196:GLU:HG3	2.01	0.42
1:A:215:MET:HG2	2:A:305:HOH:O	2.17	0.42
1:D:161:THR:OG1	1:D:165:GLY:N	2.40	0.42
1:E:67:THR:O	1:E:73:SER:HB2	2.19	0.42
1:F:114:VAL:HG11	1:F:187:TRP:CH2	2.55	0.42
1:A:6:VAL:HG22	1:A:84:LEU:HD21	2.02	0.42
1:B:71:GLY:HA2	1:B:74:THR:HB	2.01	0.42
1:D:113:ALA:HB3	1:D:130:ALA:HB3	2.01	0.42
1:E:252:LEU:HA	1:E:252:LEU:HD23	1.80	0.42
1:F:175:ARG:HG2	1:F:176:VAL:N	2.34	0.42
1:B:39:ASP:O	1:B:56:GLU:N	2.39	0.42
1:B:106:ASP:O	1:B:219:VAL:N	2.48	0.42
1:D:224:THR:O	2:D:309:HOH:O	2.22	0.42
1:E:54:ARG:HG3	1:E:63:ILE:HD13	2.02	0.42
1:B:9:LEU:O	1:B:47:HIS:ND1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:PHE:HE2	1:D:207:ALA:HB3	1.83	0.42
1:F:30:ARG:HG2	1:F:34:ILE:HD11	2.02	0.42
1:F:105:GLY:HA2	1:F:237:THR:OG1	2.20	0.42
1:A:160:ASP:HB3	1:B:119:ALA:HA	2.01	0.42
1:C:22:ALA:HA	1:C:63:ILE:O	2.20	0.42
1:E:74:THR:O	1:E:78:VAL:HG23	2.18	0.42
1:E:75:SER:HA	1:E:205:MET:SD	2.60	0.42
1:F:159:SER:OG	1:F:165:GLY:HA3	2.19	0.42
1:A:28:PRO:HA	1:A:31:VAL:HG23	2.02	0.42
1:E:118:GLY:HA3	1:F:118:GLY:HA3	2.00	0.42
1:F:242:VAL:O	1:F:245:VAL:HG12	2.18	0.42
1:C:166:GLN:HA	1:C:195:TYR:CE1	2.54	0.42
1:F:5:ASP:OD1	1:F:12:THR:HG22	2.20	0.42
1:B:117:ASP:HA	1:B:160:ASP:HB2	2.02	0.41
1:C:98:ILE:HG22	1:C:223:ARG:HD3	2.02	0.41
1:B:161:THR:O	1:B:166:GLN:HG3	2.19	0.41
1:C:43:HIS:HE2	1:C:46:SER:HG	1.66	0.41
1:C:49:GLU:CG	1:D:49:GLU:HB2	2.43	0.41
1:C:92:ILE:HD13	1:C:93:GLY:N	2.34	0.41
1:C:143:ALA:HB1	1:C:247:GLU:HB3	2.02	0.41
1:E:115:ARG:HD2	1:E:130:ALA:HB2	2.02	0.41
1:F:185:GLU:HA	1:F:188:GLN:OE1	2.20	0.41
1:A:8:HIS:NE2	1:A:76:ILE:HD13	2.35	0.41
1:B:31:VAL:HG13	1:B:64:VAL:HG12	2.02	0.41
1:D:50:PHE:CE1	1:D:77:ALA:HB2	2.54	0.41
1:D:99:GLN:OE1	1:D:100:PRO:HD2	2.20	0.41
1:D:116:LEU:HD21	1:D:187:TRP:CZ2	2.55	0.41
1:A:44:LEU:HB2	1:A:52:SER:OG	2.20	0.41
1:C:71:GLY:N	1:C:72:PRO:HD2	2.36	0.41
1:D:84:LEU:HD23	1:D:84:LEU:HA	1.94	0.41
1:B:58:ASP:OD2	1:B:250:ARG:NH1	2.53	0.41
1:B:104:VAL:HG12	1:B:221:VAL:HA	2.02	0.41
1:C:9:LEU:HD23	1:C:80:GLU:HB2	2.02	0.41
1:E:5:ASP:HB2	1:E:12:THR:HA	2.02	0.41
1:C:123:PHE:CE1	1:D:164:PRO:HG3	2.55	0.41
1:F:27:ASP:HA	1:F:28:PRO:HD3	1.95	0.41
1:F:75:SER:HA	1:F:205:MET:SD	2.61	0.41
1:A:88:THR:OG1	1:A:212:ARG:NE	2.52	0.41
