



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:35 AM GMT

PDB ID : 3BDB  
Title : Crystal Structure of Novel Immune-Type Receptor 11 Extracellular Fragment from *Ictalurus punctatus* including Stalk Region  
Authors : Ostrov, D.A.; Hernandez Prada, J.A.; Haire, R.N.; Cannon, J.P.; Magis, A.T.; Bailey, K.M.; Litman, G.W.  
Deposited on : 2007-11-14  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

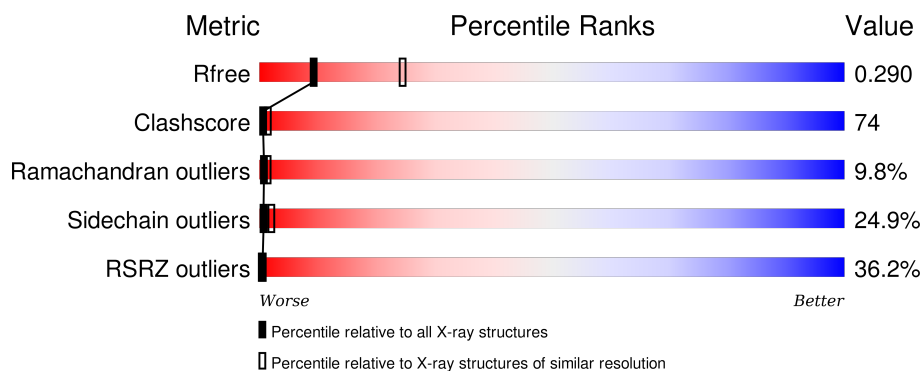
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	137	<div> <div>39%</div> <div>25% 32% 29% 6% 8%</div> </div>
1	B	137	<div> <div>36%</div> <div>25% 39% 20% 9% 8%</div> </div>
1	C	137	<div> <div>34%</div> <div>21% 44% 21% 6% 8%</div> </div>
1	D	137	<div> <div>31%</div> <div>20% 45% 21% 5% 8%</div> </div>
1	E	137	<div> <div>31%</div> <div>21% 42% 25% • 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	137	<p>28% 16% 42% 29% 8%</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6021 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 Novel immune-type receptor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			995	620	170	199	6			
1	B	126	Total	C	N	O	S	0	0	0
			995	620	170	199	6			
1	C	126	Total	C	N	O	S	0	0	0
			995	620	170	199	6			
1	D	126	Total	C	N	O	S	0	0	0
			995	620	170	199	6			
1	E	126	Total	C	N	O	S	0	0	0
			995	620	170	199	6			
1	F	126	Total	C	N	O	S	0	0	0
			995	620	170	199	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q8UWK4
B	1	MET	-	INITIATING METHIONINE	UNP Q8UWK4
C	1	MET	-	INITIATING METHIONINE	UNP Q8UWK4
D	1	MET	-	INITIATING METHIONINE	UNP Q8UWK4
E	1	MET	-	INITIATING METHIONINE	UNP Q8UWK4
F	1	MET	-	INITIATING METHIONINE	UNP Q8UWK4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	11	Total	O	0	0
			11	11		
2	C	8	Total	O	0	0
			8	8		

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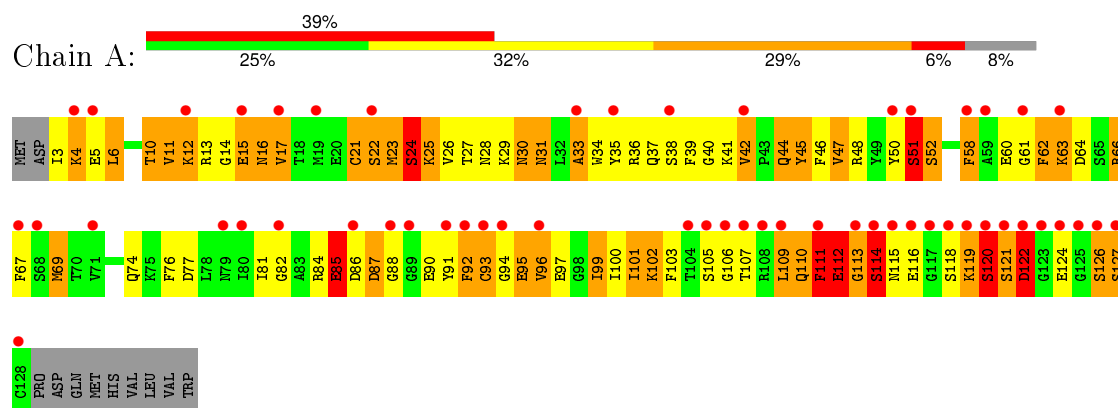
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	9	Total	O	0	0
			9	9		
2	E	7	Total	O	0	0
			7	7		
2	F	7	Total	O	0	0
			7	7		

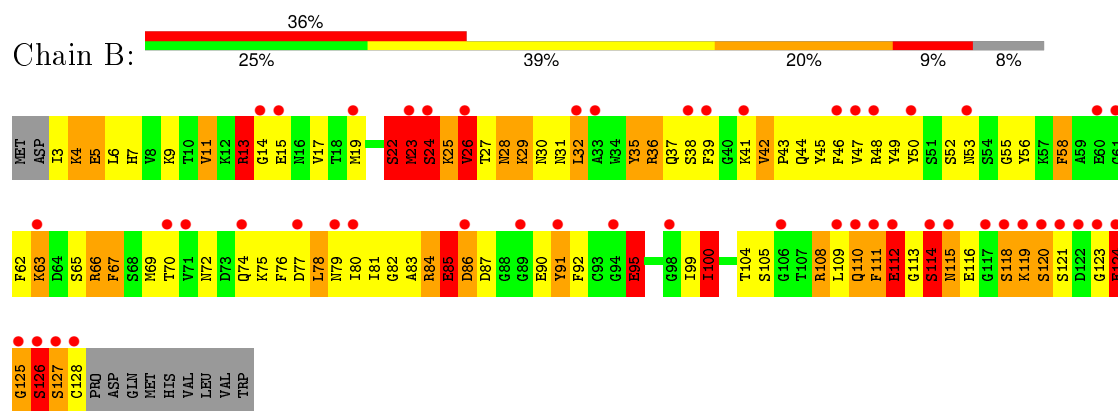
### 3 Residue-property plots [i](#)

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

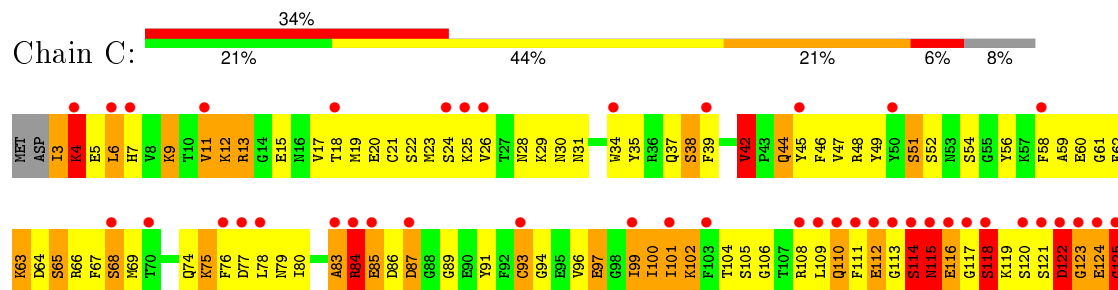
#### • Molecule 1: Novel immune-type receptor 11

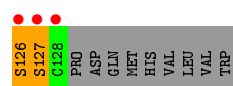


#### • Molecule 1: Novel immune-type receptor 11

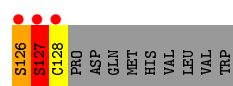
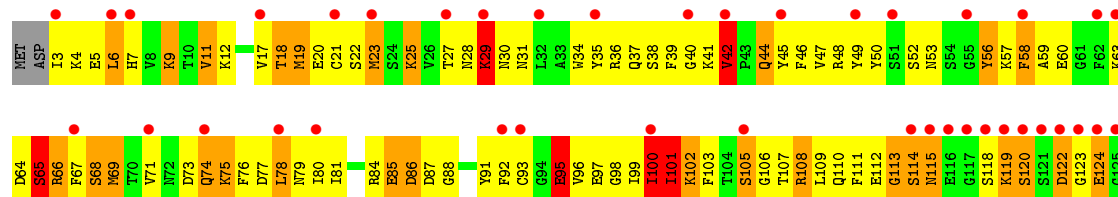
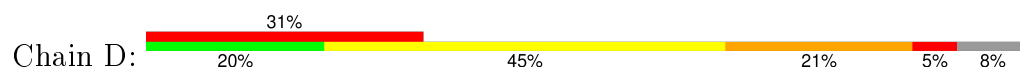


#### • Molecule 1: Novel immune-type receptor 11

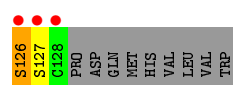
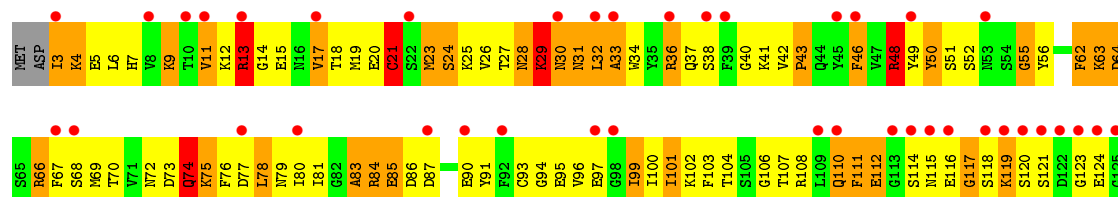
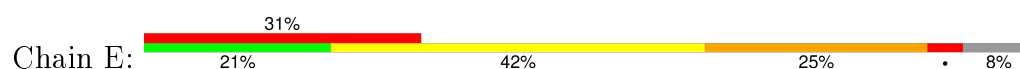




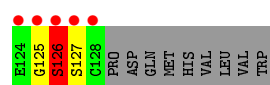
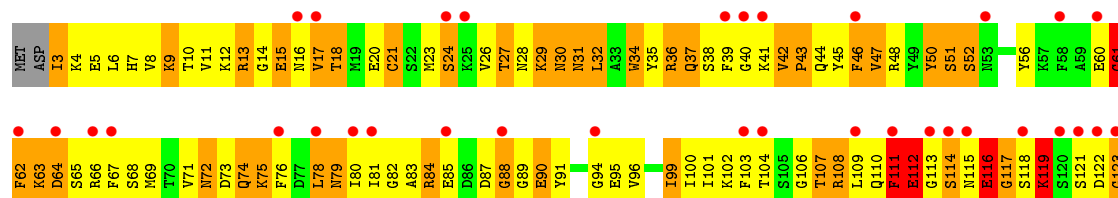
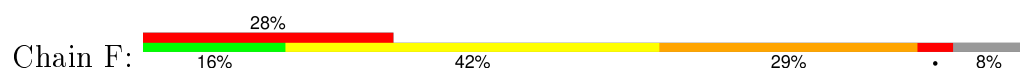
• Molecule 1: Novel immune-type receptor 11



• Molecule 1: Novel immune-type receptor 11



• Molecule 1: Novel immune-type receptor 11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.58Å 91.34Å 115.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.51 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.80) 99.3 (29.51-2.81)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	27.26 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.284 , 0.291 0.286 , 0.290	Depositor DCC
$R_{free}$ test set	1231 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.1	EDS
Estimated twinning fraction	0.427 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 23963 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.30	8/1013 (0.8%)	1.13	7/1353 (0.5%)
1	B	1.35	7/1013 (0.7%)	1.12	4/1353 (0.3%)
1	C	1.43	12/1013 (1.2%)	1.20	4/1353 (0.3%)
1	D	1.46	10/1013 (1.0%)	1.25	9/1353 (0.7%)
1	E	1.46	5/1013 (0.5%)	1.22	4/1353 (0.3%)
1	F	1.65	11/1013 (1.1%)	1.40	7/1353 (0.5%)
All	All	1.45	53/6078 (0.9%)	1.22	35/8118 (0.4%)

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	13
1	B	0	13
1	C	0	13
1	D	0	13
1	E	0	14
1	F	0	8
All	All	0	74

