



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:42 am BST

PDB ID : 2WWT  
Title : Intracellular subtilisin precursor from *B. clausii*  
Authors : Vevodova, J.; Gamble, M.; Ariza, A.; Dodson, E.; Jones, D.D.; Wilson, K.S.  
Deposited on : 2009-10-27  
Resolution : 2.68 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

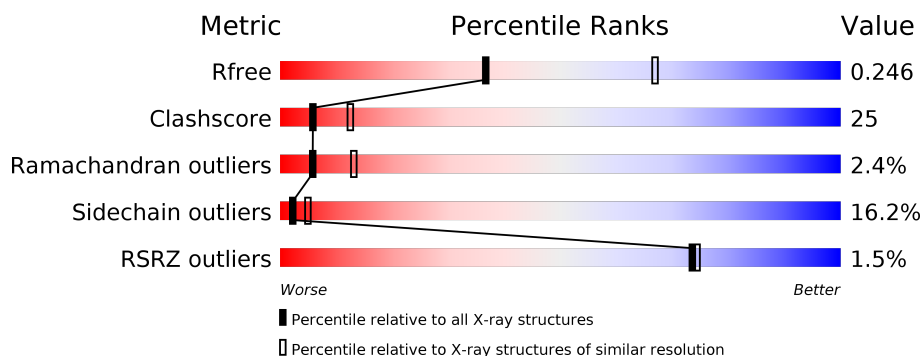
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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  $\geq 3$ , 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	329	
1	B	329	
1	C	329	
1	D	329	
1	E	329	
1	F	329	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13310 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 INTRACELLULAR SUBTILISIN PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2200	1387	373	433	7			
1	B	298	Total	C	N	O	S	0	0	0
			2194	1384	372	431	7			
1	C	300	Total	C	N	O	S	0	0	0
			2209	1392	374	436	7			
1	D	306	Total	C	N	O	S	0	0	0
			2258	1421	382	448	7			
1	E	299	Total	C	N	O	S	6	0	0
			2200	1387	373	433	7			
1	F	302	Total	C	N	O	S	0	0	0
			2224	1401	376	440	7			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	LEU	-	expression tag	UNP D0AB41
A	323	GLU	-	expression tag	UNP D0AB41
A	324	HIS	-	expression tag	UNP D0AB41
A	325	HIS	-	expression tag	UNP D0AB41
A	326	HIS	-	expression tag	UNP D0AB41
A	327	HIS	-	expression tag	UNP D0AB41
A	328	HIS	-	expression tag	UNP D0AB41
A	329	HIS	-	expression tag	UNP D0AB41
A	250	ALA	SER	engineered mutation	UNP D0AB41
B	322	LEU	-	expression tag	UNP D0AB41
B	323	GLU	-	expression tag	UNP D0AB41
B	324	HIS	-	expression tag	UNP D0AB41
B	325	HIS	-	expression tag	UNP D0AB41
B	326	HIS	-	expression tag	UNP D0AB41
B	327	HIS	-	expression tag	UNP D0AB41
B	328	HIS	-	expression tag	UNP D0AB41
B	329	HIS	-	expression tag	UNP D0AB41

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Chain	Residue	Modelled	Actual	Comment	Reference
B	250	ALA	SER	engineered mutation	UNP D0AB41
C	322	LEU	-	expression tag	UNP D0AB41
C	323	GLU	-	expression tag	UNP D0AB41
C	324	HIS	-	expression tag	UNP D0AB41
C	325	HIS	-	expression tag	UNP D0AB41
C	326	HIS	-	expression tag	UNP D0AB41
C	327	HIS	-	expression tag	UNP D0AB41
C	328	HIS	-	expression tag	UNP D0AB41
C	329	HIS	-	expression tag	UNP D0AB41
C	250	ALA	SER	engineered mutation	UNP D0AB41
D	322	LEU	-	expression tag	UNP D0AB41
D	323	GLU	-	expression tag	UNP D0AB41
D	324	HIS	-	expression tag	UNP D0AB41
D	325	HIS	-	expression tag	UNP D0AB41
D	326	HIS	-	expression tag	UNP D0AB41
D	327	HIS	-	expression tag	UNP D0AB41
D	328	HIS	-	expression tag	UNP D0AB41
D	329	HIS	-	expression tag	UNP D0AB41
D	250	ALA	SER	engineered mutation	UNP D0AB41
E	322	LEU	-	expression tag	UNP D0AB41
E	323	GLU	-	expression tag	UNP D0AB41
E	324	HIS	-	expression tag	UNP D0AB41
E	325	HIS	-	expression tag	UNP D0AB41
E	326	HIS	-	expression tag	UNP D0AB41
E	327	HIS	-	expression tag	UNP D0AB41
E	328	HIS	-	expression tag	UNP D0AB41
E	329	HIS	-	expression tag	UNP D0AB41
E	250	ALA	SER	engineered mutation	UNP D0AB41
F	322	LEU	-	expression tag	UNP D0AB41
F	323	GLU	-	expression tag	UNP D0AB41
F	324	HIS	-	expression tag	UNP D0AB41
F	325	HIS	-	expression tag	UNP D0AB41
F	326	HIS	-	expression tag	UNP D0AB41
F	327	HIS	-	expression tag	UNP D0AB41
F	328	HIS	-	expression tag	UNP D0AB41
F	329	HIS	-	expression tag	UNP D0AB41
F	250	ALA	SER	engineered mutation	UNP D0AB41

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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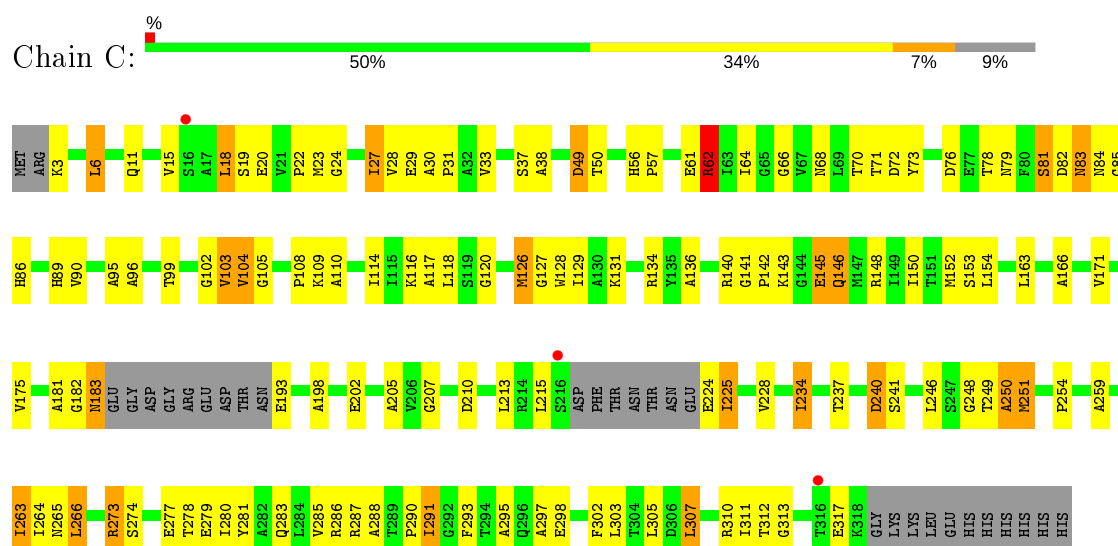
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0

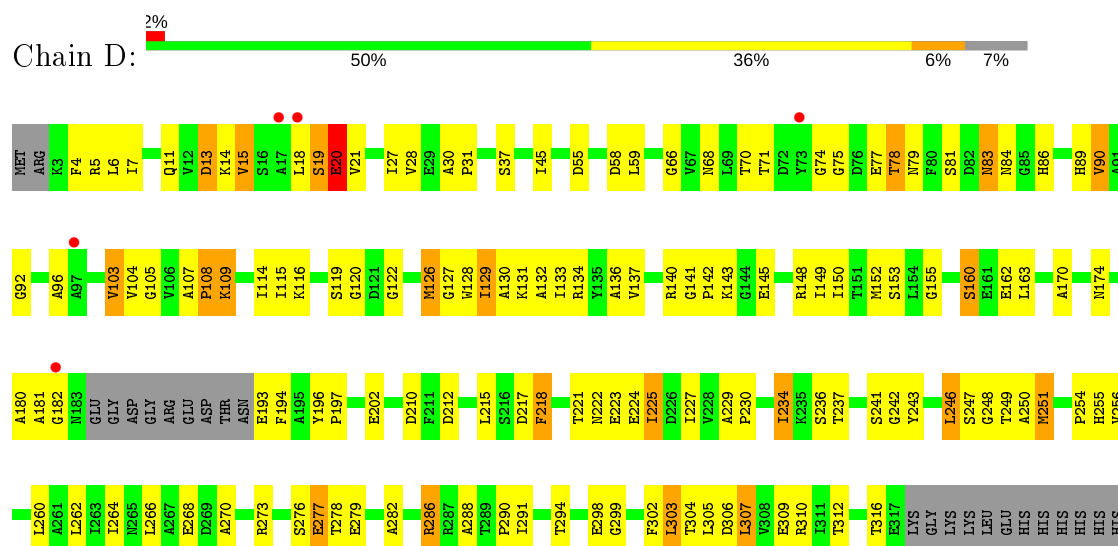
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	3	Total O 3 3	0	0
3	C	4	Total O 4 4	0	0
3	D	3	Total O 3 3	0	0
3	E	3	Total O 3 3	0	0
3	F	3	Total O 3 3	0	0