1:A:110:THR:HA	1:A:154:GLY:O	2.21	0.41
1:A:165:GLY:HA2	1:A:180:PHE:CE1	2.56	0.41
1:D:233:THR:HG23	1:D:234:MET:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:LEU:HD22	1:E:63:ILE:CD1	2.51	0.41
1:E:104:VAL:HG11	1:E:229:PRO:HG3	2.03	0.41
1:D:183:SER:O	1:D:187:TRP:CD1	2.73	0.41
1:E:209:GLN:HG2	1:F:173:SER:CB	2.49	0.41
1:B:37:LEU:HD12	1:B:242:VAL:HG12	2.03	0.41
1:B:96:GLY:HA2	1:B:219:VAL:HG13	2.03	0.41
1:C:99:GLN:HB2	1:C:102:ILE:HD12	2.02	0.41
1:C:130:ALA:HB2	1:C:204:THR:OG1	2.20	0.41
1:D:53:TRP:N	1:D:64:VAL:O	2.47	0.41
1:D:108:LEU:HD13	1:D:193:MET:HB3	2.01	0.41
1:D:128:PHE:HD2	1:D:204:THR:HG23	1.85	0.41
1:E:15:ASP:O	1:E:54:ARG:NH1	2.54	0.41
1:E:35:ALA:O	1:E:41:PRO:HB3	2.21	0.41
1:E:47:HIS:O	1:E:48:ARG:HB2	2.21	0.41
1:F:117:ASP:HB2	1:F:160:ASP:OD1	2.20	0.41
1:F:128:PHE:HE1	1:F:207:ALA:HB3	1.86	0.41
1:F:178:ARG:HA	1:F:181:LYS:HB2	2.03	0.41
1:A:34:ILE:HB	1:A:64:VAL:HG11	2.03	0.41
1:A:41:PRO:HB2	1:A:53:TRP:HZ3	1.83	0.41
1:B:143:ALA:O	1:B:147:VAL:HG23	2.21	0.41
1:C:8:HIS:HB3	1:C:50:PHE:CE2	2.56	0.41
1:D:94:THR:HB	1:D:220:ILE:CG2	2.51	0.41
1:D:167:GLU:HG3	1:D:176:VAL:HG11	2.03	0.41
1:F:30:ARG:O	1:F:34:ILE:N	2.50	0.41
1:A:5:ASP:OD1	1:A:5:ASP:N	2.44	0.40
1:A:99:GLN:HA	1:A:100:PRO:HD2	1.89	0.40
1:B:185:GLU:H	1:B:185:GLU:HG3	1.57	0.40
1:C:105:GLY:HA2	1:C:237:THR:CG2	2.51	0.40
1:D:57:LEU:HG	1:D:58:ASP:OD1	2.21	0.40
1:F:99:GLN:NE2	1:F:188:GLN:O	2.54	0.40
1:C:177:VAL:O	1:C:180:PHE:N	2.54	0.40
1:D:93:GLY:O	1:D:217:ALA:HA	2.21	0.40
1:E:167:GLU:HB2	1:E:184:MET:HG2	2.03	0.40
1:A:40:ASN:N	1:A:41:PRO:HD3	2.37	0.40
1:B:8:HIS:HB2	1:B:80:GLU:OE2	2.22	0.40
1:C:158:SER:HB2	1:C:200:ALA:HB2	2.03	0.40
1:D:52:SER:HA	1:D:64:VAL:O	2.21	0.40
1:D:76:ILE:O	1:D:80:GLU:HB2	2.21	0.40
1:D:234:MET:HG2	1:D:238:GLU:HB2	2.03	0.40
1:A:48:ARG:NE	1:B:27:ASP:HB3	2.36	0.40
1:A:125:PRO:C	1:A:127:GLU:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:GLU:H	1:C:185:GLU:HG3	1.37	0.40
1:B:97:ALA:HB2	1:B:219:VAL:HG11	2.03	0.40
1:C:165:GLY:CA	1:D:122:HIS:HD2	2.34	0.40
1:D:45:ALA:O	1:D:51:THR:HA	2.22	0.40
1:D:102:ILE:CG2	1:D:219:VAL:HG21	2.52	0.40
1:E:85:GLY:HA2	1:E:87:ARG:NH1	2.37	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	248/253 (98%)	228 (92%)	20 (8%)	0	100	100
