



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:30 am BST

PDB ID : 3GNT  
Title : Crystal Structure of the Staphylococcus aureus Enoyl-Acyl Carrier Protein Reductase (FabI) in apo form (two molecules in AU)  
Authors : Priyadarshi, A.; Hwang, K.Y.  
Deposited on : 2009-03-18  
Resolution : 2.75 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

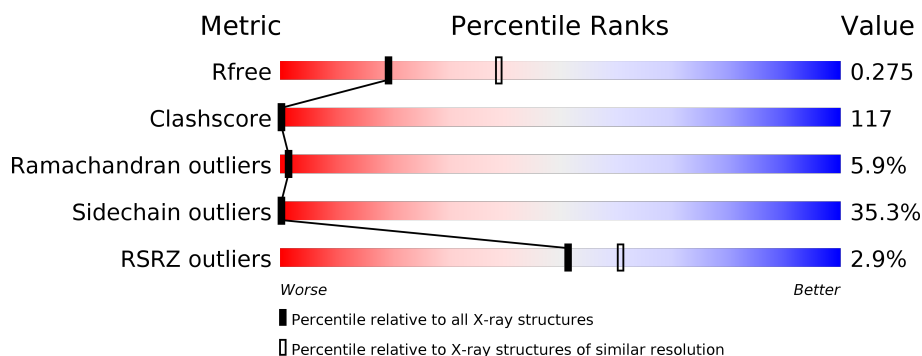
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	256	<div> <div>4%</div> <div>9%</div> <div>26%</div> <div>32%</div> <div>14%</div> <div>19%</div> </div>
1	B	256	<div> <div>%</div> <div>5%</div> <div>34%</div> <div>28%</div> <div>11%</div> <div>22%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3157 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.

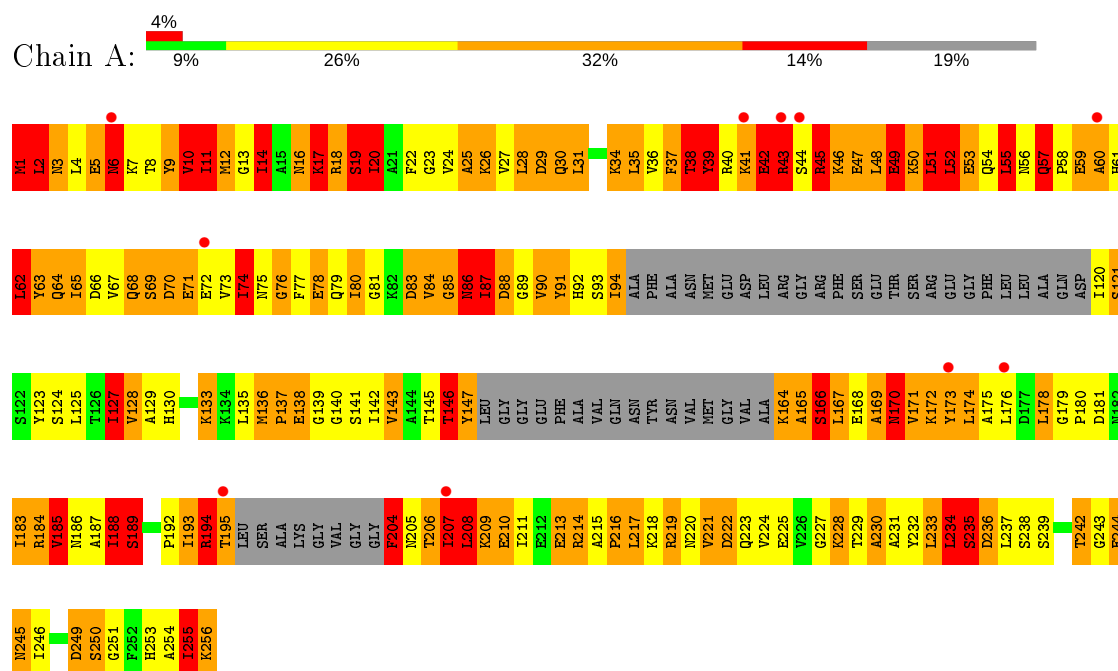
- Molecule 1 is a protein called Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1608	1017	276	312	3			
1	B	200	Total	C	N	O	S	0	0	0
			1549	978	267	301	3			