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	GLU	CD-OE2	5.99	1.32	1.25
1	A	76	PHE	CD2-CE2	5.99	1.51	1.39
1	F	35	TYR	CD1-CE1	5.98	1.48	1.39
1	D	103	PHE	CE1-CZ	5.90	1.48	1.37
1	F	71	VAL	CA-CB	-5.90	1.42	1.54
1	B	29	LYS	CD-CE	5.89	1.66	1.51
1	D	56	TYR	N-CA	-5.88	1.34	1.46
1	B	95	GLU	CB-CG	-5.88	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	15	GLU	CD-OE1	5.87	1.32	1.25
1	C	5	GLU	C-O	-5.85	1.12	1.23
1	B	22	SER	CA-CB	5.80	1.61	1.52
1	D	106	GLY	CA-C	-5.78	1.42	1.51
1	F	43	PRO	N-CA	5.75	1.57	1.47
1	C	89	GLY	CA-C	-5.71	1.42	1.51
1	D	58	PHE	CE2-CZ	5.70	1.48	1.37
1	C	4	LYS	CD-CE	5.68	1.65	1.51
1	D	103	PHE	CG-CD1	-5.65	1.30	1.38
1	E	108	ARG	CG-CD	5.64	1.66	1.51
1	C	76	PHE	N-CA	-5.60	1.35	1.46
1	E	50	TYR	CD1-CE1	-5.60	1.30	1.39
1	C	19	MET	C-O	-5.60	1.12	1.23
1	E	3	ILE	CA-CB	5.59	1.67	1.54
1	A	93	CYS	N-CA	-5.59	1.35	1.46
1	B	90	GLU	CG-CD	5.56	1.60	1.51
1	E	93	CYS	CB-SG	-5.54	1.72	1.81
1	A	87	ASP	C-O	5.49	1.33	1.23
1	D	66	ARG	C-O	5.48	1.33	1.23
1	C	9	LYS	CG-CD	5.47	1.71	1.52
1	F	72	ASN	CA-C	5.46	1.67	1.52
1	F	89	GLY	C-O	5.40	1.32	1.23
1	D	106	GLY	C-O	-5.28	1.15	1.23
1	F	27	THR	C-O	5.28	1.33	1.23
1	F	4	LYS	N-CA	5.27	1.56	1.46
1	F	116	GLU	CG-CD	5.27	1.59	1.51
1	C	44	GLN	CG-CD	5.24	1.63	1.51
1	F	50	TYR	CG-CD2	5.22	1.46	1.39
1	A	30	ASN	CA-C	-5.21	1.39	1.52
1	A	51	SER	N-CA	5.20	1.56	1.46
1	E	43	PRO	N-CA	5.18	1.56	1.47
1	B	58	PHE	CD2-CE2	5.17	1.49	1.39
1	F	34	TRP	CA-CB	-5.16	1.42	1.53
1	D	98	GLY	N-CA	-5.16	1.38	1.46
1	C	5	GLU	CB-CG	5.13	1.61	1.52
1	C	20	GLU	C-O	-5.13	1.13	1.23
1	D	66	ARG	CB-CG	-5.10	1.38	1.52
1	C	12	LYS	CB-CG	5.08	1.66	1.52
1	B	91	TYR	CG-CD2	5.08	1.45	1.39
1	C	65	SER	CB-OG	5.08	1.48	1.42
1	A	67	PHE	CE1-CZ	5.05	1.47	1.37
1	C	83	ALA	CA-CB	-5.04	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	PHE	CE1-CZ	5.04	1.47	1.37
1	A	21	CYS	CB-SG	-5.04	1.73	1.81
1	D	35	TYR	CG-CD1	5.03	1.45	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	83	ALA	N-CA-CB	-5.99	101.72	110.10
1	F	36	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	C	9	LYS	N-CA-C	-5.84	95.22	111.00
1	E	23	MET	CG-SD-CE	-5.83	90.87	100.20
1	D	18	THR	OG1-CB-CG2	-5.79	96.69	110.00
1	B	28	ASN	CB-CA-C	-5.73	98.93	110.40
1	A	100	ILE	CG1-CB-CG2	-5.72	98.83	111.40
1	D	71	VAL	CG1-CB-CG2	-5.63	101.89	110.90
1	A	62	PHE	N-CA-C	5.61	126.14	111.00
1	F	117	GLY	N-CA-C	5.57	127.02	113.10
1	A	41	LYS	CD-CE-NZ	-5.57	98.90	111.70
1	B	95	GLU	OE1-CD-OE2	-5.55	116.63	123.30
1	D	108	ARG	CA-CB-CG	-5.55	101.20	113.40
1	F	29	LYS	N-CA-C	5.51	125.87	111.00
1	D	35	TYR	CB-CG-CD1	5.45	124.27	121.00
1	D	19	MET	CG-SD-CE	5.35	108.77	100.20
1	D	122	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	16	ASN	N-CA-C	-5.30	96.70	111.00
1	F	36	ARG	CG-CD-NE	5.29	122.92	111.80
1	C	42	VAL	N-CA-C	-5.29	96.73	111.00
1	D	44	GLN	CB-CA-C	-5.28	99.84	110.40
1	B	100	ILE	CA-CB-CG1	-5.26	101.01	111.00
1	A	87	ASP	CB-CG-OD1	5.25	123.02	118.30
1	E	4	LYS	N-CA-C	5.21	125.06	111.00
1	F	111	PHE	N-CA-C	5.19	125.02	111.00
1	F	112	GLU	CB-CA-C	5.16	120.71	110.40
1	A	88	GLY	N-CA-C	-5.15	100.22	113.10
1	C	42	VAL	CB-CA-C	5.14	121.16	111.40
1	D	95	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	B	67	PHE	C-N-CA	-5.10	108.96	121.70
1	C	11	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	A	47	VAL	CA-CB-CG1	-5.07	103.30	110.90
1	D	108	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	E	77	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	F	30	ASN	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (74) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	THR	Peptide
1	A	105	SER	Peptide
1	A	111	PHE	Peptide
1	A	112	GLU	Peptide
1	A	113	GLY	Peptide
1	A	114	SER	Peptide
1	A	120	SER	Peptide
1	A	126	SER	Peptide
1	A	22	SER	Peptide
1	A	23	MET	Peptide
1	A	33	ALA	Peptide
1	A	82	GLY	Peptide
1	A	95	GLU	Peptide
1	B	105	SER	Peptide
1	B	111	PHE	Peptide
1	B	112	GLU	Peptide
1	B	114	SER	Peptide
1	B	120	SER	Peptide
1	B	124	GLU	Peptide
1	B	125	GLY	Peptide
1	B	126	SER	Peptide
1	B	127	SER	Peptide
1	B	22	SER	Peptide
1	B	24	SER	Peptide
1	B	26	VAL	Peptide
1	B	76	PHE	Peptide
1	C	113	GLY	Peptide
1	C	114	SER	Peptide
1	C	115	ASN	Peptide
1	C	118	SER	Peptide
1	C	122	ASP	Peptide
1	C	123	GLY	Peptide
1	C	124	GLU	Peptide
1	C	125	GLY	Peptide
1	C	54	SER	Peptide
1	C	61	GLY	Peptide
1	C	83	ALA	Peptide
1	C	84	ARG	Peptide
1	C	99	ILE	Peptide
1	D	101	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	D	105	SER	Peptide
1	D	113	GLY	Peptide
1	D	119	LYS	Peptide
1	D	120	SER	Peptide
1	D	127	SER	Peptide
1	D	20	GLU	Peptide
1	D	25	LYS	Peptide
1	D	29	LYS	Peptide
1	D	42	VAL	Peptide
1	D	69	MET	Peptide
1	D	74	GLN	Peptide
1	D	88	GLY	Peptide
1	E	104	THR	Peptide
1	E	110	GLN	Peptide
1	E	120	SER	Peptide
1	E	17	VAL	Peptide
1	E	21	CYS	Peptide
1	E	28	ASN	Peptide
1	E	29	LYS	Peptide
1	E	30	ASN	Peptide
1	E	33	ALA	Peptide
1	E	48	ARG	Peptide
1	E	55	GLY	Peptide
1	E	73	ASP	Peptide
1	E	74	GLN	Peptide
1	E	84	ARG	Peptide
1	F	104	THR	Peptide
1	F	107	THR	Peptide
1	F	111	PHE	Peptide
1	F	114	SER	Peptide
1	F	21	CYS	Peptide
1	F	61	GLY	Peptide
1	F	62	PHE	Peptide
1	F	84	ARG	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	995	0	945	151	0
1	B	995	0	945	166	0
1	C	995	0	945	181	0
1	D	995	0	947	130	0
1	E	995	0	945	166	0
1	F	995	0	945	149	0
2	A	9	0	0	2	0
2	B	11	0	0	7	0
2	C	8	0	0	1	0
2	D	9	0	0	4	0
2	E	7	0	0	2	0
2	F	7	0	0	7	0
All	All	6021	0	5672	858	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 74.