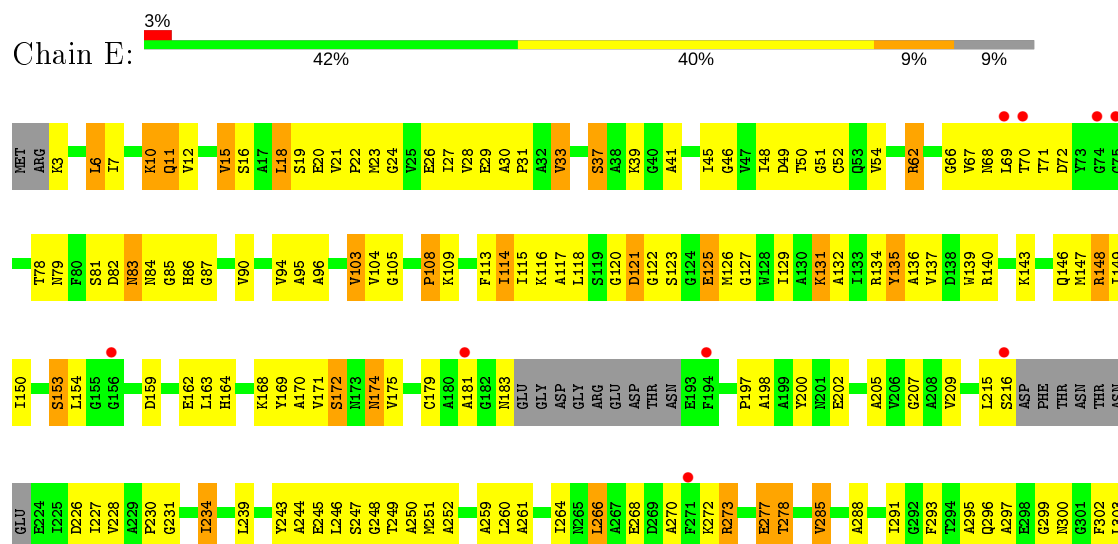


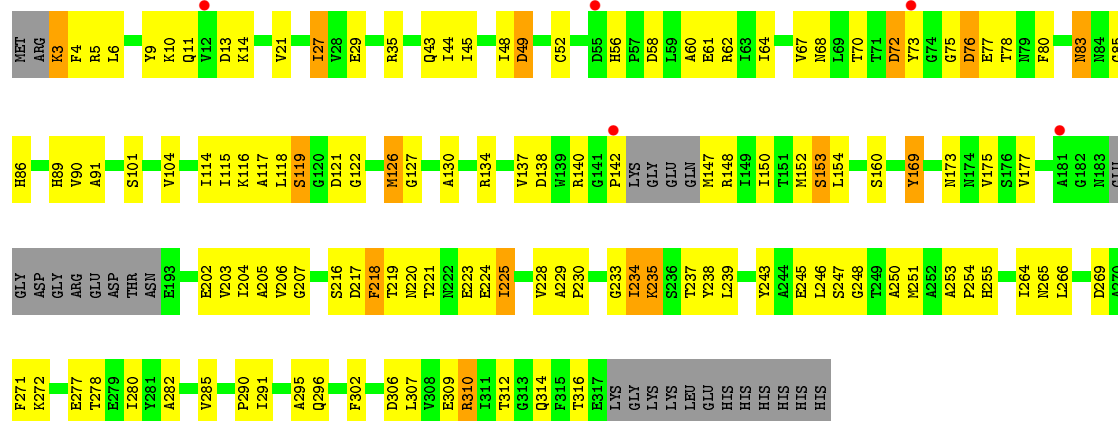


- Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE



- Molecule 1: INTRACELLULAR SUBTILISIN PROTEASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.64Å 121.64Å 106.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	105.57 – 2.68 105.34 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.8 (105.57-2.68) 99.0 (105.34-2.68)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.166 , 0.252 0.166 , 0.246	Depositor DCC
$R_{free}$ test set	2514 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 15.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.094 for -h,-k,l 0.097 for h,-h-k,-l 0.245 for -k,-h,-l	Xtriage
Reported twinning fraction	0.720 for H, K, L 0.280 for -H, H+K, -L	Depositor
Outliers	0 of 48934 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13310	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.95	2/2237 (0.1%)	0.98	5/3039 (0.2%)
1	B	0.75	0/2231	0.88	1/3031 (0.0%)
1	C	0.93	1/2246 (0.0%)	0.99	2/3051 (0.1%)
1	D	0.83	0/2297	0.90	0/3123
1	E	0.80	2/2237 (0.1%)	0.87	1/3039 (0.0%)
1	F	0.74	0/2261	0.84	0/3073
All	All	0.84	5/13509 (0.0%)	0.91	9/18356 (0.0%)

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	A	0	2
1	C	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	ARG	CB-CG	-6.47	1.35	1.52
1	A	179	CYS	CB-SG	-6.05	1.72	1.82
1	A	259	ALA	CA-CB	-5.67	1.40	1.52
1	C	193	GLU	CB-CG	5.53	1.62	1.52
1	E	309	GLU	CB-CG	5.05	1.61	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	C	266	LEU	CB-CG-CD1	-5.96	100.86	111.00
1	E	140	ARG	CA-CB-CG	5.90	126.38	113.40
1	A	196	TYR	C-N-CD	-5.85	107.72	120.60
1	A	112	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	65	GLY	N-CA-C	-5.39	99.62	113.10
1	B	303	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	13	ASP	CB-CA-C	-5.04	100.31	110.40
1	A	19	SER	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ASP	Peptide
1	A	181	ALA	Peptide
1	C	313	GLY	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	2200	0	2166	78	0
1	B	2194	0	2160	146	0
1	C	2209	0	2172	101	0
1	D	2258	0	2211	133	0
1	E	2200	0	2166	120	0
1	F	2224	0	2175	113	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	1	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	3	0	0	0	0
All	All	13310	0	13050	664	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 25.