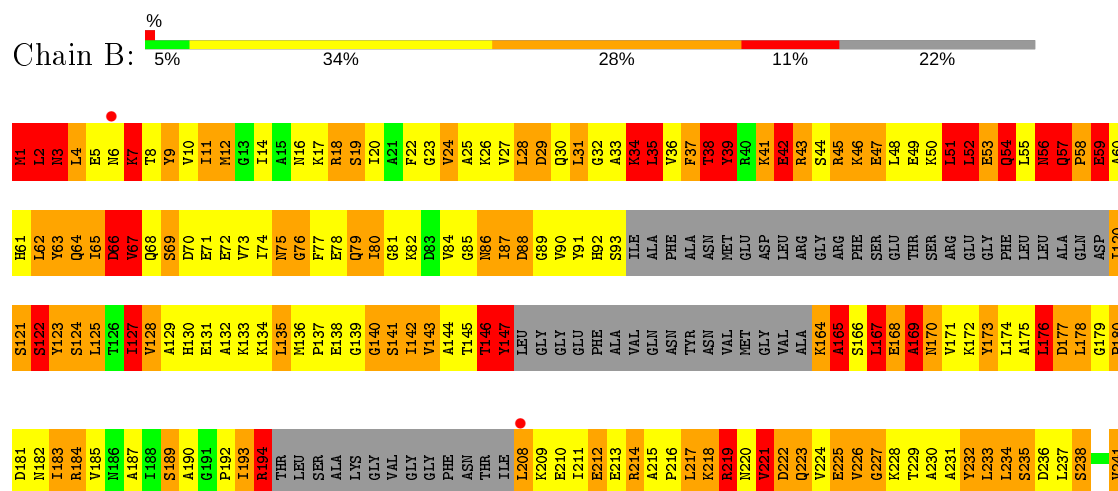
### 3 Residue-property plots

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

#### • Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



#### • Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



T242	G243	E244	N245	I246	H247	V248	D249	S250	G251	F252	H253	A254	I255	LYS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.10Å 74.46Å 70.61Å 90.00° 119.35° 90.00°	Depositor
Resolution (Å)	34.96 – 2.75 34.06 – 2.75	Depositor EDS
% Data completeness (in resolution range)	84.0 (34.96-2.75) 84.0 (34.06-2.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.242 , 0.278 0.252 , 0.275	Depositor DCC
$R_{free}$ test set	564 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 77.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.030 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	3157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.79% 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 ⓘ

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	2.09	47/1627 (2.9%)	2.08	65/2190 (3.0%)
1	B	2.01	40/1567 (2.6%)	1.96	46/2110 (2.2%)
All	All	2.05	87/3194 (2.7%)	2.02	111/4300 (2.6%)