All (858) 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:F:62:PHE:CZ	1:F:64:ASP:HB2	1.66	1.30
1:C:12:LYS:HA	1:C:112:GLU:CG	1.61	1.29
1:B:126:SER:HB2	1:B:127:SER:CA	1.65	1.21
1:C:85:GLU:HA	1:C:111:PHE:CZ	1.75	1.20
1:A:99:ILE:HG21	1:B:31:ASN:ND2	1.54	1.19
1:E:48:ARG:HG3	1:E:49:TYR:C	1.63	1.19
1:A:12:LYS:HB3	1:A:112:GLU:OE2	1.43	1.18
1:E:48:ARG:HG3	1:E:49:TYR:O	1.46	1.15
1:B:126:SER:CB	1:B:127:SER:HA	1.76	1.15
1:C:97:GLU:HB3	1:C:102:LYS:NZ	1.62	1.13
1:D:23:MET:HB2	1:D:74:GLN:O	1.46	1.13
1:B:13:ARG:HG2	1:F:81:ILE:HD11	1.15	1.13
1:C:79:ASN:O	1:C:80:ILE:HD13	1.49	1.12
1:C:13:ARG:NH2	1:C:85:GLU:HB3	1.66	1.11
1:A:96:VAL:H	1:A:101:ILE:HD12	0.96	1.11
1:F:62:PHE:CZ	1:F:67:PHE:CD2	2.37	1.11
1:C:12:LYS:CG	1:C:112:GLU:HG2	1.79	1.10
1:C:12:LYS:CA	1:C:112:GLU:HG3	1.81	1.10
1:C:85:GLU:HA	1:C:111:PHE:CE1	1.88	1.08
1:F:112:GLU:HB3	1:F:113:GLY:HA3	1.15	1.08
1:A:11:VAL:HG23	1:A:12:LYS:H	0.91	1.07
1:C:97:GLU:HB3	1:C:102:LYS:HZ1	1.13	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:HG3	1:B:85:GLU:OE1	1.55	1.07
1:F:62:PHE:HZ	1:F:67:PHE:CD2	1.70	1.06
1:C:12:LYS:HG2	1:C:112:GLU:HG2	1.36	1.06
1:B:127:SER:HB2	1:B:128:CYS:HA	1.34	1.06
1:A:96:VAL:N	1:A:101:ILE:HD12	1.71	1.05
1:E:48:ARG:CD	1:E:49:TYR:O	2.05	1.05
1:E:48:ARG:CG	1:E:49:TYR:O	2.04	1.05
1:A:11:VAL:HG23	1:A:12:LYS:N	1.58	1.05
1:F:62:PHE:CZ	1:F:67:PHE:CE2	2.45	1.04
1:B:26:VAL:HG12	1:B:27:THR:N	1.68	1.03
1:C:84:ARG:H	1:C:111:PHE:HZ	1.04	1.03
1:E:69:MET:HA	1:E:79:ASN:ND2	1.73	1.03
1:A:23:MET:H	1:A:24:SER:CB	1.72	1.02
1:F:62:PHE:CZ	1:F:64:ASP:CB	2.42	1.01
1:C:13:ARG:NH2	1:C:85:GLU:CB	2.23	1.01
1:F:17:VAL:HG11	1:F:109:LEU:HD13	1.40	1.01
1:A:35:TYR:CE2	1:A:45:TYR:HB2	1.95	1.01
1:C:6:LEU:HD11	1:D:42:VAL:HG23	1.41	1.00
1:E:62:PHE:O	1:E:62:PHE:CD2	2.15	0.99
1:B:13:ARG:CG	1:F:81:ILE:HD11	1.92	0.99
1:E:62:PHE:O	1:E:62:PHE:HD2	1.42	0.98
1:E:23:MET:HE3	1:E:29:LYS:HE2	1.46	0.97
1:F:112:GLU:CB	1:F:113:GLY:HA3	1.92	0.97
1:A:11:VAL:CG2	1:A:12:LYS:H	1.78	0.97
1:F:62:PHE:CE1	1:F:64:ASP:HB2	2.00	0.96
1:D:100:ILE:HG22	1:D:100:ILE:O	1.65	0.96
1:A:33:ALA:CB	1:A:35:TYR:CE1	2.48	0.95
1:F:62:PHE:CZ	1:F:67:PHE:HD2	1.81	0.95
1:C:6:LEU:CD1	1:D:42:VAL:HG23	1.97	0.94
1:A:33:ALA:HB3	1:A:35:TYR:HE1	1.33	0.94
1:E:69:MET:CA	1:E:79:ASN:ND2	2.32	0.92
1:B:24:SER:O	1:B:25:LYS:HB2	1.65	0.92
1:E:62:PHE:CD2	1:E:62:PHE:C	2.42	0.92
1:A:84:ARG:O	1:A:85:GLU:HG3	1.68	0.92
1:A:11:VAL:CG2	1:A:12:LYS:N	2.30	0.90
1:A:39:PHE:HA	2:A:146:HOH:O	1.70	0.90
1:D:68:SER:HA	2:D:143:HOH:O	1.69	0.90
1:C:11:VAL:HG11	1:C:109:LEU:HD11	1.50	0.90
1:A:15:GLU:O	1:A:16:ASN:OD1	1.91	0.89
1:B:120:SER:OG	1:B:121:SER:HB2	1.73	0.89
1:C:116:GLU:OE1	1:C:116:GLU:HA	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:GLY:HA2	1:E:103:PHE:HA	1.52	0.88
1:B:85:GLU:OE2	1:B:86:ASP:N	2.07	0.88
1:B:114:SER:CB	1:B:116:GLU:N	2.37	0.88
1:B:13:ARG:HG2	1:F:81:ILE:CD1	2.03	0.88
1:F:112:GLU:HB3	1:F:113:GLY:CA	2.04	0.88
1:C:79:ASN:C	1:C:80:ILE:HD13	1.94	0.87
1:C:13:ARG:HH21	1:C:85:GLU:CB	1.87	0.87
1:E:23:MET:HB2	1:E:74:GLN:O	1.73	0.86
1:D:21:CYS:HG	1:D:93:CYS:HG	0.87	0.86
1:B:112:GLU:N	1:B:113:GLY:HA2	1.88	0.86
1:D:67:PHE:CE1	1:D:80:ILE:HG13	2.11	0.86
1:F:16:ASN:OD1	1:F:81:ILE:HD13	1.74	0.85
1:D:38:SER:O	1:D:41:LYS:HB2	1.76	0.85
1:A:118:SER:O	1:A:119:LYS:HG2	1.76	0.85
1:F:16:ASN:CG	1:F:81:ILE:HD13	1.97	0.85
1:B:39:PHE:HB2	2:B:148:HOH:O	1.77	0.85
1:A:33:ALA:HB3	1:A:35:TYR:CE1	2.09	0.84
1:E:85:GLU:HA	1:E:111:PHE:CE2	2.12	0.84
1:E:48:ARG:CG	1:E:49:TYR:C	2.45	0.84
1:A:10:THR:O	1:A:11:VAL:HG12	1.77	0.83
1:B:26:VAL:HG12	1:B:27:THR:H	1.42	0.83
1:F:11:VAL:HG13	1:F:111:PHE:CE1	2.13	0.83
1:E:32:LEU:N	1:E:32:LEU:HD13	1.91	0.83
1:B:126:SER:OG	1:B:127:SER:HB3	1.79	0.83
1:A:35:TYR:CD2	1:A:45:TYR:HA	2.14	0.82
1:A:97:GLU:HB3	1:A:102:LYS:NZ	1.94	0.82
1:C:12:LYS:HA	1:C:112:GLU:HG3	0.84	0.82
1:C:12:LYS:CA	1:C:112:GLU:CG	2.49	0.82
1:B:26:VAL:CG1	1:B:27:THR:N	2.41	0.82
1:B:124:GLU:HG3	1:B:125:GLY:H	1.43	0.82
1:A:27:THR:HB	1:A:95:GLU:OE2	1.79	0.81
1:F:94:GLY:HA2	1:F:103:PHE:HA	1.60	0.81
1:C:97:GLU:CB	1:C:102:LYS:NZ	2.44	0.81
1:D:84:ARG:O	1:D:111:PHE:CZ	2.32	0.81
1:C:3:ILE:HD13	1:D:44:GLN:NE2	1.96	0.81
1:B:127:SER:HB2	1:B:128:CYS:CA	2.10	0.81
1:E:23:MET:CB	1:E:74:GLN:O	2.29	0.81
1:C:12:LYS:HB3	1:C:112:GLU:OE2	1.81	0.81
1:C:126:SER:O	1:C:127:SER:HB2	1.80	0.81
1:A:99:ILE:HG21	1:B:31:ASN:HD21	1.44	0.80
1:B:114:SER:HB3	1:B:116:GLU:N	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLU:HA	1:C:111:PHE:CE2	2.16	0.80
1:C:122:ASP:C	1:C:124:GLU:H	1.84	0.80
1:C:12:LYS:HG3	1:C:112:GLU:HG2	1.64	0.80
1:E:48:ARG:HD2	1:E:49:TYR:O	1.80	0.80
1:E:41:LYS:HD2	1:F:3:ILE:HG13	1.63	0.80
1:F:29:LYS:C	1:F:31:ASN:H	1.79	0.80
1:A:23:MET:H	1:A:24:SER:HB2	1.47	0.79
1:A:69:MET:HB3	1:A:77:ASP:O	1.82	0.79
1:B:123:GLY:O	1:B:124:GLU:HB2	1.80	0.79
1:A:96:VAL:H	1:A:101:ILE:CD1	1.87	0.79
1:E:37:GLN:HA	2:E:138:HOH:O	1.82	0.79
1:A:6:LEU:CD1	1:B:42:VAL:HG23	2.12	0.79
1:A:85:GLU:OE1	1:A:86:ASP:N	2.13	0.79
1:F:62:PHE:CZ	1:F:67:PHE:HE2	1.99	0.79
1:C:13:ARG:HE	1:C:111:PHE:HD1	1.30	0.79
1:C:125:GLY:C	1:C:127:SER:H	1.86	0.79
1:F:46:PHE:CE2	1:F:78:LEU:HD11	2.18	0.79
1:B:126:SER:CB	1:B:127:SER:CA	2.42	0.79
1:C:85:GLU:CA	1:C:111:PHE:CE1	2.66	0.79
1:F:6:LEU:HD21	1:F:90:GLU:OE2	1.83	0.79
1:C:12:LYS:HG2	1:C:112:GLU:CG	2.12	0.78
1:A:116:GLU:HG3	1:A:116:GLU:O	1.81	0.78
1:C:12:LYS:CG	1:C:112:GLU:CG	2.60	0.78
1:B:127:SER:OG	1:B:128:CYS:HB2	1.83	0.78
1:B:114:SER:HB2	1:B:116:GLU:N	1.99	0.78
1:C:67:PHE:CD1	1:C:80:ILE:HD12	2.17	0.78
1:E:32:LEU:N	1:E:32:LEU:CD1	2.47	0.78
1:C:44:GLN:NE2	1:D:3:ILE:HD12	1.98	0.78
1:E:11:VAL:O	1:E:111:PHE:HA	1.84	0.78
1:A:23:MET:H	1:A:24:SER:HB3	1.46	0.78
1:C:122:ASP:C	1:C:124:GLU:N	2.37	0.78
1:B:126:SER:HB2	1:B:127:SER:HA	0.83	0.77
1:E:78:LEU:HD23	1:E:79:ASN:H	1.48	0.77
1:E:42:VAL:HG22	1:E:43:PRO:HD2	1.66	0.77
1:A:35:TYR:CD2	1:A:45:TYR:CA	2.67	0.77
1:D:123:GLY:O	1:D:124:GLU:HB2	1.83	0.77
1:E:5:GLU:HG2	1:F:40:GLY:O	1.83	0.77
1:C:104:THR:O	1:C:105:SER:HB3	1.84	0.77
1:C:85:GLU:CA	1:C:111:PHE:CZ	2.64	0.77
1:F:17:VAL:HG11	1:F:109:LEU:CD1	2.14	0.77
1:A:31:ASN:HD22	1:A:31:ASN:N	1.79	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:CZ	1:C:85:GLU:HB3	2.14	0.77
1:A:97:GLU:HB3	1:A:102:LYS:HZ1	1.49	0.77
1:E:96:VAL:HG11	1:F:99:ILE:HG22	1.67	0.76
1:D:100:ILE:CG2	1:D:100:ILE:O	2.34	0.76
1:B:127:SER:CB	1:B:128:CYS:HA	2.15	0.76
1:C:42:VAL:CG2	1:D:105:SER:O	2.33	0.76
1:D:23:MET:HB2	1:D:74:GLN:C	2.06	0.75
1:A:4:LYS:HG3	1:A:5:GLU:N	2.01	0.75
1:B:26:VAL:HG12	1:B:28:ASN:N	2.02	0.75
1:C:31:ASN:ND2	1:D:99:ILE:HG22	2.02	0.74
1:A:13:ARG:HD2	1:A:112:GLU:OE1	1.87	0.74
1:A:47:VAL:O	1:A:47:VAL:HG13	1.87	0.74
1:E:62:PHE:HE1	1:E:67:PHE:CD2	2.05	0.74
1:D:38:SER:HB2	1:D:41:LYS:HG3	1.70	0.74
1:A:99:ILE:CG2	1:B:31:ASN:ND2	2.45	0.74
1:F:29:LYS:C	1:F:31:ASN:N	2.38	0.74
1:D:101:ILE:O	1:D:101:ILE:CG2	2.36	0.74
1:C:125:GLY:CA	1:C:126:SER:HB2	2.17	0.74
1:F:56:TYR:CD2	1:F:69:MET:HB2	2.23	0.73
1:B:45:TYR:OH	1:B:48:ARG:HG2	1.88	0.73
1:B:50:TYR:O	1:B:55:GLY:HA2	1.87	0.73
1:E:69:MET:HA	1:E:79:ASN:HD22	1.51	0.73
1:C:67:PHE:CE1	1:C:80:ILE:HD12	2.24	0.73
1:E:6:LEU:HD21	1:E:90:GLU:OE2	1.87	0.73
1:E:85:GLU:HA	1:E:111:PHE:CZ	2.24	0.73
1:C:11:VAL:O	1:C:112:GLU:N	2.22	0.72
1:F:112:GLU:CB	1:F:113:GLY:CA	2.66	0.72
1:F:44:GLN:NE2	2:F:141:HOH:O	2.23	0.72
1:E:72:ASN:HD21	1:E:75:LYS:NZ	1.87	0.72
1:F:62:PHE:HZ	1:F:67:PHE:CE2	1.93	0.72
1:E:23:MET:CE	1:E:29:LYS:HE2	2.18	0.72
1:D:108:ARG:HE	1:D:110:GLN:NE2	1.87	0.72
1:B:66:ARG:HB2	1:B:66:ARG:HH11	1.54	0.72
1:A:84:ARG:C	1:A:85:GLU:HG3	2.10	0.72
1:E:97:GLU:HG2	1:E:97:GLU:O	1.88	0.72
1:E:66:ARG:HB2	1:E:66:ARG:NH1	2.04	0.72
1:A:33:ALA:HB1	1:A:35:TYR:CE1	2.25	0.72
1:E:94:GLY:CA	1:E:103:PHE:HA	2.20	0.72
1:C:125:GLY:N	1:C:126:SER:HB2	2.04	0.71
1:E:62:PHE:CE1	1:E:67:PHE:CD2	2.77	0.71
1:C:3:ILE:HD12	1:C:4:LYS:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLY:O	1:A:114:SER:HB2	1.88	0.71
1:A:23:MET:O	1:A:26:VAL:HB	1.90	0.71
1:C:31:ASN:ND2	1:D:99:ILE:CG2	2.52	0.71
1:C:22:SER:OG	1:C:24:SER:HB2	1.91	0.71
1:B:85:GLU:OE2	1:B:86:ASP:HB3	1.91	0.71
1:A:92:PHE:HA	1:A:106:GLY:HA3	1.71	0.71
1:A:91:TYR:O	1:A:107:THR:N	2.23	0.71
1:A:84:ARG:O	1:A:85:GLU:CG	2.38	0.70
1:A:28:ASN:O	1:A:30:ASN:N	2.24	0.70
1:F:51:SER:O	1:F:52:SER:HB3	1.92	0.70
1:F:111:PHE:CE1	2:F:142:HOH:O	2.43	0.70
1:C:45:TYR:CE2	1:C:59:ALA:HB2	2.27	0.70
1:F:26:VAL:HG13	1:F:95:GLU:OE1	1.91	0.70
1:C:11:VAL:HG11	1:C:109:LEU:CD1	2.20	0.70
1:C:45:TYR:CE2	1:C:59:ALA:CB	2.75	0.70
1:E:69:MET:CA	1:E:79:ASN:HD21	2.03	0.70
1:F:46:PHE:HE2	1:F:78:LEU:HD11	1.54	0.70
1:E:42:VAL:HG22	1:E:43:PRO:CD	2.21	0.70
1:C:23:MET:HB2	1:C:74:GLN:O	1.91	0.70
1:B:7:HIS:CD2	1:B:9:LYS:HE3	2.26	0.70
1:E:48:ARG:NE	1:E:50:TYR:HD1	1.90	0.69
1:E:6:LEU:CD1	1:F:41:LYS:C	2.60	0.69
1:C:122:ASP:HB3	1:C:124:GLU:H	1.55	0.69
1:C:24:SER:O	1:C:25:LYS:HB2	1.91	0.69
1:C:42:VAL:HG21	1:D:105:SER:O	1.92	0.69
1:E:99:ILE:HG22	1:F:96:VAL:HG11	1.74	0.69
1:D:36:ARG:HG3	1:D:91:TYR:CE2	2.27	0.69
1:A:11:VAL:O	1:A:111:PHE:HA	1.92	0.69
1:E:69:MET:CA	1:E:79:ASN:HD22	2.04	0.69