All (664) 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:234:ILE:HD11	1:A:251:MET:CB	1.55	1.36
1:A:234:ILE:CD1	1:A:251:MET:HB3	1.55	1.34
1:F:234:ILE:HD11	1:F:251:MET:HB3	1.20	1.14
1:C:285:VAL:HG21	1:D:282:ALA:HB1	1.31	1.08
1:C:136:ALA:HB3	1:C:150:ILE:HD11	1.31	1.08
1:C:136:ALA:CB	1:C:150:ILE:HD11	1.83	1.08
1:E:234:ILE:HD11	1:E:251:MET:HB3	1.33	1.08
1:E:273:ARG:HH12	1:F:224:GLU:HB3	1.20	1.07
1:D:221:THR:HG22	1:D:222:ASN:N	1.72	1.04
1:E:66:GLY:HA3	1:E:114:ILE:O	1.58	1.03
1:F:150:ILE:HD12	1:F:175:VAL:HG11	1.42	1.01
1:E:136:ALA:CB	1:E:150:ILE:HD11	1.89	1.00
1:B:68:ASN:OD1	1:B:70:THR:HG22	1.62	0.99
1:C:278:THR:HG23	1:D:278:THR:HG23	1.41	0.99
1:E:18:LEU:HD22	1:E:20:GLU:HG2	1.45	0.98
1:B:314:GLN:HA	1:B:314:GLN:HE21	1.25	0.97
1:C:234:ILE:HD11	1:C:251:MET:HB3	1.45	0.96
1:C:70:THR:HG22	1:C:72:ASP:H	1.30	0.94
1:E:121:ASP:OD1	1:E:123:SER:OG	1.86	0.94
1:E:6:LEU:HD13	1:E:118:LEU:CD1	1.98	0.94
1:E:136:ALA:HB1	1:E:150:ILE:HD11	1.49	0.94
1:F:216:SER:O	1:F:220:ASN:HB2	1.68	0.93
1:C:22:PRO:HG3	1:C:103:VAL:HG22	1.50	0.92
1:D:234:ILE:HD11	1:D:251:MET:HG2	1.51	0.92
1:E:273:ARG:NH1	1:F:224:GLU:HB3	1.85	0.91
1:A:78:THR:HG22	1:A:78:THR:O	1.72	0.89
1:A:278:THR:HG23	1:B:278:THR:HG23	1.53	0.89
1:A:70:THR:HG23	1:A:72:ASP:H	1.36	0.89
1:E:264:ILE:O	1:E:268:GLU:HG3	1.73	0.89
1:F:234:ILE:CD1	1:F:251:MET:HB3	2.03	0.89
1:B:234:ILE:CD1	1:B:251:MET:HB3	2.04	0.87
1:B:215:LEU:HD12	1:B:215:LEU:H	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLN:HB3	1:B:56:HIS:HB2	1.57	0.87
1:D:221:THR:HG22	1:D:222:ASN:H	1.36	0.87
1:D:136:ALA:HB1	1:D:150:ILE:HD11	1.57	0.86
1:C:141:GLY:HA3	1:C:145:GLU:HG2	1.59	0.85
1:D:19:SER:O	1:D:20:GLU:HB2	1.76	0.84
1:B:6:LEU:HD21	1:B:86:HIS:ND1	1.92	0.84
1:E:69:LEU:CD1	1:E:132:ALA:HB2	2.07	0.84
1:B:234:ILE:HD13	1:B:251:MET:HB3	1.57	0.83
1:D:225:ILE:H	1:D:225:ILE:HD13	1.41	0.83
1:B:136:ALA:HB1	1:B:150:ILE:HD11	1.59	0.83
1:F:310:ARG:HG3	1:F:310:ARG:HH21	1.42	0.83
1:D:86:HIS:O	1:D:90:VAL:HG23	1.78	0.83
1:B:6:LEU:HD21	1:B:86:HIS:CE1	2.14	0.82
1:B:83:ASN:ND2	1:B:120:GLY:HA2	1.94	0.82
1:E:234:ILE:HD11	1:E:251:MET:CB	2.09	0.82
1:B:293:PHE:O	1:B:298:GLU:OE1	1.95	0.82
1:C:234:ILE:HD11	1:C:251:MET:CB	2.10	0.81
1:E:136:ALA:O	1:E:147:MET:HE3	1.81	0.81
1:E:96:ALA:HB3	1:E:105:GLY:N	1.96	0.81
1:E:70:THR:HG22	1:E:72:ASP:H	1.45	0.80
1:C:291:ILE:HG13	1:C:298:GLU:OE2	1.82	0.80
1:C:70:THR:HG22	1:C:72:ASP:N	1.97	0.80
1:C:285:VAL:CG2	1:D:282:ALA:HB1	2.11	0.80
1:F:153:SER:HB3	1:F:250:ALA:HB1	1.64	0.80
1:B:136:ALA:CB	1:B:147:MET:HE2	2.12	0.79
1:E:127:GLY:O	1:E:131:LYS:HB2	1.81	0.79
1:E:316:THR:HG22	1:E:317:GLU:H	1.46	0.79
1:F:234:ILE:HD11	1:F:251:MET:CB	2.07	0.79
1:D:221:THR:CG2	1:D:222:ASN:N	2.43	0.79
1:E:136:ALA:O	1:E:147:MET:CE	2.30	0.79
1:E:136:ALA:HB3	1:E:150:ILE:HD11	1.64	0.79
1:C:234:ILE:CD1	1:C:251:MET:HB3	2.12	0.79
1:B:136:ALA:HA	1:B:147:MET:CE	2.13	0.79
1:F:235:LYS:HD3	1:F:245:GLU:HB2	1.65	0.78
1:A:136:ALA:HB1	1:A:150:ILE:HD11	1.65	0.78
1:C:56:HIS:CD2	1:C:241:SER:HA	2.19	0.78
1:E:234:ILE:CD1	1:E:251:MET:HB3	2.13	0.78
1:D:221:THR:HG22	1:D:223:GLU:N	1.99	0.77
1:D:153:SER:HB2	1:D:250:ALA:HB1	1.65	0.77
1:B:136:ALA:HB1	1:B:147:MET:HE2	1.66	0.77
1:B:262:LEU:O	1:B:266:LEU:HG	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ALA:CB	1:E:150:ILE:CD1	2.61	0.77
1:A:312:THR:O	1:B:290:PRO:O	2.01	0.77
1:A:263:ILE:CD1	1:A:287:ARG:HD2	2.15	0.77
1:F:150:ILE:HD12	1:F:175:VAL:CG1	2.14	0.76
1:D:221:THR:HG22	1:D:223:GLU:H	1.49	0.76
1:F:225:ILE:H	1:F:225:ILE:HD13	1.48	0.76
1:A:215:LEU:HD12	1:A:215:LEU:H	1.49	0.76
1:D:221:THR:CG2	1:D:222:ASN:H	1.97	0.76
1:C:312:THR:HG23	1:D:290:PRO:HB2	1.68	0.76
1:E:168:LYS:O	1:E:172:SER:HB2	1.86	0.75
1:E:312:THR:O	1:F:290:PRO:O	2.03	0.75
1:B:169:TYR:O	1:B:173:ASN:ND2	2.20	0.75
1:D:83:ASN:H	1:D:83:ASN:HD22	1.34	0.75
1:D:74:GLY:N	1:D:75:GLY:HA2	2.00	0.75
1:E:137:VAL:HG21	1:E:170:ALA:HA	1.69	0.74
1:B:83:ASN:HD21	1:B:120:GLY:HA2	1.52	0.74
1:D:68:ASN:OD1	1:D:70:THR:OG1	2.04	0.74
1:B:136:ALA:CA	1:B:147:MET:HE2	2.18	0.73
1:E:137:VAL:HG22	1:E:175:VAL:HG21	1.70	0.73
1:F:90:VAL:HG13	1:F:254:PRO:HG3	1.71	0.73
1:C:22:PRO:CG	1:C:103:VAL:HG22	2.19	0.72
1:B:67:VAL:HG13	1:B:69:LEU:HD13	1.71	0.72
1:B:168:LYS:O	1:B:172:SER:HB2	1.89	0.72
1:C:143:LYS:N	1:C:145:GLU:OE2	2.22	0.71
1:C:62:ARG:NH1	1:C:110:ALA:O	2.23	0.71
1:B:43:GLN:HE22	1:B:148:ARG:HG3	1.56	0.71
1:E:69:LEU:HD13	1:E:132:ALA:HB2	1.70	0.71
1:C:90:VAL:HG13	1:C:254:PRO:HG3	1.72	0.71
1:F:154:LEU:HD12	1:F:154:LEU:O	1.90	0.71
1:B:314:GLN:HA	1:B:314:GLN:NE2	2.01	0.70
1:F:235:LYS:CD	1:F:245:GLU:HB2	2.19	0.70
1:A:39:LYS:HB2	1:A:109:LYS:HB2	1.73	0.70
1:D:248:GLY:N	1:D:251:MET:HE2	2.07	0.70
1:B:3:LYS:HD3	1:B:123:SER:HB2	1.72	0.70
1:D:71:THR:HG23	1:D:128:TRP:HZ2	1.56	0.70
1:D:225:ILE:H	1:D:225:ILE:CD1	2.04	0.70
1:F:29:GLU:OE1	1:F:306:ASP:OD1	2.10	0.69
1:B:48:ILE:HD12	1:B:150:ILE:HG23	1.74	0.69
1:E:33:VAL:O	1:E:37:SER:OG	2.09	0.69
1:C:264:ILE:HG12	1:C:280:ILE:HD12	1.73	0.69
1:C:62:ARG:HA	1:C:62:ARG:NH1	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ALA:O	1:D:286:ARG:HB3	1.93	0.69
1:F:83:ASN:HD22	1:F:83:ASN:H	1.39	0.69
1:B:28:VAL:HG22	1:B:303:LEU:HG	1.74	0.69
1:D:148:ARG:HD2	1:D:174:ASN:O	1.92	0.69
1:C:290:PRO:O	1:D:312:THR:O	2.11	0.69
1:D:141:GLY:HA3	1:D:145:GLU:HG2	1.75	0.69
1:F:126:MET:HG3	1:F:127:GLY:N	2.06	0.69
1:B:59:LEU:HD21	1:B:237:THR:HG21	1.75	0.69
1:D:234:ILE:HD12	1:D:251:MET:HB3	1.74	0.69
1:B:269:ASP:O	1:B:272:LYS:HE3	1.93	0.68
1:C:84:ASN:HB2	1:C:120:GLY:O	1.94	0.68
1:C:273:ARG:HG2	1:C:274:SER:O	1.94	0.68
1:C:24:GLY:O	1:C:28:VAL:HB	1.94	0.68
1:B:83:ASN:HD22	1:B:83:ASN:C	1.97	0.68
1:B:161:GLU:OE1	1:B:161:GLU:HA	1.94	0.68
1:B:136:ALA:HA	1:B:147:MET:HE2	1.73	0.67
1:F:44:ILE:CG2	1:F:64:ILE:HD11	2.24	0.67
1:E:29:GLU:OE2	1:E:310:ARG:NH2	2.27	0.67
1:E:62:ARG:HG3	1:E:95:ALA:O	1.94	0.67
1:B:215:LEU:HD12	1:B:215:LEU:N	2.10	0.66
1:B:83:ASN:HD21	1:B:120:GLY:CA	2.08	0.66
1:F:21:VAL:HG13	1:F:104:VAL:CG1	2.26	0.66
1:B:83:ASN:ND2	1:B:120:GLY:CA	2.57	0.66
1:D:21:VAL:HG22	1:D:104:VAL:HG11	1.77	0.66
1:F:169:TYR:HE1	1:F:173:ASN:HD21	1.44	0.66
1:B:215:LEU:HD11	1:B:293:PHE:CZ	2.31	0.66
1:A:90:VAL:HG13	1:A:254:PRO:HG3	1.78	0.65
1:B:89:HIS:HA	1:B:237:THR:O	1.96	0.65
1:E:23:MET:O	1:E:27:ILE:HB	1.95	0.65
1:B:6:LEU:CD1	1:B:9:TYR:HE2	2.10	0.65
1:C:234:ILE:HG12	1:C:246:LEU:O	1.96	0.65
1:D:148:ARG:HG3	1:D:148:ARG:HH11	1.62	0.65
1:F:309:GLU:HA	1:F:309:GLU:OE1	1.97	0.64
1:A:78:THR:O	1:A:78:THR:CG2	2.43	0.64
1:A:70:THR:HG23	1:A:71:THR:N	2.12	0.64
1:B:3:LYS:CD	1:B:123:SER:HB2	2.27	0.64
1:C:207:GLY:O	1:C:228:VAL:HA	1.98	0.64
1:A:20:GLU:O	1:A:22:PRO:HD3	1.97	0.64
1:E:10:LYS:HG3	1:E:11:GLN:N	2.12	0.64
1:A:29:GLU:OE2	1:A:310:ARG:NH2	2.30	0.64
1:D:234:ILE:CD1	1:D:251:MET:HG2	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:VAL:HB	1:B:245:GLU:HG2	1.79	0.63
1:C:153:SER:HB3	1:C:250:ALA:HB1	1.80	0.63
1:E:136:ALA:HB3	1:E:150:ILE:CD1	2.25	0.63
1:F:225:ILE:CD1	1:F:225:ILE:H	2.11	0.63
1:C:288:ALA:HA	1:C:302:PHE:O	1.98	0.63
1:B:62:ARG:HD2	1:B:97:ALA:HB2	1.80	0.63
1:C:136:ALA:HB3	1:C:150:ILE:CD1	2.20	0.63
1:F:217:ASP:O	1:F:218:PHE:HB3	1.97	0.63
1:F:49:ASP:OD1	1:F:86:HIS:ND1	2.29	0.63
1:C:62:ARG:HA	1:C:62:ARG:CZ	2.28	0.63
1:D:6:LEU:HD13	1:D:122:GLY:O	1.98	0.63
1:D:86:HIS:O	1:D:90:VAL:CG2	2.46	0.63
1:D:92:GLY:HA3	1:D:236:SER:OG	1.98	0.63
1:A:234:ILE:HD11	1:A:251:MET:HB3	0.72	0.63
1:B:136:ALA:HA	1:B:147:MET:HE1	1.79	0.62
1:B:38:ALA:C	1:B:40:GLY:H	2.01	0.62
1:D:221:THR:HG21	1:D:223:GLU:HB2	1.80	0.62
1:E:28:VAL:HG13	1:E:303:LEU:HG	1.80	0.62
1:E:316:THR:HG22	1:E:317:GLU:N	2.12	0.62
1:C:136:ALA:HB1	1:C:150:ILE:HD11	1.79	0.62
1:A:240:ASP:O	1:A:241:SER:HB2	1.99	0.62
1:F:310:ARG:CG	1:F:310:ARG:HH21	2.10	0.62
1:E:96:ALA:HB3	1:E:105:GLY:H	1.64	0.62
1:B:234:ILE:HD11	1:B:251:MET:HB3	1.81	0.62
1:D:180:ALA:CB	1:D:250:ALA:HA	2.29	0.62
1:B:7:ILE:HG22	1:B:8:PRO:CD	2.29	0.62
1:D:268:GLU:HG2	1:D:273:ARG:O	2.00	0.62
1:D:89:HIS:HA	1:D:237:THR:O	2.00	0.62
1:C:30:ALA:HB3	1:C:31:PRO:HD3	1.82	0.61
1:D:15:VAL:HB	1:D:18:LEU:HD11	1.82	0.61
1:B:158:THR:O	1:B:158:THR:HG22	2.01	0.61
1:B:314:GLN:HE21	1:B:314:GLN:CA	1.99	0.61
1:E:6:LEU:HD13	1:E:118:LEU:HD12	1.80	0.61
1:A:263:ILE:HD12	1:A:287:ARG:HD2	1.83	0.60
1:B:167:VAL:HG21	1:B:200:TYR:CD2	2.35	0.60
1:F:44:ILE:HG21	1:F:64:ILE:HD11	1.81	0.60
1:B:70:THR:HG23	1:B:72:ASP:H	1.65	0.60
1:D:89:HIS:CE1	1:D:246:LEU:HG	2.37	0.60
1:B:205:ALA:N	1:B:226:ASP:OD1	2.25	0.60
1:E:227:ILE:HD12	1:E:288:ALA:HB2	1.82	0.60
1:F:169:TYR:CE1	1:F:173:ASN:ND2	2.70	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ARG:HG3	1:D:148:ARG:NH1	2.16	0.60
1:B:248:GLY:N	1:B:251:MET:CE	2.65	0.59
1:A:133:ILE:O	1:A:137:VAL:HG23	2.02	0.59
1:A:234:ILE:HD11	1:A:251:MET:CG	2.28	0.59
1:F:3:LYS:NZ	1:F:3:LYS:HB3	2.17	0.59
1:E:84:ASN:ND2	1:E:120:GLY:O	2.35	0.59
1:E:67:VAL:HG22	1:E:68:ASN:N	2.18	0.59
1:E:164:HIS:CD2	1:E:200:TYR:CD1	2.90	0.59
1:B:6:LEU:HD11	1:B:9:TYR:HE2	1.67	0.59
1:D:304:THR:O	1:D:306:ASP:N	2.36	0.59
1:A:203:VAL:HG12	1:A:204:ILE:N	2.18	0.59
1:D:136:ALA:HB1	1:D:150:ILE:CD1	2.30	0.59
1:B:142:PRO:HD2	1:B:145:GLU:OE1	2.03	0.59
1:A:203:VAL:CG1	1:A:204:ILE:N	2.66	0.58
1:A:260:LEU:HD21	1:A:284:LEU:HD22	1.85	0.58
1:E:295:ALA:O	1:E:299:GLY:N	2.36	0.58
1:B:25:VAL:O	1:B:28:VAL:HG12	2.03	0.58
1:D:223:GLU:HG3	1:D:224:GLU:N	2.18	0.58
1:D:248:GLY:N	1:D:251:MET:CE	2.66	0.58
1:A:291:ILE:HD11	1:A:302:PHE:HB2	1.85	0.58
1:D:83:ASN:N	1:D:83:ASN:HD22	1.99	0.58
1:E:66:GLY:HA2	1:E:113:PHE:CE2	2.39	0.58
1:A:70:THR:CG2	1:A:72:ASP:H	2.11	0.58
1:A:126:MET:HE1	1:A:162:GLU:HB3	1.86	0.57
1:A:248:GLY:N	1:A:251:MET:CE	2.66	0.57
1:F:235:LYS:HD3	1:F:245:GLU:CB	2.34	0.57