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	19
1	B	0	24
All	All	0	43

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	ASP	CB-CG	-9.62	1.31	1.51
1	A	11	ILE	CA-CB	-8.74	1.34	1.54
1	A	78	GLU	CG-CD	7.79	1.63	1.51
1	B	147	TYR	CE2-CZ	7.60	1.48	1.38
1	B	39	TYR	CD1-CE1	7.38	1.50	1.39
1	A	138	GLU	CG-CD	-7.31	1.41	1.51
1	B	180	PRO	N-CA	-7.02	1.35	1.47
1	A	147	TYR	CE1-CZ	7.01	1.47	1.38
1	B	39	TYR	CD2-CE2	7.00	1.49	1.39
1	B	131	GLU	CG-CD	6.98	1.62	1.51
1	A	72	GLU	CG-CD	6.97	1.62	1.51
1	A	147	TYR	CG-CD1	6.92	1.48	1.39
1	A	173	TYR	CB-CG	-6.91	1.41	1.51
1	B	241	VAL	CA-CB	-6.90	1.40	1.54
1	B	230	ALA	CA-CB	-6.83	1.38	1.52
1	A	1	MET	CG-SD	6.76	1.98	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	TYR	CG-CD1	6.75	1.48	1.39
1	B	164	LYS	CE-NZ	6.73	1.65	1.49
1	A	37	PHE	CE1-CZ	6.58	1.49	1.37
1	A	20	ILE	CB-CG2	-6.54	1.32	1.52
1	A	10	VAL	CB-CG2	-6.41	1.39	1.52
1	B	19	SER	C-O	6.37	1.35	1.23
1	B	232	TYR	CE2-CZ	-6.24	1.30	1.38
1	A	235	SER	CA-CB	6.12	1.62	1.52
1	B	35	LEU	N-CA	-6.05	1.34	1.46
1	B	38	THR	N-CA	-5.89	1.34	1.46
1	A	184	ARG	CG-CD	-5.88	1.37	1.51
1	B	140	GLY	C-O	5.88	1.33	1.23
1	A	170	ASN	C-O	-5.87	1.12	1.23
1	B	189	SER	CA-CB	5.85	1.61	1.52
1	A	22	PHE	CD1-CE1	5.82	1.50	1.39
1	A	170	ASN	CA-C	-5.81	1.37	1.52
1	A	76	GLY	N-CA	5.77	1.54	1.46
1	B	138	GLU	CB-CG	5.72	1.63	1.52
1	A	39	TYR	CE1-CZ	5.70	1.46	1.38
1	A	147	TYR	CE2-CZ	5.68	1.46	1.38
1	A	78	GLU	CD-OE1	5.67	1.31	1.25
1	A	230	ALA	CA-CB	-5.65	1.40	1.52
1	B	190	ALA	CA-CB	5.64	1.64	1.52
1	A	194	ARG	N-CA	5.62	1.57	1.46
1	A	47	GLU	CG-CD	5.58	1.60	1.51