1:E:13:ARG:HH22	1:E:85:GLU:HB3	1.57	0.69
1:C:118:SER:HA	1:C:120:SER:OG	1.92	0.69
1:C:47:VAL:HG23	1:C:58:PHE:HA	1.74	0.69
1:F:42:VAL:HG22	1:F:43:PRO:HD2	1.75	0.69
1:C:118:SER:OG	1:C:119:LYS:N	2.26	0.69
1:C:12:LYS:CB	1:C:112:GLU:OE2	2.40	0.69
1:E:69:MET:HA	1:E:79:ASN:HD21	1.57	0.69
1:D:17:VAL:CG2	1:D:80:ILE:HB	2.23	0.68
1:E:5:GLU:CG	1:F:40:GLY:O	2.40	0.68
1:C:3:ILE:CD1	1:D:44:GLN:NE2	2.56	0.68
1:D:11:VAL:HG21	1:D:17:VAL:CG1	2.23	0.68
1:C:84:ARG:N	1:C:111:PHE:CZ	2.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:LEU:HD13	1:F:41:LYS:CA	2.24	0.68
1:E:23:MET:HG2	1:E:74:GLN:O	1.94	0.67
1:A:31:ASN:ND2	1:B:99:ILE:HG21	2.08	0.67
1:F:62:PHE:CE2	2:F:140:HOH:O	2.47	0.67
1:B:124:GLU:HG3	1:B:125:GLY:N	2.09	0.67
1:A:124:GLU:O	1:A:126:SER:HB3	1.94	0.67
1:B:75:LYS:HD2	1:B:77:ASP:OD2	1.95	0.67
1:F:62:PHE:HZ	1:F:64:ASP:CB	2.04	0.67
1:A:91:TYR:O	1:A:106:GLY:HA3	1.95	0.67
1:D:64:ASP:O	1:D:66:ARG:N	2.28	0.67
1:E:15:GLU:O	1:E:83:ALA:HB2	1.95	0.67
1:E:48:ARG:NE	1:E:50:TYR:CD1	2.62	0.67
1:B:127:SER:OG	1:B:128:CYS:CB	2.44	0.66
1:A:35:TYR:CD2	1:A:45:TYR:HB2	2.30	0.66
1:D:119:LYS:O	1:D:120:SER:OG	2.12	0.66
1:F:62:PHE:CE1	1:F:67:PHE:HE2	2.11	0.66
1:B:84:ARG:HG2	1:B:84:ARG:O	1.94	0.66
1:B:84:ARG:O	1:B:86:ASP:N	2.28	0.66
1:A:11:VAL:HG11	1:A:15:GLU:OE2	1.94	0.66
1:D:11:VAL:HG21	1:D:17:VAL:HG11	1.78	0.66
1:E:103:PHE:HB3	1:F:42:VAL:HG21	1.76	0.66
1:D:123:GLY:O	1:D:124:GLU:CB	2.44	0.66
1:C:3:ILE:HD12	1:C:4:LYS:N	2.09	0.66
1:D:7:HIS:CD2	1:D:9:LYS:HE2	2.30	0.66
1:B:127:SER:CB	1:B:128:CYS:CA	2.70	0.66
1:A:112:GLU:HA	1:A:112:GLU:OE2	1.96	0.66
1:D:47:VAL:HG23	1:D:57:LYS:O	1.95	0.66
1:A:6:LEU:HD12	1:B:42:VAL:HG23	1.76	0.65
1:B:67:PHE:CE1	1:B:80:ILE:HG13	2.31	0.65
1:C:84:ARG:NH2	1:C:86:ASP:OD1	2.29	0.65
1:E:69:MET:N	1:E:79:ASN:HD22	1.95	0.65
1:C:125:GLY:CA	1:C:127:SER:H	2.09	0.65
1:F:11:VAL:HG21	1:F:17:VAL:HG22	1.78	0.65
1:D:84:ARG:NH2	1:D:86:ASP:OD1	2.29	0.65
1:B:11:VAL:HG21	1:B:17:VAL:CG1	2.27	0.65
1:D:23:MET:HG3	1:D:73:ASP:O	1.96	0.65
1:E:32:LEU:CD1	1:E:95:GLU:HB2	2.26	0.65
1:F:94:GLY:CA	1:F:103:PHE:HA	2.26	0.65
1:C:85:GLU:N	1:C:85:GLU:OE1	2.30	0.65
1:A:85:GLU:CD	1:A:86:ASP:H	2.00	0.65
1:F:17:VAL:CG1	1:F:109:LEU:HD13	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ILE:N	1:D:80:ILE:HD12	2.12	0.65
1:E:96:VAL:HG21	1:F:99:ILE:O	1.97	0.65
1:B:111:PHE:C	1:B:113:GLY:HA2	2.15	0.64
1:B:114:SER:HB3	1:B:115:ASN:C	2.17	0.64
1:C:99:ILE:O	1:C:100:ILE:HG13	1.97	0.64
1:A:31:ASN:CG	1:B:99:ILE:HG22	2.17	0.64
1:B:112:GLU:N	1:B:113:GLY:CA	2.60	0.64
1:B:112:GLU:OE2	1:B:116:GLU:HB3	1.97	0.64
1:C:11:VAL:HG22	1:C:12:LYS:N	2.13	0.64
1:A:11:VAL:HG21	1:A:15:GLU:CD	2.17	0.64
1:D:50:TYR:HD2	1:D:52:SER:HB2	1.61	0.64
1:B:108:ARG:NH1	1:B:110:GLN:HE22	1.94	0.64
1:E:48:ARG:HG3	1:E:49:TYR:N	2.12	0.64
1:A:45:TYR:OH	1:A:48:ARG:HD3	1.97	0.64
1:F:121:SER:O	1:F:123:GLY:N	2.30	0.64
1:E:78:LEU:CD2	1:E:79:ASN:H	2.09	0.64
1:B:24:SER:O	1:B:25:LYS:CB	2.45	0.64
1:F:37:GLN:HG3	1:F:43:PRO:HG3	1.77	0.64
1:F:5:GLU:O	1:F:6:LEU:C	2.36	0.63
1:B:69:MET:HA	1:B:77:ASP:O	1.98	0.63
1:F:23:MET:O	1:F:26:VAL:HG23	1.99	0.63
1:B:70:THR:HG23	2:B:146:HOH:O	1.98	0.63
1:C:125:GLY:C	1:C:127:SER:N	2.52	0.63
1:A:31:ASN:ND2	1:B:99:ILE:CG2	2.62	0.63
1:E:6:LEU:HD13	1:F:41:LYS:C	2.18	0.63
1:E:36:ARG:HB2	1:E:91:TYR:CE2	2.34	0.63
1:B:111:PHE:O	1:B:113:GLY:HA2	1.98	0.63
1:C:13:ARG:NH2	1:C:85:GLU:HG3	2.14	0.63
1:E:36:ARG:HB2	1:E:91:TYR:CD2	2.34	0.63
1:A:6:LEU:HD22	1:B:41:LYS:O	1.99	0.63
1:F:60:GLU:O	1:F:62:PHE:N	2.32	0.62
1:A:12:LYS:CB	1:A:112:GLU:OE2	2.35	0.62
1:B:67:PHE:CE1	1:B:80:ILE:CG1	2.82	0.62
1:C:84:ARG:HH21	1:C:86:ASP:CG	2.02	0.62
1:F:16:ASN:OD1	1:F:81:ILE:HA	1.99	0.62
1:A:13:ARG:HE	1:A:85:GLU:HB3	1.64	0.62
1:E:13:ARG:O	1:E:15:GLU:N	2.32	0.62
1:C:13:ARG:NH2	1:C:85:GLU:CG	2.61	0.62
1:F:62:PHE:CD2	2:F:140:HOH:O	2.52	0.62
1:C:6:LEU:CD1	1:D:42:VAL:CG2	2.75	0.62
1:C:13:ARG:HH21	1:C:85:GLU:HB2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:SER:CA	2:B:143:HOH:O	2.46	0.62
1:E:48:ARG:HG3	1:E:49:TYR:CA	2.29	0.62
1:E:13:ARG:NH2	1:E:85:GLU:HB3	2.15	0.62
1:E:42:VAL:CG2	1:E:43:PRO:CD	2.77	0.62
1:C:125:GLY:HA2	1:C:126:SER:HB2	1.80	0.61
1:B:13:ARG:NH2	1:B:85:GLU:HB3	2.16	0.61
1:B:126:SER:OG	1:B:127:SER:CB	2.48	0.61
1:D:27:THR:HB	1:D:95:GLU:OE2	2.00	0.61
1:C:37:GLN:HG2	1:C:38:SER:O	2.00	0.61
1:C:13:ARG:HD2	1:C:13:ARG:H	1.65	0.61
1:D:31:ASN:O	1:D:95:GLU:HA	2.00	0.61
1:A:42:VAL:HB	1:B:4:LYS:O	2.00	0.61
1:D:97:GLU:OE2	1:D:102:LYS:NZ	2.31	0.61
1:B:85:GLU:N	1:B:111:PHE:CZ	2.68	0.61
1:E:48:ARG:CD	1:E:50:TYR:HD1	2.13	0.61
1:F:107:THR:HG22	1:F:108:ARG:C	2.21	0.61
1:F:60:GLU:O	1:F:61:GLY:C	2.39	0.61
1:C:13:ARG:HH22	1:C:85:GLU:HG3	1.65	0.61
1:D:67:PHE:CE1	1:D:80:ILE:CG1	2.84	0.61
1:C:13:ARG:HD2	1:C:13:ARG:N	2.17	0.60
1:C:18:THR:HG23	1:C:78:LEU:O	2.00	0.60
1:C:85:GLU:HA	1:C:111:PHE:CD1	2.36	0.60
1:E:48:ARG:HD2	1:E:50:TYR:HD1	1.66	0.60
1:A:45:TYR:CG	1:B:100:ILE:HD12	2.36	0.60
1:D:50:TYR:HD2	1:D:52:SER:CB	2.15	0.60
1:A:21:CYS:HB2	1:A:34:TRP:CZ2	2.36	0.60
1:F:10:THR:HA	1:F:110:GLN:O	2.01	0.60
1:B:114:SER:HB2	1:B:116:GLU:HB2	1.84	0.60
1:D:99:ILE:HD12	1:D:100:ILE:HG12	1.84	0.60
1:B:7:HIS:HD2	1:B:9:LYS:HE3	1.67	0.60
1:E:31:ASN:C	1:E:32:LEU:HD13	2.23	0.59
1:A:60:GLU:O	1:A:62:PHE:N	2.35	0.59
1:A:84:ARG:O	1:A:85:GLU:CB	2.50	0.59
1:D:17:VAL:HG22	1:D:80:ILE:HB	1.85	0.59
1:C:31:ASN:HD21	1:D:99:ILE:CG2	2.13	0.59
1:D:84:ARG:O	1:D:111:PHE:HZ	1.82	0.59
1:F:62:PHE:CE2	1:F:67:PHE:HD2	2.21	0.59
1:F:68:SER:O	1:F:78:LEU:HD23	2.01	0.59
1:B:11:VAL:HG21	1:B:17:VAL:HG11	1.83	0.59
1:D:56:TYR:N	1:D:56:TYR:CD2	2.70	0.59
1:C:114:SER:O	1:C:115:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:GLU:HG3	1:F:117:GLY:H	1.66	0.59
1:F:87:ASP:O	1:F:88:GLY:C	2.41	0.59
1:E:28:ASN:CG	1:E:29:LYS:O	2.41	0.59
1:E:23:MET:CG	1:E:74:GLN:O	2.51	0.59
1:D:28:ASN:O	1:D:30:ASN:N	2.36	0.59
1:F:66:ARG:NH2	1:F:84:ARG:HG2	2.17	0.59
1:B:23:MET:O	1:B:25:LYS:N	2.36	0.59
1:E:66:ARG:NH2	1:E:87:ASP:OD2	2.36	0.58
1:B:108:ARG:CZ	1:B:110:GLN:NE2	2.67	0.58
1:E:7:HIS:NE2	1:E:9:LYS:HE3	2.18	0.58
1:A:23:MET:N	1:A:24:SER:HB3	2.16	0.58
1:E:23:MET:N	1:E:74:GLN:O	2.36	0.58
1:C:31:ASN:N	1:C:31:ASN:HD22	2.00	0.58
1:E:103:PHE:HB3	1:F:42:VAL:CG2	2.33	0.58
1:C:23:MET:HA	1:C:26:VAL:CG2	2.34	0.58
1:C:42:VAL:HB	1:D:4:LYS:O	2.03	0.58
1:C:7:HIS:CD2	1:C:9:LYS:HE3	2.39	0.58
1:B:26:VAL:CG1	1:B:27:THR:H	2.10	0.58
1:F:37:GLN:HG3	1:F:43:PRO:CG	2.34	0.58
1:F:88:GLY:HA2	1:F:109:LEU:O	2.04	0.58
1:C:44:GLN:CD	1:D:3:ILE:HD12	2.24	0.58
1:F:66:ARG:CZ	1:F:84:ARG:HD3	2.34	0.57
1:E:12:LYS:O	1:E:13:ARG:C	2.41	0.57
1:D:50:TYR:CD2	1:D:52:SER:HB2	2.39	0.57
1:F:118:SER:N	2:F:144:HOH:O	2.37	0.57
1:A:120:SER:O	1:A:121:SER:HB2	2.03	0.57
1:B:32:LEU:HB2	1:B:95:GLU:HB2	1.87	0.57
1:D:21:CYS:CB	1:D:93:CYS:HG	2.15	0.57
1:B:66:ARG:NH2	1:B:87:ASP:OD2	2.38	0.57
1:F:99:ILE:H	1:F:99:ILE:HD12	1.69	0.57
1:D:101:ILE:O	1:D:101:ILE:HG23	2.05	0.57
1:C:21:CYS:HB2	1:C:34:TRP:CZ2	2.39	0.57
1:B:26:VAL:HG12	1:B:27:THR:C	2.25	0.57
1:A:96:VAL:HG23	1:A:101:ILE:HD12	1.86	0.57
1:E:68:SER:C	1:E:79:ASN:HD22	2.08	0.57
1:C:26:VAL:HG11	1:C:29:LYS:HG2	1.87	0.57
1:C:104:THR:O	1:C:105:SER:CB	2.47	0.57
1:C:13:ARG:HH21	1:C:85:GLU:HB3	1.48	0.57
1:A:113:GLY:O	1:A:114:SER:CB	2.52	0.57
1:E:32:LEU:HD12	1:E:95:GLU:HB2	1.86	0.57
1:E:33:ALA:O	1:E:76:PHE:HE2	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ARG:CG	1:B:81:ILE:O	2.52	0.56
1:A:22:SER:O	1:A:26:VAL:HG21	2.05	0.56
1:C:29:LYS:HB3	1:C:49:TYR:CE1	2.40	0.56
1:B:126:SER:CB	1:B:127:SER:CB	2.82	0.56
1:D:23:MET:CB	1:D:74:GLN:O	2.38	0.56
1:C:67:PHE:O	1:C:68:SER:HB3	2.05	0.56
1:E:21:CYS:HB2	1:E:34:TRP:CZ2	2.41	0.56
1:F:99:ILE:HD12	1:F:100:ILE:HD12	1.87	0.56
1:A:3:ILE:O	1:A:3:ILE:HG23	2.04	0.56
1:E:24:SER:O	1:E:25:LYS:HB2	2.05	0.56
1:A:23:MET:HB2	1:A:74:GLN:O	2.06	0.56
1:A:47:VAL:HB	1:A:58:PHE:CD1	2.40	0.56
1:E:66:ARG:CZ	1:E:66:ARG:HB2	2.35	0.56
1:F:121:SER:C	1:F:123:GLY:H	2.08	0.56
1:D:115:ASN:HD21	1:D:126:SER:HB3	1.69	0.56
1:C:11:VAL:CG2	1:C:12:LYS:N	2.68	0.56
1:C:74:GLN:HB3	1:C:75:LYS:HG2	1.88	0.56
1:A:90:GLU:CD	1:B:37:GLN:HE22	2.09	0.56
1:A:11:VAL:O	1:A:111:PHE:CA	2.53	0.56
1:C:110:GLN:HG2	1:C:110:GLN:O	2.05	0.56
1:A:13:ARG:CD	1:A:112:GLU:OE1	2.52	0.56
1:E:111:PHE:O	1:E:112:GLU:C	2.44	0.56
1:B:14:GLY:HA2	1:F:81:ILE:HG21	1.86	0.56
1:F:85:GLU:HG3	2:F:142:HOH:O	2.06	0.56
1:E:5:GLU:HG3	1:F:41:LYS:HG2	1.87	0.56
1:D:66:ARG:HG2	1:D:81:ILE:O	2.05	0.56
1:D:29:LYS:O	1:D:49:TYR:CD1	2.59	0.56
1:D:84:ARG:HH21	1:D:86:ASP:CG	2.10	0.56
1:F:64:ASP:OD2	1:F:66:ARG:NH1	2.38	0.55
1:A:35:TYR:CD2	1:A:45:TYR:CB	2.89	0.55
1:B:13:ARG:CG	1:F:81:ILE:CD1	2.75	0.55
1:A:26:VAL:CG1	1:A:27:THR:N	2.68	0.55
1:B:35:TYR:CD2	1:B:45:TYR:N	2.75	0.55
1:E:4:LYS:HD3	1:E:5:GLU:H	1.71	0.55
1:C:114:SER:O	1:C:115:ASN:CB	2.54	0.55
1:F:7:HIS:NE2	1:F:8:VAL:O	2.40	0.55
1:B:114:SER:HB3	1:B:116:GLU:CA	2.36	0.55
1:C:67:PHE:CE1	1:C:80:ILE:CD1	2.89	0.55
1:A:91:TYR:O	1:A:106:GLY:CA	2.55	0.55
1:E:56:TYR:CD2	1:E:69:MET:HB2	2.41	0.55