1:A:247:SER:C	1:A:251:MET:CE	2.73	0.57
1:E:139:TRP:O	1:E:146:GLN:NE2	2.37	0.57
1:C:281:TYR:O	1:C:285:VAL:HG13	2.04	0.57
1:C:83:ASN:H	1:C:83:ASN:ND2	2.02	0.57
1:D:7:ILE:HD13	1:D:182:GLY:HA2	1.86	0.57
1:D:174:ASN:HA	1:D:277:GLU:HB3	1.87	0.57
1:B:18:LEU:O	1:B:102:GLY:HA2	2.03	0.57
1:D:13:ASP:OD2	1:D:15:VAL:HG22	2.03	0.57
1:C:213:LEU:HB3	1:C:291:ILE:HD13	1.85	0.57
1:E:30:ALA:HB3	1:E:31:PRO:HD3	1.86	0.57
1:E:312:THR:HA	1:F:290:PRO:HB2	1.87	0.57
1:D:291:ILE:O	1:D:291:ILE:HG22	2.05	0.56
1:E:69:LEU:HD12	1:E:117:ALA:HB2	1.87	0.56
1:B:107:ALA:O	1:B:109:LYS:N	2.38	0.56
1:E:24:GLY:HA2	1:E:27:ILE:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:PHE:CD1	1:B:4:PHE:N	2.71	0.56
1:B:70:THR:HG23	1:B:72:ASP:HB2	1.86	0.56
1:F:248:GLY:N	1:F:251:MET:HE2	2.19	0.56
1:B:167:VAL:HG12	1:B:202:GLU:HG3	1.87	0.56
1:E:86:HIS:CE1	1:E:90:VAL:CG2	2.88	0.56
1:E:136:ALA:HB1	1:E:150:ILE:CD1	2.30	0.56
1:B:28:VAL:CG2	1:B:303:LEU:HG	2.35	0.56
1:E:247:SER:C	1:E:251:MET:CE	2.74	0.56
1:E:104:VAL:O	1:E:104:VAL:HG13	2.04	0.56
1:D:217:ASP:O	1:D:218:PHE:HB3	2.06	0.56
1:B:260:LEU:HA	1:B:263:ILE:HD12	1.88	0.55
1:C:307:LEU:HD22	1:C:311:ILE:CG2	2.36	0.55
1:C:68:ASN:OD1	1:C:70:THR:HB	2.06	0.55
1:B:39:LYS:HB3	1:B:108:PRO:HG2	1.89	0.55
1:F:233:GLY:N	1:F:247:SER:OG	2.34	0.55
1:F:203:VAL:HG12	1:F:204:ILE:N	2.21	0.55
1:B:248:GLY:CA	1:B:251:MET:HE2	2.36	0.55
1:B:266:LEU:HD12	1:B:267:ALA:N	2.21	0.55
1:E:94:VAL:HG12	1:E:95:ALA:HB2	1.89	0.55
1:B:38:ALA:C	1:B:40:GLY:N	2.58	0.55
1:F:119:SER:HB2	1:F:121:ASP:OD2	2.07	0.55
1:F:225:ILE:HD13	1:F:225:ILE:N	2.20	0.54
1:A:59:LEU:O	1:A:60:ALA:C	2.45	0.54
1:E:67:VAL:CG2	1:E:68:ASN:N	2.69	0.54
1:A:74:GLY:N	1:A:75:GLY:HA2	2.23	0.54
1:D:45:ILE:HD12	1:D:45:ILE:N	2.22	0.54
1:F:45:ILE:HD12	1:F:45:ILE:N	2.22	0.54
1:B:62:ARG:CZ	1:B:62:ARG:HA	2.37	0.54
1:E:41:ALA:HB2	1:E:109:LYS:HB3	1.90	0.54
1:D:141:GLY:O	1:D:143:LYS:N	2.41	0.54
1:E:6:LEU:HD13	1:E:118:LEU:HD13	1.89	0.54
1:B:70:THR:HG21	1:B:116:LYS:HE2	1.90	0.54
1:C:6:LEU:HD13	1:C:118:LEU:CD1	2.37	0.54
1:C:279:GLU:O	1:C:283:GLN:HG2	2.07	0.54
1:D:77:GLU:C	1:D:78:THR:O	2.46	0.54
1:B:107:ALA:C	1:B:109:LYS:H	2.09	0.54
1:D:71:THR:HG23	1:D:128:TRP:CZ2	2.42	0.54
1:E:68:ASN:HB2	1:E:79:ASN:O	2.08	0.54
1:C:49:ASP:OD1	1:C:50:THR:HG23	2.07	0.53
1:D:107:ALA:O	1:D:109:LYS:N	2.40	0.53
1:C:18:LEU:HD21	1:C:20:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ARG:CZ	1:B:308:VAL:HG21	2.38	0.53
1:D:160:SER:HB3	1:D:163:LEU:H	1.73	0.53
1:D:83:ASN:H	1:D:83:ASN:ND2	2.06	0.53
1:E:171:VAL:HG22	1:E:277:GLU:CD	2.29	0.53
1:F:169:TYR:CD1	1:F:173:ASN:ND2	2.77	0.53
1:F:221:THR:OG1	1:F:223:GLU:HB3	2.08	0.53
1:B:136:ALA:CB	1:B:150:ILE:HD11	2.34	0.53
1:D:217:ASP:O	1:D:218:PHE:CB	2.56	0.53
1:D:221:THR:CG2	1:D:223:GLU:H	2.20	0.53
1:D:247:SER:C	1:D:251:MET:HE1	2.29	0.53
1:E:115:ILE:HG21	1:E:132:ALA:HB1	1.90	0.53
1:C:224:GLU:HA	1:D:273:ARG:NH2	2.24	0.53
1:C:183:ASN:OD1	1:C:183:ASN:C	2.47	0.53
1:A:70:THR:CG2	1:A:71:THR:N	2.71	0.53
1:D:264:ILE:O	1:D:268:GLU:HB2	2.08	0.53
1:D:210:ASP:OD1	1:D:210:ASP:C	2.48	0.52
1:B:70:THR:CG2	1:B:72:ASP:HB2	2.39	0.52
1:B:67:VAL:CG1	1:B:69:LEU:HD13	2.39	0.52
1:F:67:VAL:O	1:F:67:VAL:HG13	2.10	0.52
1:A:291:ILE:O	1:A:291:ILE:HG22	2.10	0.52
1:B:130:ALA:O	1:B:134:ARG:HG3	2.10	0.52
1:C:90:VAL:HG13	1:C:254:PRO:CG	2.40	0.52
1:B:215:LEU:HD11	1:B:293:PHE:CE2	2.45	0.52
1:F:76:ASP:OD1	1:F:76:ASP:C	2.48	0.52
1:B:52:CYS:O	1:B:81:SER:HA	2.09	0.52
1:D:148:ARG:CG	1:D:148:ARG:HH11	2.22	0.52
1:F:83:ASN:ND2	1:F:83:ASN:H	2.07	0.52
1:E:285:VAL:HG21	1:F:282:ALA:HB1	1.90	0.52
1:A:28:VAL:O	1:A:29:GLU:HB2	2.09	0.52
1:F:306:ASP:N	1:F:306:ASP:OD1	2.36	0.52
1:E:247:SER:C	1:E:251:MET:HE3	2.31	0.51
1:E:291:ILE:HD11	1:E:302:PHE:HB2	1.92	0.51
1:B:55:ASP:HA	1:B:60:ALA:HB2	1.92	0.51
1:B:6:LEU:HD11	1:B:9:TYR:CE2	2.44	0.51
1:C:83:ASN:H	1:C:83:ASN:HD22	1.59	0.51
1:C:96:ALA:H	1:C:105:GLY:HA3	1.74	0.51
1:E:67:VAL:CG2	1:E:68:ASN:H	2.24	0.51
1:F:85:GLY:HA3	1:F:238:TYR:CE1	2.45	0.51
1:B:4:PHE:HD1	1:B:4:PHE:N	2.08	0.51
1:D:21:VAL:HA	1:D:104:VAL:HG12	1.91	0.51
1:D:180:ALA:HB2	1:D:250:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ALA:HB3	1:D:270:ALA:C	2.31	0.51
1:B:153:SER:HB3	1:B:250:ALA:HB1	1.93	0.51
1:B:248:GLY:N	1:B:251:MET:HE2	2.26	0.51
1:F:44:ILE:HG23	1:F:64:ILE:HD11	1.92	0.51
1:D:66:GLY:HA2	1:D:114:ILE:O	2.10	0.51
1:A:236:SER:OG	1:A:237:THR:N	2.43	0.51
1:B:31:PRO:O	1:B:33:VAL:N	2.44	0.51
1:F:73:TYR:C	1:F:75:GLY:HA2	2.31	0.51
1:D:260:LEU:O	1:D:264:ILE:HG13	2.11	0.51
1:A:28:VAL:HG22	1:A:303:LEU:O	2.11	0.50
1:B:171:VAL:HG21	1:B:202:GLU:HB2	1.94	0.50
1:C:126:MET:HG3	1:C:127:GLY:N	2.26	0.50
1:C:22:PRO:HG3	1:C:103:VAL:CG2	2.31	0.50
1:F:235:LYS:HD3	1:F:245:GLU:OE1	2.11	0.50
1:D:120:GLY:C	1:D:122:GLY:H	2.14	0.50
1:E:296:GLN:HB3	1:F:271:PHE:O	2.11	0.50
1:A:8:PRO:HD3	1:A:194:PHE:CZ	2.46	0.50
1:A:308:VAL:HG13	1:B:290:PRO:HG2	1.94	0.50
1:D:181:ALA:HB2	1:D:225:ILE:HG22	1.94	0.50
1:E:70:THR:CG2	1:E:71:THR:N	2.74	0.50
1:B:38:ALA:O	1:B:40:GLY:N	2.45	0.50
1:C:140:ARG:CZ	1:C:146:GLN:HE21	2.25	0.50
1:E:18:LEU:CD2	1:E:20:GLU:HG2	2.32	0.50
1:E:7:ILE:HD13	1:E:181:ALA:O	2.11	0.50
1:A:267:ALA:O	1:A:271:PHE:HD1	1.95	0.50
1:C:136:ALA:CB	1:C:150:ILE:CD1	2.75	0.50
1:C:28:VAL:HG13	1:C:303:LEU:HD23	1.92	0.50
1:E:29:GLU:OE1	1:E:304:THR:HB	2.12	0.50
1:B:225:ILE:HD13	1:B:225:ILE:H	1.77	0.50
1:E:66:GLY:CA	1:E:114:ILE:O	2.45	0.50
1:E:296:GLN:HG3	1:E:297:ALA:N	2.27	0.50
1:E:82:ASP:CG	1:E:85:GLY:H	2.15	0.50
1:F:216:SER:HB3	1:F:219:THR:OG1	2.12	0.50
1:B:46:GLY:HA3	1:B:147:MET:HE3	1.94	0.49
1:B:247:SER:C	1:B:251:MET:CE	2.80	0.49
1:A:278:THR:HG23	1:B:278:THR:CG2	2.36	0.49
1:C:24:GLY:HA2	1:C:27:ILE:HG22	1.93	0.49
1:C:37:SER:O	1:C:265:ASN:ND2	2.45	0.49
1:C:89:HIS:HA	1:C:237:THR:O	2.12	0.49
1:A:11:GLN:HE22	1:A:14:LYS:HG3	1.77	0.49
1:E:154:LEU:HD12	1:E:154:LEU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:THR:CG2	1:E:317:GLU:H	2.21	0.49
1:B:28:VAL:HG21	1:B:303:LEU:HD23	1.94	0.49
1:C:82:ASP:OD2	1:C:85:GLY:N	2.44	0.49
1:D:90:VAL:HG12	1:D:254:PRO:HB3	1.95	0.49
1:C:240:ASP:O	1:C:241:SER:HB2	2.12	0.49
1:C:66:GLY:CA	1:C:114:ILE:O	2.60	0.49
1:E:48:ILE:CD1	1:E:150:ILE:CG2	2.91	0.49
1:F:310:ARG:NH2	1:F:310:ARG:CG	2.74	0.49
1:E:234:ILE:O	1:E:245:GLU:HA	2.13	0.49
1:F:247:SER:C	1:F:251:MET:HE3	2.33	0.49
1:A:39:LYS:HB3	1:A:108:PRO:HD2	1.94	0.49
1:B:104:VAL:HG23	1:B:108:PRO:HB3	1.95	0.49
1:B:163:LEU:O	1:B:167:VAL:HG23	2.11	0.49
1:C:117:ALA:O	1:C:128:TRP:HE3	1.95	0.49
1:F:235:LYS:HD3	1:F:245:GLU:CG	2.43	0.49
1:A:59:LEU:O	1:A:61:GLU:N	2.46	0.49
1:C:248:GLY:HA3	1:C:251:MET:HE1	1.94	0.49
1:D:78:THR:HG22	1:D:79:ASN:H	1.78	0.49
1:D:294:THR:O	1:D:298:GLU:HG2	2.13	0.48
1:F:225:ILE:CD1	1:F:225:ILE:N	2.75	0.48
1:B:116:LYS:HE3	1:B:118:LEU:O	2.12	0.48
1:B:74:GLY:HA3	1:B:76:ASP:H	1.78	0.48
1:F:177:VAL:HG12	1:F:203:VAL:HG13	1.93	0.48
1:F:217:ASP:O	1:F:218:PHE:CB	2.60	0.48
1:F:237:THR:HG22	1:F:243:TYR:CE1	2.48	0.48
1:A:68:ASN:OD1	1:A:70:THR:HB	2.13	0.48
1:B:247:SER:C	1:B:251:MET:HE1	2.33	0.48
1:E:231:GLY:O	1:E:248:GLY:N	2.42	0.48
1:E:86:HIS:CE1	1:E:90:VAL:HG21	2.49	0.48
1:F:237:THR:HG22	1:F:243:TYR:HE1	1.79	0.48
1:B:53:GLN:O	1:B:55:ASP:N	2.47	0.48
1:C:154:LEU:HD12	1:C:154:LEU:C	2.34	0.48
1:D:143:LYS:HB3	1:D:145:GLU:OE2	2.13	0.48
1:A:238:TYR:O	1:A:239:LEU:O	2.31	0.48
1:C:141:GLY:HA3	1:C:145:GLU:CG	2.37	0.48
1:F:89:HIS:HE1	1:F:234:ILE:O	1.96	0.48
1:B:167:VAL:HG21	1:B:200:TYR:HD2	1.77	0.48
1:B:88:THR:O	1:B:237:THR:OG1	2.32	0.48
1:D:129:ILE:O	1:D:130:ALA:C	2.52	0.48
1:E:137:VAL:O	1:E:146:GLN:NE2	2.47	0.48
1:A:83:ASN:H	1:A:83:ASN:ND2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:SER:O	1:B:275:LEU:HD23	2.14	0.48
1:B:291:ILE:HG13	1:B:298:GLU:OE2	2.13	0.48
1:C:248:GLY:CA	1:C:251:MET:HE1	2.43	0.48
1:D:247:SER:C	1:D:251:MET:CE	2.82	0.48
1:D:90:VAL:HG13	1:D:254:PRO:HG3	1.95	0.48
1:E:39:LYS:HB3	1:E:108:PRO:HG2	1.96	0.48
1:E:86:HIS:CE1	1:E:90:VAL:HG23	2.48	0.48
1:C:259:ALA:HB1	1:C:305:LEU:HD21	1.95	0.48
1:E:66:GLY:HA2	1:E:113:PHE:CZ	2.49	0.48
1:E:209:VAL:HG21	1:E:302:PHE:CE1	2.49	0.48
1:F:234:ILE:HD12	1:F:255:HIS:HE1	1.79	0.48
1:B:229:ALA:HB1	1:B:230:PRO:CD	2.44	0.47
1:A:296:GLN:OE1	1:B:272:LYS:HG3	2.14	0.47
1:B:45:ILE:N	1:B:45:ILE:HD12	2.28	0.47
1:D:242:GLY:C	1:D:243:TYR:CD2	2.87	0.47
1:A:133:ILE:CG2	1:A:166:ALA:HB1	2.44	0.47
1:A:210:ASP:OD1	1:A:210:ASP:C	2.50	0.47
1:B:83:ASN:CG	1:B:116:LYS:HZ3	2.17	0.47
1:D:223:GLU:CG	1:D:224:GLU:N	2.77	0.47
1:E:179:CYS:O	1:E:205:ALA:HA	2.14	0.47
1:E:52:CYS:HB2	1:E:114:ILE:HD12	1.96	0.47
1:B:281:TYR:O	1:B:285:VAL:HG13	2.13	0.47
1:C:6:LEU:HD13	1:C:118:LEU:HD13	1.96	0.47
1:A:37:SER:OG	1:A:266:LEU:HD23	2.15	0.47
1:C:251:MET:N	1:C:251:MET:HE2	2.29	0.47
1:D:249:THR:C	1:D:251:MET:H	2.17	0.47
1:C:83:ASN:HD22	1:C:83:ASN:N	2.12	0.47
1:D:303:LEU:HD12	1:D:304:THR:N	2.29	0.47
1:F:117:ALA:O	1:F:118:LEU:HG	2.14	0.47
1:E:278:THR:HG23	1:F:278:THR:OG1	2.14	0.47
1:D:15:VAL:CB	1:D:18:LEU:HD11	2.44	0.47
1:C:79:ASN:OD1	1:C:81:SER:OG	2.30	0.47
1:D:66:GLY:CA	1:D:114:ILE:O	2.63	0.47
1:A:121:ASP:OD1	1:A:123:SER:OG	2.22	0.47
1:B:48:ILE:CD1	1:B:150:ILE:HG23	2.44	0.47
1:C:116:LYS:NZ	1:C:118:LEU:O	2.48	0.47
1:D:58:ASP:O	1:D:59:LEU:HD23	2.14	0.47
1:E:307:LEU:HD22	1:E:311:ILE:HG23	1.97	0.47
1:A:253:ALA:HB3	1:A:254:PRO:HD3	1.96	0.47
1:C:307:LEU:HD22	1:C:311:ILE:HG23	1.97	0.47
1:B:215:LEU:CD1	1:B:215:LEU:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:PHE:CE1	1:D:126:MET:HB3	2.50	0.47
1:D:180:ALA:HB1	1:D:250:ALA:HA	1.97	0.47
1:B:131:LYS:O	1:B:135:TYR:HB2	2.15	0.46
1:D:83:ASN:HD21	1:D:116:LYS:HZ1	1.62	0.46
1:B:143:LYS:N	1:B:145:GLU:OE2	2.47	0.46