1	B	248/253 (98%)	236 (95%)	11 (4%)	1 (0%)	34	32
1	C	248/253 (98%)	227 (92%)	17 (7%)	4 (2%)	9	4
1	D	248/253 (98%)	229 (92%)	18 (7%)	1 (0%)	34	32
1	E	248/253 (98%)	228 (92%)	18 (7%)	2 (1%)	19	14
1	F	248/253 (98%)	233 (94%)	15 (6%)	0	100	100
All	All	1488/1518 (98%)	1381 (93%)	99 (7%)	8 (0%)	29	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	MET
1	C	221	VAL
1	C	116	LEU
1	B	176	VAL
1	C	176	VAL
1	D	221	VAL

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Mol	Chain	Res	Type
1	E	229	PRO
1	E	176	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	201/203 (99%)	179 (89%)	22 (11%)	6	3
1	B	201/203 (99%)	173 (86%)	28 (14%)	3	1
1	C	201/203 (99%)	174 (87%)	27 (13%)	4	2
1	D	201/203 (99%)	174 (87%)	27 (13%)	4	2
1	E	201/203 (99%)	173 (86%)	28 (14%)	3	1
1	F	201/203 (99%)	181 (90%)	20 (10%)	7	4
All	All	1206/1218 (99%)	1054 (87%)	152 (13%)	4	2

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	6	VAL
1	A	12	THR
1	A	27	ASP
1	A	49	GLU
1	A	62	VAL
1	A	73	SER
1	A	75	SER
1	A	127	GLU
1	A	135	SER
1	A	160	ASP
1	A	172	PHE
1	A	178	ARG
1	A	184	MET
1	A	185	GLU
1	A	202	LEU

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Mol	Chain	Res	Type
1	A	227	GLU
1	A	238	GLU
1	A	247	GLU
1	A	250	ARG
1	A	251	HIS
1	A	252	LEU
1	B	12	THR
1	B	17	GLN
1	B	42	VAL
1	B	54	ARG
1	B	56	GLU
1	B	62	VAL
1	B	92	ILE
1	B	95	THR
1	B	106	ASP
1	B	145	LYS
1	B	159	SER
1	B	160	ASP
1	B	170	ASP
1	B	171	THR
1	B	175	ARG
1	B	177	VAL
1	B	183	SER
1	B	185	GLU
1	B	188	GLN
1	B	195	TYR
1	B	196	GLU
1	B	209	GLN
1	B	227	GLU
1	B	230	ASN
1	B	231	GLU
1	B	233	THR
1	B	234	MET
1	B	245	VAL
1	C	9	LEU
1	C	24	VAL
1	C	30	ARG
1	C	37	LEU
1	C	48	ARG
1	C	52	SER
1	C	57	LEU
1	C	60	LYS

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Mol	Chain	Res	Type
1	C	72	PRO
1	C	75	SER
1	C	92	ILE
1	C	117	ASP
1	C	135	SER
1	C	146	SER
1	C	160	ASP
1	C	167	GLU
1	C	168	ARG
1	C	169	TYR
1	C	172	PHE
1	C	185	GLU
1	C	226	GLN
1	C	230	ASN
1	C	231	GLU
1	C	232	GLU
1	C	233	THR
1	C	234	MET
1	C	238	GLU
1	D	9	LEU
1	D	14	ASN
1	D	17	GLN
1	D	20	THR
1	D	27	ASP
1	D	37	LEU
1	D	43	HIS
1	D	48	ARG
1	D	54	ARG
1	D	58	ASP
1	D	80	GLU
1	D	135	SER
1	D	138	THR
1	D	147	VAL
1	D	151	THR