1:E:31:ASN:C	1:E:32:LEU:CD1	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:VAL:HG22	1:F:43:PRO:CD	2.36	0.55
1:E:66:ARG:CB	1:E:66:ARG:CZ	2.85	0.55
1:F:118:SER:O	1:F:119:LYS:HB2	2.07	0.55
1:B:114:SER:HB2	1:B:116:GLU:H	1.72	0.55
1:C:122:ASP:CB	1:C:124:GLU:H	2.19	0.55
1:E:41:LYS:HD2	1:F:3:ILE:CG1	2.36	0.55
1:E:99:ILE:HG13	1:E:100:ILE:HD12	1.89	0.55
1:F:30:ASN:C	1:F:31:ASN:HD22	2.10	0.55
1:A:31:ASN:ND2	1:A:31:ASN:N	2.49	0.55
1:B:75:LYS:HD2	1:B:77:ASP:CG	2.27	0.55
1:B:112:GLU:OE2	1:B:116:GLU:CB	2.56	0.54
1:B:66:ARG:HG2	1:B:81:ILE:O	2.07	0.54
1:C:122:ASP:O	1:C:124:GLU:HG2	2.07	0.54
1:A:99:ILE:HG21	1:B:31:ASN:CG	2.25	0.54
1:A:24:SER:C	1:A:25:LYS:HG3	2.27	0.54
1:A:4:LYS:HG3	1:A:5:GLU:H	1.72	0.54
1:E:78:LEU:CD2	1:E:79:ASN:N	2.69	0.54
1:E:11:VAL:N	1:E:110:GLN:O	2.36	0.54
1:D:101:ILE:O	1:D:101:ILE:HG22	2.07	0.54
1:F:117:GLY:HA2	2:F:144:HOH:O	2.07	0.54
1:B:26:VAL:HG12	1:B:27:THR:CA	2.36	0.54
1:C:67:PHE:CD1	1:C:80:ILE:CD1	2.89	0.54
1:A:46:PHE:HE1	1:A:62:PHE:CE1	2.26	0.54
1:B:66:ARG:CB	1:B:66:ARG:HH11	2.19	0.54
1:D:69:MET:HG2	1:D:78:LEU:HD23	1.89	0.54
1:A:45:TYR:CZ	1:A:48:ARG:HD3	2.42	0.54
1:C:18:THR:HA	1:C:78:LEU:O	2.08	0.54
1:B:85:GLU:N	1:B:111:PHE:CE1	2.76	0.54
1:B:108:ARG:CZ	1:B:110:GLN:HE22	2.20	0.54
1:C:66:ARG:HH22	1:C:87:ASP:CG	2.11	0.53
1:E:62:PHE:CZ	1:E:67:PHE:HD2	2.26	0.53
1:C:31:ASN:HD21	1:D:99:ILE:HG22	1.73	0.53
1:C:44:GLN:NE2	1:D:3:ILE:CD1	2.70	0.53
1:B:19:MET:N	1:B:78:LEU:O	2.31	0.53
1:F:62:PHE:CE2	1:F:67:PHE:CD2	2.95	0.53
1:A:109:LEU:HD21	1:A:111:PHE:CE2	2.43	0.53
1:C:124:GLU:HG3	1:C:124:GLU:O	2.08	0.53
1:D:97:GLU:CD	1:D:102:LYS:NZ	2.62	0.53
1:C:11:VAL:CG1	1:C:109:LEU:HD11	2.32	0.53
1:A:92:PHE:HB2	1:A:103:PHE:CD1	2.44	0.53
1:A:124:GLU:HG2	1:A:124:GLU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:GLU:CG	1:F:117:GLY:H	2.22	0.53
1:A:66:ARG:NH2	1:A:87:ASP:OD2	2.42	0.53
1:E:48:ARG:HG2	1:E:50:TYR:HB2	1.90	0.53
1:B:22:SER:HA	2:B:143:HOH:O	2.08	0.53
1:A:23:MET:N	1:A:24:SER:CB	2.56	0.53
1:B:50:TYR:HD2	1:B:52:SER:HB2	1.73	0.53
1:B:114:SER:CB	1:B:116:GLU:CA	2.87	0.53
1:F:6:LEU:CD2	1:F:90:GLU:OE2	2.55	0.53
1:E:13:ARG:C	1:E:15:GLU:H	2.10	0.53
1:A:22:SER:O	1:A:26:VAL:CG2	2.57	0.52
1:F:47:VAL:HG13	1:F:47:VAL:O	2.10	0.52
1:C:45:TYR:HE1	1:C:48:ARG:HB3	1.73	0.52
1:C:91:TYR:O	1:C:106:GLY:HA3	2.09	0.52
1:F:91:TYR:O	1:F:106:GLY:HA2	2.09	0.52
1:F:11:VAL:O	1:F:111:PHE:CD1	2.63	0.52
1:E:96:VAL:CG1	1:F:99:ILE:HG22	2.36	0.52
1:A:10:THR:HA	1:A:110:GLN:O	2.09	0.52
1:E:78:LEU:HD23	1:E:79:ASN:N	2.21	0.52
1:A:28:ASN:C	1:A:30:ASN:H	2.13	0.52
1:E:5:GLU:HA	1:F:41:LYS:HA	1.92	0.52
1:F:72:ASN:HD21	1:F:75:LYS:NZ	2.08	0.52
1:F:38:SER:O	1:F:39:PHE:C	2.48	0.52
1:E:37:GLN:NE2	1:F:90:GLU:OE2	2.39	0.52
1:C:62:PHE:CZ	1:C:64:ASP:HB3	2.44	0.52
1:E:67:PHE:CD1	1:E:80:ILE:HG12	2.45	0.52
1:B:9:LYS:O	1:B:109:LEU:HD12	2.10	0.52
1:A:36:ARG:H	1:A:46:PHE:HB2	1.75	0.52
1:A:23:MET:CB	1:A:74:GLN:O	2.58	0.52
1:E:62:PHE:HE1	1:E:67:PHE:CE2	2.27	0.52
1:E:46:PHE:CE2	1:E:78:LEU:HD11	2.45	0.52
1:F:62:PHE:CD1	1:F:63:LYS:N	2.78	0.51
1:A:17:VAL:HG21	1:A:109:LEU:HD13	1.91	0.51
1:A:26:VAL:HG12	1:A:27:THR:N	2.24	0.51
1:B:23:MET:N	2:B:143:HOH:O	2.42	0.51
1:B:114:SER:CB	1:B:116:GLU:HB2	2.39	0.51
1:E:50:TYR:N	1:E:55:GLY:O	2.36	0.51
1:A:96:VAL:HG23	1:A:101:ILE:CD1	2.39	0.51
1:F:99:ILE:H	1:F:99:ILE:CD1	2.23	0.51
1:E:72:ASN:HD21	1:E:75:LYS:HZ1	1.58	0.51
1:D:28:ASN:OD1	1:D:28:ASN:C	2.48	0.51
1:B:28:ASN:OD1	1:B:30:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:GLU:CA	1:F:41:LYS:HD3	2.40	0.51
1:D:37:GLN:CG	1:D:41:LYS:O	2.57	0.51
1:A:120:SER:O	1:A:121:SER:CB	2.58	0.51
1:C:68:SER:O	1:C:78:LEU:HD23	2.09	0.51
1:E:91:TYR:O	1:E:106:GLY:HA2	2.10	0.51
1:E:69:MET:N	1:E:79:ASN:ND2	2.57	0.51
1:A:35:TYR:HD2	1:A:45:TYR:N	2.07	0.51
1:E:72:ASN:HD21	1:E:75:LYS:HZ3	1.55	0.51
1:C:45:TYR:CE1	1:C:48:ARG:HB3	2.46	0.51
1:E:40:GLY:O	1:F:5:GLU:HG3	2.11	0.51
1:C:69:MET:HA	1:C:77:ASP:O	2.11	0.51
1:B:26:VAL:CG1	1:B:95:GLU:OE2	2.59	0.51
1:E:32:LEU:HD12	1:E:95:GLU:CB	2.42	0.51
1:E:48:ARG:HD2	1:E:50:TYR:HA	1.93	0.50
1:E:42:VAL:CG2	1:E:43:PRO:HD2	2.38	0.50
1:E:29:LYS:C	1:E:31:ASN:H	2.15	0.50
1:B:62:PHE:HZ	1:B:67:PHE:CD2	2.29	0.50
1:B:47:VAL:HG23	1:B:58:PHE:HA	1.94	0.50
1:A:28:ASN:C	1:A:30:ASN:N	2.62	0.50
1:C:23:MET:HA	1:C:26:VAL:HG23	1.94	0.50
1:B:108:ARG:CG	1:B:108:ARG:O	2.59	0.50
1:E:33:ALA:HB3	2:E:144:HOH:O	2.11	0.50
1:E:26:VAL:HG12	1:E:26:VAL:O	2.11	0.50
1:B:49:TYR:CD1	1:B:50:TYR:N	2.80	0.50
1:B:79:ASN:C	1:B:80:ILE:HD12	2.32	0.50
1:D:23:MET:CG	1:D:73:ASP:O	2.60	0.50
1:B:120:SER:CB	1:B:121:SER:HB2	2.42	0.50
1:E:81:ILE:HD12	1:E:81:ILE:N	2.26	0.50
1:F:67:PHE:HA	1:F:79:ASN:O	2.11	0.50
1:A:96:VAL:N	1:A:101:ILE:CD1	2.59	0.50
1:C:122:ASP:O	1:C:124:GLU:N	2.44	0.50
1:E:72:ASN:ND2	1:E:75:LYS:NZ	2.57	0.50
1:B:127:SER:CB	1:B:128:CYS:CB	2.90	0.50
1:C:31:ASN:ND2	1:D:99:ILE:HG21	2.26	0.50
1:F:14:GLY:HA2	1:F:82:GLY:HA2	1.94	0.50
1:A:44:GLN:NE2	1:B:3:ILE:HG13	2.26	0.50
1:B:23:MET:CE	1:B:29:LYS:HD3	2.42	0.50
1:A:47:VAL:O	1:A:47:VAL:CG1	2.59	0.50
1:F:45:TYR:OH	1:F:48:ARG:HD3	2.12	0.50
1:D:38:SER:HB2	1:D:41:LYS:CG	2.40	0.49
1:B:49:TYR:C	1:B:49:TYR:CD1	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLU:CD	1:D:102:LYS:HZ3	2.16	0.49
1:A:22:SER:HB3	1:A:24:SER:CB	2.42	0.49
1:E:19:MET:HG2	1:E:107:THR:HG21	1.94	0.49
1:E:41:LYS:HA	1:F:5:GLU:HA	1.93	0.49
1:A:3:ILE:HG13	1:B:44:GLN:NE2	2.27	0.49
1:A:64:ASP:OD1	1:A:66:ARG:NH1	2.45	0.49
1:D:75:LYS:HD2	1:D:77:ASP:OD2	2.12	0.49
1:B:35:TYR:N	1:B:35:TYR:CD1	2.80	0.49
1:A:124:GLU:O	1:A:124:GLU:CG	2.59	0.49
1:C:94:GLY:HA3	1:C:101:ILE:CD1	2.42	0.49
1:C:108:ARG:NH1	1:D:40:GLY:HA2	2.26	0.49
1:F:9:LYS:NZ	1:F:18:THR:O	2.45	0.49
1:B:17:VAL:CG2	1:B:80:ILE:HB	2.42	0.49
1:A:37:GLN:HG2	1:A:38:SER:O	2.11	0.49
1:B:85:GLU:OE2	1:B:86:ASP:CB	2.60	0.49
1:C:45:TYR:CD1	1:D:100:ILE:HD11	2.47	0.49
1:D:28:ASN:O	1:D:28:ASN:OD1	2.31	0.49
1:C:7:HIS:HD2	1:C:9:LYS:HE3	1.76	0.49
1:C:66:ARG:NH2	1:C:84:ARG:HB3	2.28	0.49
1:E:46:PHE:HE2	1:E:78:LEU:HD11	1.78	0.49
1:D:86:ASP:O	1:D:86:ASP:OD2	2.30	0.49
1:C:124:GLU:CG	1:C:124:GLU:O	2.59	0.49
1:B:50:TYR:CD2	1:B:52:SER:HB2	2.46	0.49
1:E:63:LYS:O	1:E:64:ASP:HB2	2.13	0.49
1:E:7:HIS:CD2	1:E:9:LYS:HE3	2.47	0.49
1:B:66:ARG:HH21	1:B:84:ARG:HD3	1.76	0.49
1:A:97:GLU:HB3	1:A:102:LYS:HZ3	1.73	0.49
1:C:125:GLY:HA2	1:C:127:SER:N	2.28	0.49
1:F:34:TRP:O	1:F:46:PHE:CB	2.60	0.49
1:B:37:GLN:HB2	1:B:43:PRO:HG3	1.95	0.49
1:E:36:ARG:HG2	1:E:36:ARG:O	2.11	0.49
1:C:97:GLU:CB	1:C:102:LYS:HZ3	2.23	0.49
1:F:11:VAL:CG1	1:F:111:PHE:CE1	2.92	0.49
1:B:115:ASN:OD1	1:B:115:ASN:O	2.30	0.48
1:C:66:ARG:NH2	1:C:87:ASP:OD2	2.43	0.48
1:D:38:SER:O	1:D:41:LYS:CB	2.55	0.48
1:F:23:MET:HB2	1:F:73:ASP:O	2.13	0.48
1:D:12:LYS:HG2	1:D:112:GLU:HG2	1.94	0.48
1:C:11:VAL:CG1	1:C:109:LEU:CD1	2.90	0.48
1:A:90:GLU:OE2	1:B:37:GLN:NE2	2.45	0.48
1:D:111:PHE:O	1:D:113:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:HIS:CD2	1:D:9:LYS:CE	2.96	0.48
1:F:69:MET:HA	1:F:79:ASN:ND2	2.28	0.48
1:C:28:ASN:OD1	1:C:30:ASN:OD1	2.32	0.48
1:C:86:ASP:C	1:C:86:ASP:OD2	2.50	0.48
1:C:108:ARG:HH12	1:D:40:GLY:HA2	1.79	0.48
1:B:82:GLY:O	1:B:83:ALA:C	2.47	0.48
1:E:115:ASN:HB2	1:E:123:GLY:HA2	1.96	0.48
1:B:22:SER:C	2:B:143:HOH:O	2.51	0.48
1:B:123:GLY:O	1:B:124:GLU:CB	2.56	0.48
1:D:21:CYS:CB	1:D:93:CYS:SG	3.00	0.48
1:E:118:SER:O	1:E:119:LYS:HG2	2.13	0.48
1:C:31:ASN:HD21	1:D:99:ILE:HG21	1.79	0.48
1:D:115:ASN:ND2	1:D:126:SER:HB3	2.29	0.48
1:E:26:VAL:CG1	1:E:32:LEU:HD21	2.43	0.48
1:C:45:TYR:CE2	1:C:59:ALA:HB1	2.48	0.48
1:D:66:ARG:NH2	1:D:87:ASP:OD2	2.47	0.47
1:A:11:VAL:O	1:A:111:PHE:C	2.53	0.47
1:A:35:TYR:HB3	1:A:44:GLN:O	2.14	0.47
1:A:45:TYR:CG	1:B:100:ILE:CD1	2.96	0.47
1:B:66:ARG:NH2	1:B:84:ARG:HD3	2.30	0.47
1:E:50:TYR:O	1:E:55:GLY:O	2.32	0.47
1:E:4:LYS:CD	1:E:5:GLU:H	2.27	0.47
1:C:125:GLY:HA2	1:C:127:SER:H	1.80	0.47
1:C:45:TYR:CZ	1:C:59:ALA:HB2	2.49	0.47
1:E:15:GLU:O	1:E:83:ALA:CB	2.62	0.47
1:B:69:MET:HG2	1:B:78:LEU:HD23	1.96	0.47
1:B:126:SER:HB2	1:B:127:SER:CB	2.37	0.47
1:B:26:VAL:CG1	1:B:28:ASN:N	2.74	0.47
1:D:78:LEU:HD22	1:D:79:ASN:H	1.78	0.47
1:D:68:SER:CB	2:D:143:HOH:O	2.63	0.47
1:F:46:PHE:HE2	1:F:78:LEU:CD1	2.23	0.47
1:C:99:ILE:C	1:C:100:ILE:HG13	2.35	0.47
1:C:122:ASP:HB3	1:C:124:GLU:HB3	1.97	0.47
1:E:37:GLN:HG3	1:E:41:LYS:O	2.14	0.47
1:B:70:THR:HA	2:B:146:HOH:O	2.14	0.47
1:D:115:ASN:HD21	1:D:126:SER:CB	2.26	0.47
1:E:119:LYS:NZ	1:E:119:LYS:O	2.40	0.47
1:A:35:TYR:CG	1:A:45:TYR:HA	2.49	0.47
1:E:90:GLU:HA	1:E:107:THR:O	2.14	0.47
1:F:99:ILE:HD12	1:F:100:ILE:CD1	2.45	0.47
1:A:110:GLN:HG2	1:A:110:GLN:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASN:O	1:C:29:LYS:C	2.51	0.47
1:D:52:SER:OG	1:D:53:ASN:N	2.47	0.47
1:C:64:ASP:C	1:C:64:ASP:OD2	2.52	0.47
1:E:123:GLY:O	1:E:126:SER:N	2.46	0.47
1:D:79:ASN:C	1:D:80:ILE:HD12	2.35	0.47
1:B:100:ILE:HA	1:B:100:ILE:HD13	1.74	0.47
1:F:118:SER:O	1:F:119:LYS:CB	2.61	0.47
1:E:48:ARG:HD2	1:E:50:TYR:CD1	2.48	0.46
1:C:84:ARG:O	1:C:86:ASP:N	2.48	0.46
1:B:26:VAL:HG12	1:B:28:ASN:H	1.77	0.46
1:E:28:ASN:OD1	1:E:29:LYS:O	2.33	0.46
1:A:6:LEU:CD1	1:B:42:VAL:CG2	2.88	0.46