1:D:130:ALA:CB	1:D:162:GLU:HG2	2.46	0.46
1:B:309:GLU:OE1	1:B:309:GLU:N	2.48	0.46
1:D:7:ILE:HB	1:D:250:ALA:HB2	1.96	0.46
1:C:18:LEU:CD2	1:C:20:GLU:OE2	2.64	0.46
1:C:62:ARG:HG3	1:C:95:ALA:O	2.16	0.46
1:D:141:GLY:HA3	1:D:145:GLU:CG	2.44	0.46
1:C:104:VAL:HG23	1:C:108:PRO:HG3	1.97	0.46
1:D:223:GLU:HG3	1:D:224:GLU:H	1.79	0.46
1:F:314:GLN:HA	1:F:314:GLN:HE21	1.81	0.46
1:B:83:ASN:OD1	1:B:116:LYS:NZ	2.40	0.46
1:C:86:HIS:CE1	1:C:90:VAL:HG21	2.51	0.46
1:D:127:GLY:O	1:D:128:TRP:C	2.53	0.46
1:D:210:ASP:OD1	1:D:212:ASP:N	2.45	0.46
1:D:288:ALA:HA	1:D:302:PHE:O	2.15	0.46
1:E:46:GLY:HA2	1:E:113:PHE:O	2.16	0.46
1:E:28:VAL:CG1	1:E:28:VAL:O	2.64	0.46
1:F:247:SER:C	1:F:251:MET:CE	2.83	0.46
1:D:229:ALA:HB1	1:D:230:PRO:HD2	1.97	0.46
1:D:256:VAL:O	1:D:260:LEU:HG	2.15	0.46
1:B:230:PRO:O	1:B:252:ALA:HA	2.16	0.46
1:E:153:SER:OG	1:E:250:ALA:HB1	2.16	0.46
1:E:48:ILE:HD11	1:E:150:ILE:HG21	1.98	0.46
1:F:85:GLY:O	1:F:86:HIS:C	2.53	0.46
1:D:103:VAL:HG11	1:D:237:THR:HG23	1.97	0.46
1:A:248:GLY:N	1:A:251:MET:HE2	2.31	0.45
1:C:251:MET:HB2	1:C:251:MET:HE3	1.70	0.45
1:D:262:LEU:HD12	1:D:305:LEU:HD13	1.98	0.45
1:D:304:THR:C	1:D:306:ASP:H	2.19	0.45
1:C:311:ILE:HD12	1:D:307:LEU:HD11	1.98	0.45
1:E:15:VAL:HG23	1:E:243:TYR:HB2	1.97	0.45
1:F:235:LYS:HD2	1:F:245:GLU:HB2	1.98	0.45
1:A:90:VAL:O	1:A:94:VAL:HG23	2.16	0.45
1:B:279:GLU:O	1:B:282:ALA:HB3	2.17	0.45
1:C:210:ASP:OD1	1:C:210:ASP:C	2.54	0.45
1:D:230:PRO:HG2	1:D:255:HIS:CE1	2.51	0.45
1:E:48:ILE:CD1	1:E:150:ILE:HG21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:ASN:O	1:F:269:ASP:HB2	2.16	0.45
1:B:52:CYS:CA	1:B:82:ASP:HB2	2.47	0.45
1:C:37:SER:O	1:C:38:ALA:C	2.55	0.45
1:D:30:ALA:N	1:D:31:PRO:CD	2.80	0.45
1:B:62:ARG:HA	1:B:62:ARG:NH1	2.32	0.45
1:E:230:PRO:O	1:E:252:ALA:HA	2.17	0.45
1:B:167:VAL:CG1	1:B:202:GLU:HG3	2.47	0.45
1:E:28:VAL:CG1	1:E:303:LEU:HG	2.46	0.45
1:F:203:VAL:CG1	1:F:204:ILE:N	2.80	0.45
1:F:70:THR:HB	1:F:72:ASP:H	1.81	0.45
1:F:89:HIS:HA	1:F:237:THR:O	2.17	0.45
1:A:210:ASP:OD1	1:A:212:ASP:N	2.50	0.45
1:B:55:ASP:O	1:B:56:HIS:C	2.55	0.45
1:C:83:ASN:ND2	1:C:83:ASN:N	2.63	0.45
1:D:276:SER:OG	1:D:279:GLU:HG3	2.17	0.45
1:E:120:GLY:C	1:E:122:GLY:H	2.20	0.45
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.75	0.44
1:B:163:LEU:HD21	1:B:197:PRO:HD3	1.98	0.44
1:D:105:GLY:O	1:D:108:PRO:HD3	2.17	0.44
1:D:130:ALA:HB2	1:D:162:GLU:HG2	1.99	0.44
1:E:226:ASP:O	1:E:300:ASN:HB2	2.16	0.44
1:F:130:ALA:O	1:F:134:ARG:HG3	2.18	0.44
1:F:13:ASP:OD2	1:F:14:LYS:N	2.50	0.44
1:B:7:ILE:CG2	1:B:8:PRO:HD3	2.47	0.44
1:B:83:ASN:C	1:B:83:ASN:ND2	2.69	0.44
1:D:11:GLN:HE22	1:D:14:LYS:HB2	1.82	0.44
1:E:22:PRO:HG3	1:E:103:VAL:CG2	2.48	0.44
1:E:83:ASN:H	1:E:83:ASN:ND2	2.15	0.44
1:F:229:ALA:HB1	1:F:230:PRO:CD	2.48	0.44
1:D:11:GLN:NE2	1:D:14:LYS:HB2	2.33	0.44
1:B:53:GLN:O	1:B:54:VAL:C	2.54	0.44
1:F:56:HIS:ND1	1:F:58:ASP:HB2	2.32	0.44
1:C:251:MET:H	1:C:251:MET:HE2	1.83	0.44
1:F:137:VAL:HG11	1:F:173:ASN:HD22	1.82	0.44
1:F:221:THR:OG1	1:F:223:GLU:CB	2.66	0.44
1:A:52:CYS:N	1:A:82:ASP:HB2	2.33	0.44
1:B:107:ALA:C	1:B:109:LYS:N	2.70	0.44
1:E:163:LEU:HD11	1:E:197:PRO:HG3	2.00	0.44
1:E:227:ILE:CD1	1:E:288:ALA:HB2	2.48	0.44
1:F:154:LEU:HD12	1:F:154:LEU:C	2.38	0.44
1:F:3:LYS:HZ3	1:F:3:LYS:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:O	1:B:61:GLU:N	2.51	0.44
1:D:107:ALA:C	1:D:109:LYS:H	2.21	0.44
1:E:260:LEU:HA	1:E:260:LEU:HD23	1.55	0.43
1:B:150:ILE:HA	1:B:150:ILE:HD13	1.69	0.43
1:F:205:ALA:HB3	1:F:225:ILE:HA	1.99	0.43
1:F:14:LYS:HG3	1:F:243:TYR:O	2.18	0.43
1:F:248:GLY:N	1:F:251:MET:CE	2.82	0.43
1:F:52:CYS:HB3	1:F:114:ILE:HG13	2.00	0.43
1:C:126:MET:HG3	1:C:127:GLY:H	1.82	0.43
1:A:6:LEU:HD22	1:A:122:GLY:CA	2.48	0.43
1:C:273:ARG:CZ	1:D:224:GLU:HB3	2.49	0.43
1:A:259:ALA:HB1	1:A:305:LEU:HD21	1.99	0.43
1:B:264:ILE:O	1:B:265:ASN:C	2.56	0.43
1:E:197:PRO:HA	1:E:200:TYR:CD2	2.53	0.43
1:E:52:CYS:O	1:E:81:SER:HA	2.18	0.43
1:F:48:ILE:HA	1:F:115:ILE:HB	2.00	0.43
1:B:105:GLY:O	1:B:108:PRO:HD3	2.18	0.43
1:C:225:ILE:HD11	1:C:297:ALA:O	2.19	0.43
1:D:137:VAL:HG21	1:D:170:ALA:HA	2.01	0.43
1:F:253:ALA:HB3	1:F:254:PRO:HD3	1.99	0.43
1:B:6:LEU:CD1	1:B:9:TYR:CE2	2.95	0.43
1:B:72:ASP:C	1:B:74:GLY:H	2.22	0.43
1:F:68:ASN:ND2	1:F:70:THR:OG1	2.52	0.43
1:A:248:GLY:HA3	1:A:251:MET:HE1	2.00	0.43
1:B:291:ILE:HD11	1:B:302:PHE:HB2	2.01	0.43
1:D:223:GLU:CG	1:D:224:GLU:H	2.32	0.43
1:F:237:THR:HA	1:F:243:TYR:HD1	1.82	0.43
1:B:213:LEU:HB3	1:B:291:ILE:HD13	2.01	0.42
1:C:99:THR:N	3:C:2002:HOH:O	2.50	0.42
1:D:115:ILE:HG21	1:D:132:ALA:HB1	2.01	0.42
1:D:152:MET:CE	1:D:197:PRO:HG2	2.49	0.42
1:D:5:ARG:HG3	1:D:194:PHE:HE1	1.84	0.42
1:D:37:SER:HB2	1:D:262:LEU:HB3	2.01	0.42
1:A:39:LYS:HD3	1:A:108:PRO:HG2	2.01	0.42
1:A:248:GLY:CA	1:A:251:MET:HE1	2.48	0.42
1:C:68:ASN:HB2	1:C:79:ASN:O	2.19	0.42
1:D:148:ARG:C	1:D:149:ILE:HG13	2.38	0.42
1:D:303:LEU:HD12	1:D:303:LEU:C	2.38	0.42
1:A:83:ASN:H	1:A:83:ASN:HD22	1.67	0.42
1:C:19:SER:HA	1:C:102:GLY:O	2.18	0.42
1:D:21:VAL:HA	1:D:104:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ILE:HB	1:F:147:MET:HB3	2.01	0.42
1:E:315:PHE:HZ	1:F:291:ILE:HA	1.84	0.42
1:F:118:LEU:HD23	1:F:122:GLY:O	2.19	0.42
1:A:273:ARG:NE	1:B:224:GLU:HG2	2.34	0.42
1:D:234:ILE:CD1	1:D:251:MET:HB3	2.47	0.42
1:E:135:TYR:CD2	1:E:135:TYR:C	2.93	0.42
1:F:138:ASP:HA	1:F:140:ARG:NH1	2.34	0.42
1:C:70:THR:HG22	1:C:71:THR:N	2.34	0.42
1:D:225:ILE:CD1	1:D:225:ILE:N	2.72	0.42
1:F:9:TYR:HB2	1:F:251:MET:HE3	2.01	0.42
1:B:314:GLN:NE2	1:B:314:GLN:CA	2.67	0.42
1:C:181:ALA:HB2	1:C:205:ALA:HB1	2.01	0.42
1:C:234:ILE:HG21	1:C:234:ILE:HD12	1.79	0.42
1:C:70:THR:CG2	1:C:71:THR:N	2.83	0.42
1:E:50:THR:O	1:E:116:LYS:HE2	2.19	0.42
1:E:259:ALA:HB1	1:E:305:LEU:HD21	2.01	0.42
1:E:316:THR:CG2	1:E:317:GLU:N	2.81	0.42
1:F:137:VAL:O	1:F:140:ARG:NH1	2.53	0.42
1:F:43:GLN:HE22	1:F:148:ARG:HG2	1.85	0.42
1:A:295:ALA:HB3	1:B:270:ALA:O	2.20	0.42
1:A:92:GLY:HA3	1:A:236:SER:OG	2.20	0.42
1:B:24:GLY:O	1:B:27:ILE:HG22	2.20	0.42
1:E:272:LYS:O	1:E:273:ARG:CB	2.68	0.42
1:F:229:ALA:HB1	1:F:230:PRO:HD2	2.02	0.42
1:F:27:ILE:HG22	1:F:302:PHE:HZ	1.84	0.42
1:A:260:LEU:O	1:A:264:ILE:HG13	2.19	0.42
1:D:133:ILE:HG22	1:D:134:ARG:N	2.34	0.42
1:D:96:ALA:CB	1:D:103:VAL:HG13	2.49	0.42
1:E:270:ALA:O	1:F:295:ALA:HB3	2.19	0.42
1:C:181:ALA:O	1:C:249:THR:HG21	2.20	0.41
1:F:207:GLY:C	1:F:228:VAL:HG12	2.41	0.41
1:F:206:VAL:HG11	1:F:253:ALA:HA	2.02	0.41
1:A:70:THR:HG23	1:A:71:THR:H	1.83	0.41
1:B:256:VAL:HG11	1:B:284:LEU:HD21	2.02	0.41
1:C:56:HIS:HA	1:C:57:PRO:HD2	1.89	0.41
1:D:248:GLY:CA	1:D:251:MET:HE2	2.50	0.41
1:F:68:ASN:OD1	1:F:116:LYS:CD	2.68	0.41
1:B:209:VAL:HA	1:B:214:ARG:O	2.20	0.41
1:D:234:ILE:HD13	1:D:246:LEU:O	2.21	0.41
1:C:295:ALA:HB3	1:D:270:ALA:O	2.20	0.41
1:A:95:ALA:O	1:A:96:ALA:C	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLY:CA	1:C:251:MET:CE	2.99	0.41
1:D:120:GLY:C	1:D:122:GLY:N	2.74	0.41
1:E:174:ASN:N	1:E:174:ASN:OD1	2.53	0.41
1:A:28:VAL:HG22	1:A:303:LEU:HB3	2.02	0.41
1:E:21:VAL:HG22	1:E:104:VAL:HG11	2.02	0.41
1:F:137:VAL:HG11	1:F:173:ASN:ND2	2.36	0.41
1:B:98:GLU:C	1:B:100:GLY:H	2.23	0.41
1:B:138:ASP:HA	1:B:140:ARG:NH1	2.35	0.41
1:B:52:CYS:HA	1:B:82:ASP:HB2	2.03	0.41
1:E:45:ILE:HD11	1:E:261:ALA:HB2	2.02	0.41
1:C:148:ARG:O	1:C:175:VAL:HA	2.21	0.41
1:E:51:GLY:O	1:E:87:GLY:HA3	2.20	0.41
1:E:69:LEU:CD1	1:E:132:ALA:CB	2.90	0.41
1:F:169:TYR:HE1	1:F:173:ASN:ND2	2.14	0.41
1:F:247:SER:O	1:F:251:MET:HE3	2.20	0.41
1:F:83:ASN:N	1:F:83:ASN:HD22	2.07	0.41
1:B:83:ASN:CG	1:B:116:LYS:NZ	2.74	0.41
1:F:264:ILE:HG12	1:F:280:ILE:HD12	2.03	0.41
1:B:22:PRO:CG	1:B:103:VAL:HG23	2.50	0.41
1:C:134:ARG:NH1	1:C:166:ALA:HA	2.36	0.41
1:D:155:GLY:HA2	1:D:196:TYR:O	2.21	0.41
1:D:15:VAL:HB	1:D:18:LEU:CD1	2.49	0.41
1:A:9:TYR:CE1	1:A:246:LEU:HD13	2.56	0.41
1:D:225:ILE:HD13	1:D:225:ILE:N	2.15	0.41
1:F:76:ASP:OD1	1:F:77:GLU:N	2.53	0.41
1:F:80:PHE:N	1:F:80:PHE:CD2	2.89	0.41
1:A:174:ASN:OD1	1:A:276:SER:HA	2.21	0.40
1:B:7:ILE:HG13	1:B:153:SER:O	2.21	0.40
1:C:263:ILE:HD13	1:C:287:ARG:HD2	2.03	0.40
1:D:236:SER:OG	1:D:237:THR:N	2.51	0.40
1:E:266:LEU:C	1:E:266:LEU:HD12	2.42	0.40
1:F:4:PHE:CE1	1:F:126:MET:HB3	2.56	0.40
1:A:68:ASN:HA	1:A:116:LYS:HB3	2.02	0.40
1:A:27:ILE:HG23	1:A:302:PHE:HZ	1.86	0.40
1:B:15:VAL:CG1	1:B:16:SER:N	2.84	0.40
1:C:129:ILE:HB	1:C:163:LEU:HD11	2.03	0.40
1:C:28:VAL:HG22	1:C:303:LEU:HB3	2.03	0.40
1:E:28:VAL:O	1:E:28:VAL:HG12	2.20	0.40
1:F:83:ASN:ND2	1:F:83:ASN:N	2.69	0.40
1:A:247:SER:C	1:A:251:MET:HE3	2.41	0.40
1:A:253:ALA:N	1:A:254:PRO:CD	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASP:OD2	1:B:83:ASN:N	2.54	0.40
1:C:234:ILE:HD13	1:C:234:ILE:HG23	1.72	0.40
1:D:58:ASP:C	1:D:59:LEU:HD23	2.41	0.40
1:F:27:ILE:HG22	1:F:302:PHE:CZ	2.57	0.40
1:A:149:ILE:O	1:A:150:ILE:HD13	2.22	0.40
1:A:277:GLU:O	1:A:281:TYR:N	2.55	0.40
1:A:30:ALA:O	1:A:31:PRO:C	2.57	0.40
1:B:68:ASN:ND2	1:B:79:ASN:O	2.48	0.40
1:F:152:MET:HB2	1:F:154:LEU:HG	2.02	0.40
1:F:245:GLU:O	1:F:246:LEU:HD23	2.21	0.40
1:B:96:ALA:HB3	1:B:104:VAL:HA	2.04	0.40
1:B:45:ILE:H	1:B:45:ILE:HD12	1.87	0.40
1:D:20:GLU:CD	1:D:21:VAL:H	2.24	0.40
1:E:148:ARG:C	1:E:149:ILE:HG13	2.41	0.40
1:E:207:GLY:O	1:E:228:VAL:HA	2.21	0.40
1:E:244:ALA:HB1	1:E:246:LEU:HD21	2.03	0.40
1:E:273:ARG:HH11	1:F:224:GLU:CD	2.25	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	293/329 (89%)	266 (91%)	23 (8%)	4 (1%)	11	25
1	B	292/329 (89%)	253 (87%)	30 (10%)	9 (3%)	4	8
1	C	294/329 (89%)	261 (89%)	25 (8%)	8 (3%)	5	11
1	D	302/329 (92%)	259 (86%)	35 (12%)	8 (3%)	5	11
1	E	293/329 (89%)	261 (89%)	22 (8%)	10 (3%)	3	7
1	F	296/329 (90%)	263 (89%)	30 (10%)	3 (1%)	15	34
All	All	1770/1974 (90%)	1563 (88%)	165 (9%)	42 (2%)	6	13