1	A	185	VAL	CB-CG1	-5.54	1.41	1.52
1	B	37	PHE	CE2-CZ	-5.53	1.26	1.37
1	A	19	SER	N-CA	-5.53	1.35	1.46
1	A	171	VAL	CA-CB	-5.53	1.43	1.54
1	A	204	PHE	CD1-CE1	5.45	1.50	1.39
1	A	91	TYR	CD2-CE2	-5.44	1.31	1.39
1	A	166	SER	CA-CB	-5.44	1.44	1.52
1	B	225	GLU	CD-OE1	-5.41	1.19	1.25
1	A	22	PHE	CD2-CE2	5.41	1.50	1.39
1	B	9	TYR	CG-CD2	5.41	1.46	1.39
1	A	63	TYR	CE1-CZ	5.40	1.45	1.38
1	B	37	PHE	CB-CG	-5.39	1.42	1.51
1	A	228	LYS	CD-CE	5.38	1.64	1.51
1	A	210	GLU	CD-OE2	5.38	1.31	1.25
1	A	14	ILE	CB-CG2	-5.36	1.36	1.52
1	B	220	ASN	C-O	5.36	1.33	1.23
1	A	213	GLU	CG-CD	5.35	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	VAL	CB-CG2	-5.35	1.41	1.52
1	B	131	GLU	CD-OE1	5.33	1.31	1.25
1	A	172	LYS	CE-NZ	5.33	1.62	1.49
1	B	145	THR	C-O	-5.31	1.13	1.23
1	B	227	GLY	C-O	-5.31	1.15	1.23
1	B	173	TYR	CE1-CZ	5.30	1.45	1.38
1	A	25	ALA	N-CA	5.28	1.56	1.46
1	B	11	ILE	CA-CB	-5.26	1.42	1.54
1	B	38	THR	CA-CB	-5.26	1.39	1.53
1	A	84	VAL	CB-CG2	5.26	1.63	1.52
1	B	192	PRO	CG-CD	-5.26	1.33	1.50
1	B	143	VAL	CB-CG1	5.25	1.63	1.52
1	A	53	GLU	CD-OE2	5.24	1.31	1.25
1	A	185	VAL	CA-CB	-5.21	1.43	1.54
1	A	30	GLN	CG-CD	5.21	1.63	1.51
1	B	232	TYR	N-CA	5.16	1.56	1.46
1	A	17	LYS	CE-NZ	5.14	1.61	1.49
1	B	238	SER	C-O	5.11	1.33	1.23
1	A	86	ASN	CA-C	5.10	1.66	1.52
1	A	86	ASN	C-O	5.10	1.33	1.23
1	B	132	ALA	CA-CB	-5.09	1.41	1.52
1	B	225	GLU	CG-CD	-5.08	1.44	1.51
1	A	85	GLY	N-CA	-5.07	1.38	1.46
1	B	42	GLU	CG-CD	5.06	1.59	1.51
1	A	80	ILE	C-O	5.04	1.32	1.23
1	A	235	SER	N-CA	5.04	1.56	1.46
1	B	42	GLU	CB-CG	5.01	1.61	1.52
1	B	244	GLU	C-O	5.01	1.32	1.23
1	B	9	TYR	CD1-CE1	-5.01	1.31	1.39