1:C:44:GLN:CG	1:D:3:ILE:CD1	2.93	0.46
1:C:47:VAL:HB	1:C:58:PHE:CD1	2.50	0.46
1:A:11:VAL:HG21	1:A:15:GLU:CB	2.45	0.46
1:E:26:VAL:CG2	1:E:32:LEU:HD21	2.45	0.46
1:E:69:MET:C	1:E:79:ASN:HD21	2.18	0.46
1:A:24:SER:C	1:A:26:VAL:H	2.19	0.46
1:C:24:SER:O	1:C:25:LYS:CB	2.60	0.46
1:D:18:THR:HG22	1:D:19:MET:N	2.28	0.46
1:D:64:ASP:OD2	1:D:66:ARG:HD3	2.16	0.46
1:B:67:PHE:CE1	1:B:80:ILE:HG12	2.51	0.46
1:A:85:GLU:CD	1:A:86:ASP:N	2.64	0.46
1:D:68:SER:HB3	2:D:143:HOH:O	2.15	0.46
1:C:101:ILE:O	1:C:101:ILE:CG2	2.64	0.46
1:A:14:GLY:O	1:A:15:GLU:O	2.34	0.46
1:E:119:LYS:HE3	1:E:119:LYS:HB3	1.44	0.46
1:C:45:TYR:HB2	1:D:100:ILE:HD12	1.98	0.46
1:A:10:THR:C	1:A:11:VAL:CG1	2.85	0.46
1:D:108:ARG:NE	1:D:110:GLN:NE2	2.60	0.46
1:A:50:TYR:HD2	1:A:52:SER:HB3	1.81	0.46
1:F:67:PHE:HD1	1:F:80:ILE:HG13	1.81	0.46
1:E:69:MET:HB3	1:E:69:MET:HE2	1.88	0.46
1:C:3:ILE:CD1	1:D:44:GLN:HE21	2.26	0.46
1:C:29:LYS:HB3	1:C:49:TYR:CD1	2.51	0.45
1:B:45:TYR:HE1	1:B:48:ARG:HB3	1.80	0.45
1:E:31:ASN:HA	1:E:31:ASN:HD22	1.43	0.45
1:D:48:ARG:HD2	1:D:49:TYR:O	2.15	0.45
1:D:17:VAL:HG23	1:D:80:ILE:HB	1.98	0.45
1:F:80:ILE:N	1:F:80:ILE:HD12	2.31	0.45
1:F:16:ASN:HA	1:F:80:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ILE:CD1	1:D:80:ILE:N	2.79	0.45
1:F:62:PHE:CE1	1:F:64:ASP:CB	2.85	0.45
1:C:97:GLU:CB	1:C:102:LYS:HZ1	2.03	0.45
1:B:110:GLN:HB3	1:B:110:GLN:HE21	1.56	0.45
1:A:121:SER:HB3	1:A:122:ASP:H	1.57	0.45
1:C:12:LYS:CB	1:C:112:GLU:CG	2.93	0.45
1:D:69:MET:HE1	1:D:76:PHE:CE2	2.52	0.45
1:A:69:MET:CB	1:A:77:ASP:O	2.62	0.45
1:D:64:ASP:O	1:D:65:SER:C	2.55	0.45
1:C:91:TYR:O	1:C:106:GLY:CA	2.64	0.45
1:C:23:MET:HA	1:C:26:VAL:HG21	1.98	0.45
1:C:7:HIS:CD2	1:C:9:LYS:CE	3.00	0.45
1:F:62:PHE:C	1:F:63:LYS:HG2	2.36	0.45
1:F:112:GLU:HG2	1:F:113:GLY:HA2	1.98	0.45
1:E:75:LYS:HB2	1:E:75:LYS:HE2	1.24	0.45
1:C:84:ARG:N	1:C:111:PHE:CE1	2.85	0.45
1:E:12:LYS:O	1:E:15:GLU:HB2	2.17	0.45
1:F:28:ASN:O	1:F:31:ASN:HB2	2.17	0.45
1:B:63:LYS:HG2	1:B:63:LYS:O	2.17	0.45
1:F:46:PHE:CE2	1:F:78:LEU:CD1	2.96	0.44
1:B:80:ILE:HD12	1:B:80:ILE:N	2.32	0.44
1:F:36:ARG:HG3	1:F:91:TYR:CE2	2.51	0.44
1:C:11:VAL:HG23	1:C:15:GLU:HB3	1.98	0.44
1:F:62:PHE:HZ	1:F:67:PHE:HD2	1.21	0.44
1:B:30:ASN:O	1:B:31:ASN:ND2	2.47	0.44
1:C:7:HIS:NE2	1:C:9:LYS:HE2	2.32	0.44
1:A:11:VAL:C	1:A:12:LYS:HG3	2.37	0.44
1:D:42:VAL:O	1:D:42:VAL:CG1	2.65	0.44
1:C:74:GLN:CB	1:C:75:LYS:HG2	2.47	0.44
1:A:4:LYS:HB2	1:A:4:LYS:HE2	1.61	0.44
1:E:72:ASN:ND2	1:E:75:LYS:HZ1	2.16	0.44
1:F:108:ARG:HH11	1:F:108:ARG:HG3	1.83	0.44
1:A:63:LYS:O	1:A:64:ASP:HB2	2.17	0.44
1:B:84:ARG:HG3	1:B:85:GLU:CD	2.34	0.44
1:D:69:MET:HA	1:D:77:ASP:O	2.17	0.44
1:D:37:GLN:HG2	1:D:41:LYS:O	2.16	0.44
1:E:64:ASP:OD1	1:E:66:ARG:NH1	2.50	0.44
1:D:47:VAL:HB	1:D:58:PHE:CD1	2.53	0.44
1:B:46:PHE:HE1	1:B:62:PHE:CE1	2.35	0.44
1:F:15:GLU:O	1:F:83:ALA:HB2	2.17	0.44
1:F:39:PHE:CE2	1:F:88:GLY:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASN:O	1:C:31:ASN:N	2.47	0.44
1:F:23:MET:O	1:F:26:VAL:N	2.41	0.44
1:C:56:TYR:HE1	1:C:58:PHE:HE2	1.66	0.44
1:D:93:CYS:HB3	1:D:105:SER:OG	2.17	0.44
1:F:116:GLU:CG	1:F:117:GLY:N	2.80	0.44
1:D:38:SER:O	1:D:41:LYS:N	2.49	0.44
1:B:38:SER:O	1:B:39:PHE:C	2.56	0.44
1:C:125:GLY:CA	1:C:127:SER:N	2.78	0.44
1:E:3:ILE:HG13	1:F:41:LYS:HD2	1.99	0.44
1:F:12:LYS:HG3	1:F:15:GLU:OE1	2.17	0.44
1:A:40:GLY:O	1:B:5:GLU:HG3	2.18	0.44
1:E:26:VAL:HG21	1:E:32:LEU:HD21	1.99	0.43
1:E:67:PHE:CE1	1:E:80:ILE:HG12	2.53	0.43
1:E:6:LEU:CD1	1:F:42:VAL:N	2.81	0.43
1:B:26:VAL:HG13	1:B:95:GLU:CD	2.38	0.43
1:B:72:ASN:OD1	1:B:74:GLN:N	2.46	0.43
1:C:46:PHE:HE1	1:C:62:PHE:CE1	2.36	0.43
1:C:108:ARG:HH12	1:D:40:GLY:CA	2.31	0.43
1:E:115:ASN:ND2	1:E:123:GLY:HA3	2.33	0.43
1:E:70:THR:N	1:E:79:ASN:HD21	2.15	0.43
1:C:34:TRP:CD2	1:C:93:CYS:HB2	2.53	0.43
1:A:39:PHE:CA	2:A:146:HOH:O	2.46	0.43
1:D:9:LYS:HE2	1:D:9:LYS:HB2	1.56	0.43
1:D:47:VAL:HG22	1:D:48:ARG:N	2.32	0.43
1:B:23:MET:HB2	1:B:74:GLN:O	2.19	0.43
1:E:6:LEU:HD13	1:F:41:LYS:N	2.34	0.43
1:B:56:TYR:CD2	1:B:69:MET:HB2	2.54	0.43
1:C:84:ARG:N	1:C:111:PHE:HZ	1.88	0.43
1:B:37:GLN:HB2	1:B:43:PRO:CB	2.49	0.43
1:E:48:ARG:CD	1:E:50:TYR:CD1	3.00	0.43
1:A:110:GLN:CG	1:A:110:GLN:O	2.67	0.43
1:E:29:LYS:C	1:E:31:ASN:N	2.71	0.43
1:C:45:TYR:OH	1:C:48:ARG:HG2	2.19	0.43
1:D:64:ASP:C	1:D:66:ARG:N	2.71	0.43
1:A:10:THR:O	1:A:11:VAL:CG1	2.57	0.43
1:E:56:TYR:CE2	1:E:69:MET:HB2	2.54	0.43
1:E:26:VAL:HG11	1:E:32:LEU:HD21	2.00	0.43
1:A:13:ARG:HH21	1:A:85:GLU:CB	2.31	0.43
1:C:11:VAL:CG2	1:C:12:LYS:H	2.31	0.42
1:C:56:TYR:CD2	1:C:69:MET:HB2	2.54	0.42
1:D:18:THR:CG2	1:D:19:MET:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:VAL:HA	2:D:146:HOH:O	2.18	0.42
1:E:103:PHE:CB	1:F:42:VAL:CG2	2.96	0.42
1:F:37:GLN:HG3	1:F:43:PRO:CB	2.49	0.42
1:D:7:HIS:NE2	1:D:9:LYS:HE2	2.34	0.42
1:F:9:LYS:HB2	1:F:9:LYS:HE3	1.74	0.42
1:C:42:VAL:HG21	1:D:105:SER:C	2.40	0.42
1:C:122:ASP:HB3	1:C:124:GLU:N	2.29	0.42
1:E:41:LYS:C	1:F:6:LEU:HD13	2.40	0.42
1:F:46:PHE:HB3	1:F:47:VAL:HG12	2.01	0.42
1:C:101:ILE:O	1:C:101:ILE:HG23	2.18	0.42
1:B:112:GLU:HG2	1:B:116:GLU:OE2	2.19	0.42
1:B:114:SER:CB	1:B:115:ASN:C	2.81	0.42
1:B:66:ARG:NH2	1:B:84:ARG:CD	2.82	0.42
1:B:86:ASP:O	1:B:86:ASP:OD2	2.38	0.42
1:A:28:ASN:OD1	1:A:28:ASN:C	2.58	0.42
1:C:35:TYR:CD2	1:C:45:TYR:HA	2.54	0.42
1:C:44:GLN:HG2	1:D:3:ILE:HD11	2.01	0.42
1:B:50:TYR:HD2	1:B:52:SER:CB	2.32	0.42
1:F:23:MET:N	1:F:74:GLN:O	2.46	0.42
1:D:47:VAL:HG23	1:D:58:PHE:HA	2.01	0.42
1:D:6:LEU:HA	1:D:6:LEU:HD12	1.83	0.42
1:B:118:SER:OG	1:B:119:LYS:N	2.51	0.42
1:A:35:TYR:N	1:A:35:TYR:CD1	2.87	0.42
1:E:62:PHE:CE1	1:E:67:PHE:HD2	2.32	0.42
1:A:6:LEU:HD13	1:B:41:LYS:O	2.20	0.42
1:C:100:ILE:H	1:D:96:VAL:HG21	1.85	0.42
1:D:39:PHE:C	1:D:41:LYS:H	2.23	0.42
1:A:31:ASN:OD1	1:B:99:ILE:HG22	2.19	0.42
1:C:63:LYS:HG2	1:C:63:LYS:O	2.20	0.42
1:B:114:SER:HB2	1:B:116:GLU:CB	2.48	0.42
1:B:30:ASN:C	1:B:31:ASN:HD22	2.21	0.42
1:A:6:LEU:HD13	1:B:42:VAL:HA	2.01	0.42
1:C:56:TYR:HE1	1:C:58:PHE:CE2	2.37	0.42
1:F:13:ARG:HH22	1:F:84:ARG:HB2	1.83	0.42
1:D:34:TRP:HA	1:D:92:PHE:O	2.19	0.42
1:A:27:THR:HB	1:A:28:ASN:H	1.66	0.42
1:B:35:TYR:HA	1:B:44:GLN:O	2.19	0.42
1:C:28:ASN:O	1:C:30:ASN:N	2.52	0.42
1:D:23:MET:HG2	1:D:75:LYS:N	2.34	0.42
1:A:28:ASN:O	1:A:29:LYS:C	2.58	0.42
1:E:5:GLU:HG3	1:F:40:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PHE:CD1	1:B:80:ILE:HG13	2.53	0.42
1:A:34:TRP:CD2	1:A:93:CYS:HB2	2.55	0.42
1:E:5:GLU:CB	1:F:41:LYS:HD3	2.50	0.41
1:D:46:PHE:O	1:D:59:ALA:HB2	2.20	0.41
1:E:20:GLU:O	1:E:34:TRP:HH2	2.02	0.41
1:E:101:ILE:HD11	1:E:103:PHE:CE1	2.55	0.41
1:B:47:VAL:HB	1:B:58:PHE:CD1	2.54	0.41
1:C:60:GLU:HB2	2:C:139:HOH:O	2.19	0.41
1:F:69:MET:CE	1:F:76:PHE:CD1	3.04	0.41
1:E:34:TRP:O	1:E:46:PHE:CB	2.68	0.41
1:E:6:LEU:CD2	1:E:90:GLU:OE2	2.64	0.41
1:E:117:GLY:HA3	1:E:118:SER:HA	1.80	0.41
1:C:87:ASP:O	1:C:111:PHE:HE2	2.04	0.41
1:A:3:ILE:O	1:A:3:ILE:CG2	2.68	0.41
1:F:23:MET:SD	1:F:32:LEU:HD21	2.60	0.41
1:C:96:VAL:CG2	1:C:101:ILE:HG13	2.51	0.41
1:A:50:TYR:CD2	1:A:52:SER:HB3	2.56	0.41
1:B:13:ARG:CZ	1:B:85:GLU:HB3	2.51	0.41
1:D:78:LEU:HD22	1:D:79:ASN:N	2.36	0.41
1:B:22:SER:OG	1:B:24:SER:HB2	2.21	0.41
1:A:4:LYS:NZ	1:A:4:LYS:CB	2.81	0.41
1:E:86:ASP:C	1:E:86:ASP:OD2	2.59	0.41
1:B:13:ARG:NH2	1:B:112:GLU:OE1	2.54	0.41
1:A:99:ILE:CG2	1:B:31:ASN:CG	2.86	0.41
1:B:52:SER:OG	1:B:53:ASN:N	2.54	0.41
1:D:108:ARG:HE	1:D:110:GLN:HE21	1.66	0.41
1:C:99:ILE:CG2	1:D:31:ASN:ND2	2.84	0.41
1:F:125:GLY:O	1:F:126:SER:HB2	2.20	0.41
1:E:48:ARG:HD2	1:E:50:TYR:CA	2.50	0.41
1:E:62:PHE:CZ	1:E:67:PHE:CD2	3.06	0.41
1:E:14:GLY:N	1:E:83:ALA:O	2.37	0.41
1:D:64:ASP:C	1:D:66:ARG:H	2.24	0.41
1:A:84:ARG:C	1:A:85:GLU:CG	2.79	0.41
1:A:94:GLY:C	1:A:101:ILE:HD11	2.41	0.41
1:A:24:SER:C	1:A:25:LYS:CG	2.88	0.41
1:A:47:VAL:HG22	1:A:48:ARG:N	2.36	0.41
1:E:5:GLU:HB2	1:F:41:LYS:HD3	2.03	0.41
1:C:122:ASP:CA	1:C:124:GLU:H	2.33	0.41
1:C:94:GLY:HA3	1:C:101:ILE:HD11	2.02	0.41
1:B:36:ARG:HB2	1:B:91:TYR:CE2	2.55	0.41
1:D:34:TRP:CD1	1:D:76:PHE:CE2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ASN:CG	1:D:99:ILE:HG22	2.41	0.41
1:F:7:HIS:C	1:F:7:HIS:CD2	2.94	0.41
1:D:19:MET:HG2	1:D:107:THR:HG21	2.03	0.41
1:B:126:SER:CB	1:B:127:SER:HB3	2.48	0.40
1:A:109:LEU:HD21	1:A:111:PHE:HE2	1.84	0.40
1:F:74:GLN:HE21	1:F:75:LYS:HZ2	1.69	0.40
1:E:3:ILE:HG23	1:F:41:LYS:HE2	2.03	0.40
1:F:48:ARG:NH2	1:F:50:TYR:HE1	2.19	0.40
1:F:62:PHE:CG	1:F:63:LYS:N	2.89	0.40
1:D:75:LYS:HB2	1:D:75:LYS:HE2	1.57	0.40
1:C:80:ILE:HD13	1:C:80:ILE:N	2.34	0.40
1:F:23:MET:O	1:F:24:SER:C	2.59	0.40
1:C:12:LYS:HG2	1:C:112:GLU:CD	2.41	0.40
1:F:69:MET:CA	1:F:79:ASN:HD21	2.34	0.40
1:D:86:ASP:C	1:D:86:ASP:OD2	2.59	0.40
1:A:126:SER:O	1:A:127:SER:CB	2.69	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	124/137 (90%)	91 (73%)	19 (15%)	14 (11%)	0	1
1	B	124/137 (90%)	96 (77%)	18 (14%)	10 (8%)	1	2
1	C	124/137 (90%)	87 (70%)	23 (18%)	14 (11%)	0	1
1	D	124/137 (90%)	92 (74%)	24 (19%)	8 (6%)	1	4
1	E	124/137 (90%)	85 (68%)	27 (22%)	12 (10%)	1	1
1	F	124/137 (90%)	88 (71%)	21 (17%)	15 (12%)	0	1
All	All	744/822 (90%)	539 (72%)	132 (18%)	73 (10%)	1	1