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	GLY
1	A	239	LEU
1	B	32	ALA
1	B	60	ALA
1	B	182	GLY
1	C	317	GLU
1	D	316	THR
1	F	60	ALA
1	A	60	ALA
1	A	316	THR
1	B	54	VAL
1	C	29	GLU
1	D	19	SER
1	D	218	PHE
1	E	125	GLU
1	E	198	ALA
1	E	239	LEU
1	C	49	ASP
1	C	250	ALA
1	D	20	GLU
1	D	78	THR
1	E	169	TYR
1	E	293	PHE
1	B	73	TYR
1	C	198	ALA
1	E	273	ARG
1	F	91	ALA
1	F	218	PHE
1	B	49	ASP
1	B	76	ASP
1	D	108	PRO
1	E	19	SER
1	B	31	PRO
1	C	142	PRO
1	C	293	PHE
1	E	121	ASP
1	B	108	PRO
1	C	182	GLY
1	D	142	PRO
1	E	108	PRO
1	D	299	GLY
1	E	12	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	224/252 (89%)	197 (88%)	27 (12%)	5	10
1	B	223/252 (88%)	184 (82%)	39 (18%)	2	4
1	C	225/252 (89%)	185 (82%)	40 (18%)	2	4
1	D	231/252 (92%)	197 (85%)	34 (15%)	3	7
1	E	224/252 (89%)	180 (80%)	44 (20%)	1	3
1	F	228/252 (90%)	193 (85%)	35 (15%)	2	6
All	All	1355/1512 (90%)	1136 (84%)	219 (16%)	2	5