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	GLU	CB-CA-C	-13.03	84.34	110.40
1	A	45	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	A	88	ASP	CB-CG-OD2	11.06	128.26	118.30
1	B	4	LEU	N-CA-C	11.04	140.81	111.00
1	B	12	MET	CB-CG-SD	-10.10	82.10	112.40
1	B	194	ARG	NE-CZ-NH1	-9.97	115.31	120.30
1	A	28	LEU	CA-CB-CG	-9.79	92.80	115.30
1	B	80	ILE	CB-CA-C	-9.72	92.16	111.60
1	A	11	ILE	CB-CA-C	-9.64	92.32	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	LEU	CB-CA-C	-9.59	91.97	110.20
1	B	184	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	B	56	ASN	N-CA-C	-8.74	87.41	111.00
1	A	45	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	1	MET	CG-SD-CE	8.64	114.03	100.20
1	A	2	LEU	CA-CB-CG	-8.58	95.57	115.30
1	A	2	LEU	CB-CG-CD1	-8.38	96.75	111.00
1	B	233	LEU	CB-CG-CD2	-8.35	96.81	111.00
1	A	1	MET	CA-CB-CG	-8.35	99.11	113.30
1	A	174	LEU	CA-CB-CG	8.30	134.40	115.30
1	A	88	ASP	CB-CG-OD1	-8.29	110.84	118.30
1	B	174	LEU	CB-CG-CD1	-8.21	97.05	111.00
1	A	136	MET	CG-SD-CE	-8.16	87.14	100.20
1	B	176	LEU	CA-CB-CG	-8.01	96.87	115.30
1	A	222	ASP	CB-CG-OD1	7.96	125.46	118.30
1	B	29	ASP	CB-CG-OD2	7.93	125.44	118.30
1	B	66	ASP	CB-CA-C	-7.71	94.97	110.40
1	A	57	GLN	C-N-CD	7.65	144.47	128.40
1	B	223	GLN	O-C-N	-7.63	110.50	122.70
1	A	62	LEU	CB-CG-CD1	7.59	123.90	111.00
1	A	194	ARG	NE-CZ-NH1	-7.59	116.51	120.30
1	A	244	GLU	OE1-CD-OE2	-7.30	114.55	123.30
1	A	2	LEU	CB-CG-CD2	7.11	123.08	111.00
1	B	1	MET	CB-CA-C	7.05	124.50	110.40
1	B	146	THR	N-CA-C	-7.04	92.00	111.00
1	A	233	LEU	CB-CG-CD1	6.98	122.87	111.00
1	B	63	TYR	N-CA-C	-6.89	92.39	111.00
1	A	169	ALA	C-N-CA	-6.87	104.53	121.70
1	B	164	LYS	CA-C-N	6.76	132.07	117.20
1	A	18	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	164	LYS	O-C-N	-6.71	111.97	122.70
1	A	12	MET	CB-CG-SD	-6.67	92.39	112.40
1	A	38	THR	CA-CB-OG1	6.57	122.79	109.00
1	A	39	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	A	83	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	143	VAL	CB-CA-C	-6.41	99.22	111.40
1	B	64	GLN	CB-CA-C	-6.39	97.61	110.40
1	A	51	LEU	N-CA-C	-6.38	93.77	111.00
1	A	18	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	142	ILE	CG1-CB-CG2	-6.31	97.52	111.40
1	A	12	MET	CA-CB-CG	6.27	123.96	113.30
1	A	188	ILE	CB-CA-C	-6.27	99.07	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	SER	N-CA-C	-6.26	94.09	111.00
1	B	194	ARG	NE-CZ-NH2	6.19	123.40	120.30
1	B	12	MET	CA-CB-CG	6.18	123.81	113.30
1	A	38	THR	CB-CA-C	-6.17	94.95	111.60
1	B	122	SER	N-CA-C	6.12	127.54	111.00
1	A	86	ASN	N-CA-C	6.08	127.42	111.00
1	A	6	ASN	CB-CA-C	-6.04	98.33	110.40
1	B	67	VAL	O-C-N	-6.00	113.09	122.70
1	B	219	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	76	GLY	N-CA-C	-5.94	98.25	113.10
1	A	1	MET	N-CA-C	5.90	126.92	111.00
1	A	39	TYR	CB-CG-CD1	5.81	124.48	121.00
1	A	234	LEU	CB-CG-CD2	-5.80	101.13	111.00
1	A	217	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	B	11	ILE	CB-CA-C	-5.68	100.24	111.60