1	D	170	ASP
1	D	172	PHE
1	D	176	VAL
1	D	177	VAL
1	D	189	SER
1	D	195	TYR
1	D	196	GLU
1	D	206	CYS

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Mol	Chain	Res	Type
1	D	208	SER
1	D	224	THR
1	D	230	ASN
1	D	240	HIS
1	E	11	LEU
1	E	12	THR
1	E	13	LYS
1	E	21	LEU
1	E	37	LEU
1	E	48	ARG
1	E	52	SER
1	E	56	GLU
1	E	73	SER
1	E	92	ILE
1	E	106	ASP
1	E	135	SER
1	E	153	ILE
1	E	158	SER
1	E	167	GLU
1	E	170	ASP
1	E	172	PHE
1	E	175	ARG
1	E	185	GLU
1	E	193	MET
1	E	196	GLU
1	E	226	GLN
1	E	233	THR
1	E	234	MET
1	E	235	LYS
1	E	237	THR
1	E	240	HIS
1	E	247	GLU
1	F	4	SER
1	F	5	ASP
1	F	11	LEU
1	F	16	LEU
1	F	24	VAL
1	F	62	VAL
1	F	138	THR
1	F	156	THR
1	F	158	SER
1	F	160	ASP

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Mol	Chain	Res	Type
1	F	170	ASP
1	F	172	PHE
1	F	181	LYS
1	F	185	GLU
1	F	196	GLU
1	F	201	THR
1	F	221	VAL
1	F	228	ILE
1	F	242	VAL
1	F	250	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	101	HIS
1	B	225	GLN
1	C	166	GLN
1	D	8	HIS
1	D	194	ASN
1	E	240	HIS
1	F	152	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	250/253 (98%)	0.17	6 (2%) 59 64	17, 31, 50, 61	0
1	B	250/253 (98%)	0.04	5 (2%) 65 69	16, 30, 44, 55	0
1	C	250/253 (98%)	0.05	4 (1%) 72 76	18, 30, 46, 53	0
1	D	250/253 (98%)	0.04	5 (2%) 65 69	16, 31, 46, 58	0
1	E	250/253 (98%)	0.19	11 (4%) 34 40	20, 32, 53, 66	0
1	F	250/253 (98%)	0.19	7 (2%) 53 59	19, 34, 50, 59	0
All	All	1500/1518 (98%)	0.11	38 (2%) 57 62	16, 32, 50, 66	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	84	LEU	5.1
1	E	169	TYR	4.4
1	B	229	PRO	4.0
1	A	4	SER	3.8
1	E	164	PRO	3.7
1	E	234	MET	3.6
1	F	224	THR	3.6
1	D	231	GLU	3.5
1	B	172	PHE	3.5
1	D	234	MET	3.4
1	E	230	ASN	3.4
1	E	232	GLU	3.0
1	E	226	GLN	3.0
1	A	13	LYS	2.9
1	E	163	TYR	2.9
1	D	233	THR	2.9
1	D	18	GLY	2.8
1	C	172	PHE	2.8
1	F	44	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	164	PRO	2.8
1	F	9	LEU	2.7
1	E	228	ILE	2.6
1	C	169	TYR	2.6
1	E	229	PRO	2.5
1	D	87	ARG	2.4
1	F	187	TRP	2.4
1	A	50	PHE	2.4
1	C	121	LEU	2.4
1	E	7	PHE	2.3
1	B	221	VAL	2.3
1	B	231	GLU	2.3
1	B	164	PRO	2.3
1	F	233	THR	2.2
1	A	234	MET	2.2
1	A	221	VAL	2.2
1	F	228	ILE	2.1
1	A	7	PHE	2.1
1	E	221	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.