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	6	LEU
1	A	10	LYS
1	A	11	GLN
1	A	15	VAL
1	A	28	VAL
1	A	33	VAL
1	A	49	ASP
1	A	67	VAL
1	A	70	THR
1	A	71	THR
1	A	73	TYR
1	A	83	ASN
1	A	103	VAL
1	A	109	LYS
1	A	126	MET
1	A	143	LYS
1	A	147	MET
1	A	172	SER
1	A	177	VAL
1	A	179	CYS
1	A	202	GLU

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Mol	Chain	Res	Type
1	A	215	LEU
1	A	277	GLU
1	A	296	GLN
1	A	307	LEU
1	A	316	THR
1	B	3	LYS
1	B	4	PHE
1	B	6	LEU
1	B	11	GLN
1	B	21	VAL
1	B	26	GLU
1	B	28	VAL
1	B	33	VAL
1	B	49	ASP
1	B	52	CYS
1	B	53	GLN
1	B	67	VAL
1	B	69	LEU
1	B	71	THR
1	B	73	TYR
1	B	77	GLU
1	B	78	THR
1	B	83	ASN
1	B	101	SER
1	B	104	VAL
1	B	119	SER
1	B	126	MET
1	B	146	GLN
1	B	152	MET
1	B	172	SER
1	B	173	ASN
1	B	176	SER
1	B	183	ASN
1	B	193	GLU
1	B	202	GLU
1	B	214	ARG
1	B	215	LEU
1	B	225	ILE
1	B	234	ILE
1	B	241	SER
1	B	285	VAL
1	B	294	THR