1	B	88	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	A	208	LEU	CA-CB-CG	-5.65	102.31	115.30
1	A	242	THR	CA-CB-CG2	-5.63	104.52	112.40
1	A	48	LEU	CB-CG-CD2	-5.61	101.47	111.00
1	B	143	VAL	N-CA-C	-5.61	95.86	111.00
1	B	214	ARG	CG-CD-NE	5.59	123.53	111.80
1	B	177	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	127	ILE	CB-CA-C	-5.58	100.44	111.60
1	A	12	MET	C-N-CA	-5.57	110.59	122.30
1	B	220	ASN	CB-CA-C	5.50	121.41	110.40
1	B	2	LEU	CB-CG-CD1	5.49	120.33	111.00
1	A	189	SER	CB-CA-C	5.48	120.51	110.10
1	A	147	TYR	CD1-CE1-CZ	-5.46	114.88	119.80
1	A	83	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	65	ILE	N-CA-C	5.45	125.71	111.00
1	A	184	ARG	CG-CD-NE	5.44	123.23	111.80
1	A	194	ARG	CG-CD-NE	-5.43	100.40	111.80
1	B	146	THR	CB-CA-C	-5.42	96.96	111.60
1	B	59	GLU	CA-CB-CG	5.39	125.25	113.40
1	A	183	ILE	C-N-CA	-5.36	108.31	121.70
1	B	64	GLN	N-CA-C	-5.34	96.58	111.00
1	A	221	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	A	255	ILE	CG1-CB-CG2	-5.33	99.66	111.40
1	A	234	LEU	CB-CA-C	-5.32	100.10	110.20
1	B	221	VAL	C-N-CA	-5.31	108.42	121.70
1	A	28	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	A	217	LEU	CB-CG-CD1	-5.28	102.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	TYR	CZ-CE2-CD2	-5.23	115.09	119.80
1	A	236	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	28	LEU	CB-CA-C	-5.22	100.28	110.20
1	A	73	VAL	CB-CA-C	5.18	121.25	111.40
1	B	75	ASN	O-C-N	5.18	132.01	123.20
1	B	57	GLN	N-CA-C	5.16	124.92	111.00
1	B	226	VAL	CA-CB-CG1	-5.14	103.18	110.90
1	A	87	ILE	N-CA-C	5.13	124.84	111.00
1	A	28	LEU	CB-CA-C	-5.11	100.50	110.20
1	B	39	TYR	CA-CB-CG	5.10	123.09	113.40
1	A	9	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	B	7	LYS	CB-CA-C	5.05	120.51	110.40
1	A	29	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	B	169	ALA	C-N-CA	-5.04	109.11	121.70
1	A	220	ASN	N-CA-C	5.03	124.58	111.00
1	A	65	ILE	CG1-CB-CG2	-5.02	100.35	111.40
1	A	55	LEU	CA-CB-CG	-5.02	103.75	115.30
1	A	43	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ILE	Peptide
1	A	127	ILE	Peptide
1	A	146	THR	Peptide
1	A	164	LYS	Peptide
1	A	165	ALA	Peptide
1	A	166	SER	Peptide
1	A	185	VAL	Peptide
1	A	2	LEU	Peptide
1	A	38	THR	Peptide
1	A	42	GLU	Peptide
1	A	49	GLU	Peptide
1	A	50	LYS	Peptide
1	A	51	LEU	Peptide
1	A	57	GLN	Peptide
1	A	59	GLU	Peptide
1	A	6	ASN	Peptide
1	A	60	ALA	Peptide
1	A	71	GLU	Mainchain
1	A	86	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	1	MET	Peptide
1	B	121	SER	Peptide
1	B	122	SER	Peptide
1	B	165	ALA	Peptide
1	B	167	LEU	Peptide
1	B	169	ALA	Peptide
1	B	176	LEU	Peptide
1	B	193	ILE	Peptide
1	B	2	LEU	Peptide
1	B	208	LEU	Peptide
1	B	221	VAL	Peptide
1	B	224	VAL	Mainchain
1	B	24	VAL	Peptide
1	B	254	ALA	Peptide
1	B	3	ASN	Peptide
1	B	34	LYS	Peptide
1	B	38	THR	Peptide
1	B	41	LYS	Peptide
1	B	42	GLU	Peptide
1	B	51	LEU	Peptide
1	B	52	LEU	Peptide
1	B	53	GLU	Peptide
1	B	54	GLN	Peptide
1	B	67	VAL	Peptide