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	51	SER
1	A	85	GLU
1	A	115	ASN
1	A	121	SER
1	B	24	SER
1	B	25	LYS
1	B	26	VAL
1	B	85	GLU
1	B	112	GLU
1	B	115	ASN
1	B	124	GLU
1	C	51	SER
1	C	100	ILE
1	C	112	GLU
1	C	115	ASN
1	C	123	GLY
1	C	126	SER
1	C	127	SER
1	D	100	ILE
1	D	127	SER
1	E	24	SER
1	E	29	LYS
1	E	30	ASN
1	E	112	GLU
1	E	124	GLU
1	E	126	SER
1	E	127	SER
1	F	24	SER
1	F	61	GLY
1	F	88	GLY
1	F	112	GLU
1	F	116	GLU
1	F	119	LYS
1	F	122	ASP
1	F	127	SER
1	A	11	VAL
1	A	24	SER
1	A	96	VAL
1	A	114	SER
1	C	38	SER
1	C	68	SER

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Mol	Chain	Res	Type
1	C	84	ARG
1	D	60	GLU
1	D	65	SER
1	E	21	CYS
1	E	117	GLY
1	F	21	CYS
1	F	52	SER
1	F	123	GLY
1	F	126	SER
1	A	66	ARG
1	A	111	PHE
1	B	13	ARG
1	D	114	SER
1	D	124	GLU
1	E	13	ARG
1	F	20	GLU
1	F	47	VAL
1	F	114	SER
1	A	127	SER
1	C	118	SER
1	C	122	ASP
1	C	125	GLY
1	E	64	ASP
1	A	122	ASP
1	B	23	MET
1	B	15	GLU
1	C	117	GLY
1	D	85	GLU
1	E	74	GLN
1	A	61	GLY
1	D	101	ILE