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Mol	Chain	Res	Type
1	B	307	LEU
1	B	314	GLN
1	C	3	LYS
1	C	6	LEU
1	C	11	GLN
1	C	15	VAL
1	C	18	LEU
1	C	23	MET
1	C	27	ILE
1	C	33	VAL
1	C	61	GLU
1	C	62	ARG
1	C	64	ILE
1	C	73	TYR
1	C	76	ASP
1	C	78	THR
1	C	81	SER
1	C	83	ASN
1	C	103	VAL
1	C	104	VAL
1	C	109	LYS
1	C	126	MET
1	C	131	LYS
1	C	145	GLU
1	C	146	GLN
1	C	152	MET
1	C	171	VAL
1	C	183	ASN
1	C	202	GLU
1	C	215	LEU
1	C	225	ILE
1	C	234	ILE
1	C	240	ASP
1	C	251	MET
1	C	263	ILE
1	C	266	LEU
1	C	273	ARG
1	C	277	GLU
1	C	286	ARG
1	C	291	ILE
1	C	307	LEU
1	C	310	ARG

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Mol	Chain	Res	Type
1	D	13	ASP
1	D	15	VAL
1	D	20	GLU
1	D	27	ILE
1	D	28	VAL
1	D	55	ASP
1	D	81	SER
1	D	83	ASN
1	D	84	ASN
1	D	90	VAL
1	D	103	VAL
1	D	109	LYS
1	D	119	SER
1	D	126	MET
1	D	129	ILE
1	D	131	LYS
1	D	140	ARG
1	D	160	SER
1	D	193	GLU
1	D	202	GLU
1	D	215	LEU
1	D	225	ILE
1	D	227	ILE
1	D	234	ILE
1	D	241	SER
1	D	246	LEU
1	D	251	MET
1	D	266	LEU
1	D	277	GLU
1	D	286	ARG
1	D	303	LEU
1	D	307	LEU
1	D	309	GLU
1	D	310	ARG
1	E	3	LYS
1	E	6	LEU
1	E	10	LYS
1	E	11	GLN
1	E	15	VAL
1	E	16	SER
1	E	18	LEU
1	E	26	GLU

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Mol	Chain	Res	Type
1	E	33	VAL
1	E	37	SER
1	E	49	ASP
1	E	54	VAL
1	E	62	ARG
1	E	78	THR
1	E	83	ASN
1	E	103	VAL
1	E	114	ILE
1	E	125	GLU
1	E	126	MET
1	E	129	ILE
1	E	131	LYS
1	E	134	ARG
1	E	135	TYR
1	E	143	LYS
1	E	148	ARG
1	E	153	SER
1	E	159	ASP
1	E	162	GLU
1	E	172	SER
1	E	174	ASN
1	E	183	ASN
1	E	202	GLU
1	E	215	LEU
1	E	216	SER
1	E	234	ILE
1	E	249	THR
1	E	266	LEU
1	E	277	GLU
1	E	278	THR
1	E	285	VAL
1	E	307	LEU
1	E	309	GLU
1	E	312	THR
1	E	314	GLN
1	F	3	LYS
1	F	5	ARG
1	F	6	LEU
1	F	10	LYS
1	F	11	GLN
1	F	27	ILE

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Mol	Chain	Res	Type
1	F	35	ARG
1	F	49	ASP
1	F	61	GLU
1	F	62	ARG
1	F	72	ASP
1	F	76	ASP
1	F	78	THR
1	F	83	ASN
1	F	101	SER
1	F	119	SER
1	F	126	MET
1	F	142	PRO
1	F	153	SER
1	F	160	SER
1	F	169	TYR
1	F	202	GLU
1	F	225	ILE
1	F	234	ILE
1	F	235	LYS
1	F	239	LEU
1	F	266	LEU
1	F	272	LYS
1	F	277	GLU
1	F	285	VAL
1	F	296	GLN
1	F	307	LEU
1	F	310	ARG
1	F	312	THR
1	F	316	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	B	43	GLN
1	B	146	GLN
1	B	173	ASN
1	B	201	ASN
1	B	314	GLN
1	C	83	ASN
1	C	146	GLN
1	C	201	ASN

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Mol	Chain	Res	Type
1	C	296	GLN
1	D	11	GLN
1	D	83	ASN
1	D	164	HIS
1	D	201	ASN
1	D	314	GLN
1	E	83	ASN
1	E	86	HIS
1	E	146	GLN
1	F	43	GLN
1	F	83	ASN
1	F	89	HIS
1	F	164	HIS
1	F	173	ASN
1	F	183	ASN
1	F	255	HIS
1	F	314	GLN

### 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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	299/329 (90%)	-0.15	0 100 100	19, 29, 44, 59	0
1	B	298/329 (90%)	0.18	5 (1%) 70 71	22, 42, 67, 89	0
1	C	300/329 (91%)	-0.09	3 (1%) 82 82	19, 28, 44, 77	0
1	D	306/329 (93%)	0.08	5 (1%) 72 73	20, 37, 56, 69	0
1	E	299/329 (90%)	0.22	9 (3%) 50 49	25, 42, 63, 70	1 (0%)
1	F	302/329 (91%)	0.26	5 (1%) 70 71	28, 48, 74, 98	0
All	All	1804/1974 (91%)	0.09	27 (1%) 73 74	19, 37, 65, 98	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	LEU	3.4
1	F	73	TYR	3.3
1	D	17	ALA	3.2
1	E	69	LEU	3.2
1	E	74	GLY	3.1
1	F	12	VAL	2.8
1	C	316	THR	2.8
1	E	216	SER	2.7
1	B	118	LEU	2.7
1	B	237	THR	2.6
1	F	55	ASP	2.6
1	D	73	TYR	2.6
1	B	95	ALA	2.4
1	F	142	PRO	2.3
1	E	181	ALA	2.3
1	B	246	LEU	2.3
1	E	70	THR	2.3
1	C	16	SER	2.2
1	E	194	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	216	SER	2.1
1	E	75	GLY	2.1
1	D	97	ALA	2.1
1	D	182	GLY	2.1
1	E	271	PHE	2.1
1	F	181	ALA	2.0
1	B	55	ASP	2.0
1	E	156	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	E	401	1/1	0.82	0.16	33,33,33,33	0
2	NA	B	401	1/1	0.88	0.08	37,37,37,37	0
2	NA	D	401	1/1	0.92	0.07	37,37,37,37	0
2	NA	F	401	1/1	0.98	0.10	44,44,44,44	0
2	NA	C	401	1/1	0.98	0.12	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.