## 5.2 Too-close contacts [i](#)

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	1608	0	1640	365	0
1	B	1549	0	1576	388	0
All	All	3157	0	3216	744	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 117.

All (744) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ILE:CG2	1:B:73:VAL:HG12	1.39	1.49
1:B:59:GLU:HG3	1:B:61:HIS:N	1.39	1.36
1:B:8:THR:CG2	1:B:87:ILE:HD11	1.55	1.36
1:B:52:LEU:HA	1:B:54:GLN:CG	1.55	1.36
1:B:89:GLY:HA2	1:B:136:MET:CE	1.60	1.31
1:B:147:TYR:CD1	1:B:147:TYR:C	1.99	1.30
1:B:75:ASN:O	1:B:79:GLN:HB2	1.35	1.26
1:B:167:LEU:O	1:B:167:LEU:HD13	1.31	1.25
1:B:167:LEU:HA	1:B:168:GLU:CB	1.69	1.20
1:A:194:ARG:NH1	1:A:194:ARG:HB3	1.56	1.20
1:B:52:LEU:CA	1:B:54:GLN:HG2	1.70	1.20
1:B:135:LEU:O	1:B:137:PRO:HD3	1.41	1.17
1:B:1:MET:HB3	1:B:2:LEU:HD23	1.26	1.16
1:B:65:ILE:HG22	1:B:73:VAL:CG1	1.76	1.16
1:B:1:MET:HB3	1:B:2:LEU:CD2	1.75	1.15
1:A:166:SER:HB3	1:A:169:ALA:CB	1.76	1.15
1:B:10:VAL:HG13	1:B:36:VAL:HG12	1.27	1.15
1:B:59:GLU:N	1:B:60:ALA:HA	1.55	1.14
1:A:39:TYR:CE1	1:A:64:GLN:HG2	1.83	1.13
1:B:59:GLU:CG	1:B:61:HIS:H	1.60	1.13
1:A:171:VAL:HG21	1:A:187:ALA:HB2	1.28	1.13
1:B:34:LYS:HB3	1:B:34:LYS:NZ	1.43	1.12
1:B:194:ARG:HH11	1:B:194:ARG:HG2	1.06	1.12
1:B:65:ILE:CG2	1:B:73:VAL:CG1	2.26	1.11
1:B:65:ILE:HG22	1:B:73:VAL:HG12	1.22	1.11
1:B:65:ILE:HG21	1:B:73:VAL:HG12	1.21	1.09
1:A:123:TYR:CG	1:A:127:ILE:HD11	1.87	1.09
1:A:93:SER:O	1:A:94:ILE:HB	1.44	1.08
1:B:194:ARG:HH11	1:B:194:ARG:CG	1.55	1.08
1:A:166:SER:HB3	1:A:169:ALA:HB3	1.17	1.08
1:B:8:THR:HB	1:B:87:ILE:CD1	1.84	1.07
1:A:123:TYR:O	1:A:127:ILE:HG13	1.55	1.06
1:B:194:ARG:HB3	1:B:194:ARG:NH1	1.68	1.06
1:B:43:ARG:O	1:B:46:LYS:HB2	1.54	1.05
1:B:194:ARG:CB	1:B:194:ARG:NH1	2.19	1.05
1:B:8:THR:CG2	1:B:87:ILE:CD1	2.37	1.03
1:B:167:LEU:CA	1:B:168:GLU:HB2	1.88	1.03
1:A:59:GLU:H	1:A:60:ALA:HA	1.20	1.02
1:B:177:ASP:HB3	1:B:178:LEU:HD13	1.39	1.02
1:B:123:TYR:HD2	1:B:123:TYR:C	1.61	1.02
1:A:39:TYR:CD1	1:A:39:TYR:C	2.33	1.02
1:B:182:ASN:O	1:B:183:ILE:HD12	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:TYR:CE2	1:B:127:ILE:CG1	2.42	1.02
1:B:124:SER:O	1:B:128:VAL:HG23	1.58	1.01
1:B:167:LEU:CA	1:B:168:GLU:CB	2.38	1.01
1:A:124:SER:O	1:A:128:VAL:HG23	1.58	1.00
1:B:8:THR:CB	1:B:87:ILE:HD11	1.90	1.00
1:B:139:GLY:HA2	1:B:183:ILE:HD11	1.38	1.00