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/120 (91%)	83 (76%)	26 (24%)	1	2
1	B	109/120 (91%)	81 (74%)	28 (26%)	0	2
1	C	109/120 (91%)	86 (79%)	23 (21%)	1	4
1	D	109/120 (91%)	80 (73%)	29 (27%)	0	1
1	E	109/120 (91%)	79 (72%)	30 (28%)	0	1
1	F	109/120 (91%)	82 (75%)	27 (25%)	1	2
All	All	654/720 (91%)	491 (75%)	163 (25%)	1	2

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	LEU
1	A	12	LYS
1	A	17	VAL
1	A	24	SER
1	A	25	LYS
1	A	31	ASN
1	A	42	VAL
1	A	44	GLN
1	A	45	TYR
1	A	51	SER
1	A	52	SER
1	A	63	LYS
1	A	69	MET
1	A	81	ILE
1	A	85	GLU
1	A	92	PHE
1	A	99	ILE
1	A	101	ILE
1	A	102	LYS
1	A	109	LEU
1	A	110	GLN
1	A	112	GLU
1	A	119	LYS
1	A	120	SER
1	A	122	ASP
1	B	4	LYS

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Mol	Chain	Res	Type
1	B	5	GLU
1	B	6	LEU
1	B	11	VAL
1	B	13	ARG
1	B	22	SER
1	B	23	MET
1	B	32	LEU
1	B	35	TYR
1	B	36	ARG
1	B	42	VAL
1	B	63	LYS
1	B	65	SER
1	B	66	ARG
1	B	78	LEU
1	B	84	ARG
1	B	85	GLU
1	B	86	ASP
1	B	92	PHE
1	B	95	GLU
1	B	100	ILE
1	B	104	THR
1	B	108	ARG
1	B	110	GLN
1	B	114	SER
1	B	118	SER
1	B	119	LYS
1	B	126	SER
1	C	3	ILE
1	C	4	LYS
1	C	6	LEU
1	C	13	ARG
1	C	17	VAL
1	C	39	PHE
1	C	42	VAL
1	C	51	SER
1	C	52	SER
1	C	63	LYS
1	C	65	SER
1	C	75	LYS
1	C	85	GLU
1	C	87	ASP
1	C	93	CYS

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Mol	Chain	Res	Type
1	C	97	GLU
1	C	101	ILE
1	C	102	LYS
1	C	110	GLN
1	C	114	SER
1	C	116	GLU
1	C	118	SER
1	C	121	SER
1	D	5	GLU
1	D	6	LEU
1	D	9	LYS
1	D	11	VAL
1	D	22	SER
1	D	23	MET
1	D	25	LYS
1	D	29	LYS
1	D	42	VAL
1	D	45	TYR
1	D	63	LYS
1	D	65	SER
1	D	68	SER
1	D	75	LYS
1	D	78	LEU
1	D	85	GLU
1	D	86	ASP
1	D	95	GLU
1	D	100	ILE
1	D	101	ILE
1	D	102	LYS
1	D	109	LEU
1	D	114	SER
1	D	115	ASN
1	D	118	SER
1	D	122	ASP
1	D	126	SER
1	D	127	SER
1	D	128	CYS
1	E	9	LYS
1	E	11	VAL
1	E	13	ARG
1	E	17	VAL
1	E	18	THR

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Mol	Chain	Res	Type
1	E	27	THR
1	E	31	ASN
1	E	32	LEU
1	E	36	ARG
1	E	38	SER
1	E	46	PHE
1	E	48	ARG
1	E	51	SER
1	E	52	SER
1	E	62	PHE
1	E	63	LYS
1	E	66	ARG
1	E	74	GLN
1	E	75	LYS
1	E	78	LEU
1	E	84	ARG
1	E	85	GLU
1	E	99	ILE
1	E	101	ILE
1	E	102	LYS
1	E	111	PHE
1	E	114	SER
1	E	116	GLU
1	E	119	LYS
1	E	121	SER
1	F	3	ILE
1	F	9	LYS
1	F	13	ARG
1	F	17	VAL
1	F	18	THR
1	F	27	THR
1	F	31	ASN
1	F	32	LEU
1	F	37	GLN
1	F	42	VAL
1	F	46	PHE
1	F	51	SER
1	F	63	LYS
1	F	64	ASP
1	F	65	SER
1	F	74	GLN
1	F	75	LYS

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Mol	Chain	Res	Type
1	F	78	LEU
1	F	79	ASN
1	F	90	GLU
1	F	99	ILE
1	F	101	ILE
1	F	102	LYS
1	F	108	ARG
1	F	115	ASN
1	F	119	LYS
1	F	126	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	31	ASN
1	A	44	GLN
1	A	74	GLN
1	A	110	GLN
1	B	7	HIS
1	B	31	ASN
1	B	37	GLN
1	B	110	GLN
1	B	115	ASN
1	C	30	ASN
1	C	31	ASN
1	C	44	GLN
1	C	110	GLN
1	D	31	ASN
1	D	44	GLN
1	D	110	GLN
1	E	31	ASN
1	E	72	ASN
1	E	79	ASN
1	F	30	ASN
1	F	31	ASN
1	F	53	ASN
1	F	74	GLN
1	F	79	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	126/137 (91%)	2.52	54 (42%) 0 0	32, 63, 100, 100	0
1	B	126/137 (91%)	2.15	49 (38%) 0 0	31, 62, 100, 100	0
1	C	126/137 (91%)	2.13	46 (36%) 0 0	33, 60, 100, 100	0
1	D	126/137 (91%)	2.16	43 (34%) 0 0	26, 61, 100, 100	0
1	E	126/137 (91%)	1.87	43 (34%) 0 0	48, 79, 100, 100	0
1	F	126/137 (91%)	1.82	39 (30%) 1 0	43, 80, 100, 100	0
All	All	756/822 (91%)	2.11	274 (36%) 0 0	26, 71, 100, 100	0

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	CYS	17.4
1	D	128	CYS	15.3
1	D	120	SER	13.8
1	C	121	SER	12.5
1	B	123	GLY	12.3
1	A	117	GLY	12.0
1	E	127	SER	11.4
1	A	127	SER	11.2
1	A	114	SER	11.1
1	E	128	CYS	10.6
1	B	128	CYS	10.5
1	D	126	SER	9.8
1	D	127	SER	9.8
1	D	122	ASP	9.4
1	C	122	ASP	9.2
1	B	127	SER	9.0
1	A	115	ASN	8.7
1	A	118	SER	8.5
1	D	123	GLY	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	106	GLY	8.1
1	F	120	SER	8.1
1	E	113	GLY	7.9
1	B	126	SER	7.9
1	A	123	GLY	7.8
1	D	116	GLU	7.7
1	A	126	SER	7.7
1	C	120	SER	7.7
1	D	118	SER	7.6
1	D	124	GLU	7.5
1	F	39	PHE	7.4
1	A	128	CYS	7.2
1	D	125	GLY	7.2
1	A	116	GLU	7.2
1	F	115	ASN	7.0
1	B	117	GLY	6.9
1	E	38	SER	6.8
1	C	127	SER	6.7
1	A	119	LYS	6.6
1	F	113	GLY	6.4
1	F	114	SER	6.4
1	A	124	GLU	6.3
1	C	124	GLU	6.2
1	D	121	SER	6.1
1	C	123	GLY	5.9
1	F	123	GLY	5.9
1	E	39	PHE	5.9
1	B	23	MET	5.7
1	E	114	SER	5.7
1	A	68	SER	5.5
1	C	125	GLY	5.3
1	D	114	SER	5.2
1	A	120	SER	5.2
1	F	94	GLY	5.2
1	E	120	SER	5.1
1	A	91	TYR	5.0
1	A	111	PHE	4.8
1	F	17	VAL	4.8
1	C	126	SER	4.8
1	D	115	ASN	4.8
1	B	112	GLU	4.7
1	D	119	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	50	TYR	4.7
1	D	117	GLY	4.7
1	E	124	GLU	4.7
1	B	122	ASP	4.6
1	B	94	GLY	4.6
1	B	118	SER	4.6
1	F	126	SER	4.6
1	B	15	GLU	4.5
1	A	121	SER	4.5
1	F	121	SER	4.3
1	B	24	SER	4.3
1	B	120	SER	4.3
1	C	109	LEU	4.3
1	B	121	SER	4.2
1	C	83	ALA	4.1
1	A	125	GLY	4.1
1	E	32	LEU	4.1
1	E	125	GLY	4.0
1	F	24	SER	4.0
1	D	105	SER	4.0
1	C	18	THR	4.0
1	F	85	GLU	3.9
1	C	117	GLY	3.9
1	D	63	LYS	3.9
1	E	115	ASN	3.9
1	F	58	PHE	3.9
1	F	64	ASP	3.9
1	B	60	GLU	3.9
1	F	128	CYS	3.9
1	C	108	ARG	3.9
1	E	118	SER	3.9
1	E	126	SER	3.9
1	E	67	PHE	3.8
1	D	29	LYS	3.8
1	B	33	ALA	3.8
1	A	94	GLY	3.8
1	F	122	ASP	3.7
1	A	92	PHE	3.7
1	A	107	THR	3.7
1	F	80	ILE	3.7
1	A	5	GLU	3.7
1	F	125	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	53	ASN	3.7
1	F	76	PHE	3.7
1	A	50	TYR	3.7
1	B	63	LYS	3.7
1	B	114	SER	3.7
1	A	89	GLY	3.6
1	E	122	ASP	3.6
1	A	93	CYS	3.6
1	E	121	SER	3.6
1	C	99	ILE	3.5
1	C	25	LYS	3.5
1	E	49	TYR	3.5
1	C	87	ASP	3.4
1	E	13	ARG	3.4
1	A	38	SER	3.3
1	A	113	GLY	3.3
1	E	87	ASP	3.3
1	E	30	ASN	3.3
1	F	111	PHE	3.3
1	B	48	ARG	3.3
1	E	17	VAL	3.3
1	C	58	PHE	3.2
1	E	45	TYR	3.2
1	A	122	ASP	3.2
1	D	6	LEU	3.2
1	D	49	TYR	3.2
1	C	78	LEU	3.2
1	E	123	GLY	3.2
1	D	51	SER	3.2
1	F	127	SER	3.2
1	C	115	ASN	3.1
1	F	81	ILE	3.1
1	A	35	TYR	3.1
1	B	115	ASN	3.1
1	D	45	TYR	3.1
1	D	80	ILE	3.1
1	C	118	SER	3.0
1	A	88	GLY	3.0
1	B	70	THR	3.0
1	A	86	ASP	3.0
1	E	36	ARG	3.0
1	E	10	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	32	LEU	3.0
1	C	34	TRP	3.0
1	F	67	PHE	3.0
1	F	46	PHE	3.0
1	A	15	GLU	2.9
1	A	51	SER	2.9
1	D	74	GLN	2.9
1	C	101	ILE	2.9
1	F	78	LEU	2.9
1	E	8	VAL	2.9
1	A	105	SER	2.9
1	B	91	TYR	2.9
1	A	33	ALA	2.9
1	F	88	GLY	2.9
1	C	70	THR	2.9
1	C	116	GLU	2.8
1	A	67	PHE	2.8
1	A	80	ILE	2.8
1	C	6	LEU	2.8
1	B	14	GLY	2.8
1	C	24	SER	2.8
1	B	110	GLN	2.8
1	E	116	GLU	2.8
1	A	17	VAL	2.8
1	D	100	ILE	2.8
1	F	104	THR	2.8
1	E	97	GLU	2.7
1	B	53	ASN	2.7
1	B	109	LEU	2.7
1	F	103	PHE	2.7
1	C	114	SER	2.7
1	B	46	PHE	2.7
1	F	124	GLU	2.7
1	D	42	VAL	2.7
1	A	108	ARG	2.6
1	A	79	ASN	2.6
1	B	50	TYR	2.6
1	A	104	THR	2.6
1	C	103	PHE	2.6
1	A	4	LYS	2.6
1	B	98	GLY	2.6
1	F	40	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	96	VAL	2.6
1	C	26	VAL	2.6
1	D	27	THR	2.5
1	D	40	GLY	2.5
1	D	55	GLY	2.5
1	B	47	VAL	2.5
1	F	16	ASN	2.5
1	E	33	ALA	2.5
1	E	80	ILE	2.5
1	D	35	TYR	2.5
1	C	93	CYS	2.5
1	C	84	ARG	2.5
1	C	4	LYS	2.5
1	F	25	LYS	2.5
1	B	89	GLY	2.5
1	F	109	LEU	2.5
1	C	110	GLN	2.5
1	F	66	ARG	2.5
1	B	71	VAL	2.4
1	E	92	PHE	2.4
1	B	74	GLN	2.4
1	E	3	ILE	2.4
1	B	41	LYS	2.4
1	A	82	GLY	2.4
1	B	124	GLU	2.4
1	E	22	SER	2.4
1	C	7	HIS	2.4
1	C	11	VAL	2.3
1	B	106	GLY	2.3
1	C	111	PHE	2.3
1	E	109	LEU	2.3
1	B	61	GLY	2.3
1	F	62	PHE	2.3
1	B	26	VAL	2.3
1	C	76	PHE	2.3
1	A	42	VAL	2.3
1	B	125	GLY	2.3
1	B	86	ASP	2.3
1	E	119	LYS	2.3
1	B	80	ILE	2.3
1	D	67	PHE	2.3
1	C	113	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	2.2
1	C	39	PHE	2.2
1	F	60	GLU	2.2
1	A	109	LEU	2.2
1	A	58	PHE	2.2
1	D	21	CYS	2.2
1	A	61	GLY	2.2
1	B	119	LYS	2.2
1	D	7	HIS	2.2
1	D	17	VAL	2.2
1	A	63	LYS	2.2
1	A	19	MET	2.2
1	D	23	MET	2.2
1	E	11	VAL	2.2
1	B	111	PHE	2.2
1	D	62	PHE	2.2
1	F	41	LYS	2.1
1	D	92	PHE	2.1
1	A	71	VAL	2.1
1	E	110	GLN	2.1
1	E	46	PHE	2.1
1	E	77	ASP	2.1
1	E	90	GLU	2.1
1	B	79	ASN	2.1
1	D	93	CYS	2.1
1	B	39	PHE	2.1
1	D	32	LEU	2.1
1	D	71	VAL	2.1
1	B	19	MET	2.1
1	B	77	ASP	2.1
1	E	68	SER	2.1
1	E	98	GLY	2.1
1	C	77	ASP	2.1
1	C	112	GLU	2.1
1	F	118	SER	2.1
1	C	45	TYR	2.0
1	A	12	LYS	2.0
1	A	22	SER	2.0
1	C	68	SER	2.0
1	C	85	GLU	2.0
1	D	78	LEU	2.0
1	E	53	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	58	PHE	2.0
1	D	3	ILE	2.0
1	B	38	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.