1:B:8:THR:HB	1:B:87:ILE:HD12	1.41	1.00
1:A:49:GLU:HG2	1:A:49:GLU:O	1.61	1.00
1:B:123:TYR:HE2	1:B:127:ILE:CD1	1.73	1.00
1:B:123:TYR:HE2	1:B:127:ILE:HD11	1.26	1.00
1:B:5:GLU:O	1:B:6:ASN:HB2	1.58	1.00
1:B:89:GLY:HA2	1:B:136:MET:HE2	1.41	0.99
1:A:4:LEU:HD12	1:A:236:ASP:CG	1.83	0.99
1:A:170:ASN:N	1:A:170:ASN:HD22	1.54	0.99
1:B:123:TYR:CD2	1:B:123:TYR:C	2.30	0.98
1:B:8:THR:HG22	1:B:87:ILE:HD11	1.01	0.98
1:B:10:VAL:HG22	1:B:36:VAL:HB	1.43	0.98
1:B:167:LEU:O	1:B:167:LEU:CD1	2.12	0.97
1:B:8:THR:CB	1:B:87:ILE:CD1	2.42	0.97
1:B:6:ASN:HA	1:B:34:LYS:HD2	1.47	0.96
1:B:34:LYS:HB3	1:B:34:LYS:HZ3	0.93	0.96
1:B:2:LEU:HB2	1:B:3:ASN:ND2	1.81	0.96
1:B:17:LYS:O	1:B:17:LYS:HG2	1.66	0.96
1:A:194:ARG:CB	1:A:194:ARG:HH11	1.78	0.96
1:A:130:HIS:O	1:A:133:LYS:HB3	1.66	0.95
1:A:55:LEU:O	1:A:57:GLN:HG3	1.66	0.95
1:B:54:GLN:O	1:B:54:GLN:HG3	1.63	0.95
1:B:8:THR:HG22	1:B:87:ILE:CD1	1.92	0.95
1:B:89:GLY:HA2	1:B:136:MET:HE3	1.49	0.95
1:B:167:LEU:HA	1:B:168:GLU:HB2	0.97	0.95
1:A:29:ASP:HB2	1:A:54:GLN:NE2	1.81	0.94
1:A:237:LEU:HD12	1:B:228:LYS:HD2	1.48	0.94
1:A:39:TYR:C	1:A:39:TYR:HD1	1.67	0.94
1:A:51:LEU:HB3	1:A:52:LEU:C	1.87	0.94
1:A:5:GLU:HG3	1:A:6:ASN:N	1.80	0.94
1:B:8:THR:HA	1:B:34:LYS:O	1.67	0.94
1:B:147:TYR:C	1:B:147:TYR:HD1	1.47	0.94
1:A:38:THR:HG23	1:A:39:TYR:H	1.30	0.94
1:B:45:ARG:HG2	1:B:45:ARG:O	1.66	0.93
1:A:194:ARG:CB	1:A:194:ARG:NH1	2.31	0.92
1:B:167:LEU:HD13	1:B:167:LEU:C	1.89	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ARG:NH1	1:B:194:ARG:CG	2.20	0.92
1:A:50:LYS:HG3	1:A:51:LEU:N	1.83	0.92
1:A:38:THR:CG2	1:A:39:TYR:N	2.33	0.91
1:B:39:TYR:CZ	1:B:64:GLN:HB2	2.06	0.91
1:B:39:TYR:CE1	1:B:64:GLN:HB2	2.06	0.91
1:B:167:LEU:HD22	1:B:168:GLU:HB3	1.51	0.91
1:A:60:ALA:O	1:A:61:HIS:CD2	2.23	0.90
1:A:4:LEU:CD1	1:A:236:ASP:CG	2.40	0.90
1:B:123:TYR:HE2	1:B:127:ILE:CG1	1.81	0.90
1:A:188:ILE:CG2	1:A:189:SER:N	2.35	0.89
1:A:60:ALA:O	1:A:61:HIS:CG	2.25	0.89
1:A:39:TYR:HE1	1:A:64:GLN:HG2	1.32	0.89
1:B:169:ALA:O	1:B:173:TYR:CD2	2.25	0.89
1:A:2:LEU:HD12	1:A:2:LEU:N	1.82	0.89
1:B:52:LEU:HA	1:B:54:GLN:HG2	0.90	0.89
1:B:139:GLY:HA2	1:B:183:ILE:CD1	2.02	0.88
1:A:23:GLY:O	1:A:27:VAL:HG23	1.73	0.88
1:B:123:TYR:CE2	1:B:127:ILE:HD11	2.08	0.88
1:B:44:SER:O	1:B:48:LEU:HD23	1.72	0.88
1:A:1:MET:HA	1:A:1:MET:HE3	1.55	0.88
1:A:207:ILE:C	1:A:207:ILE:HD12	1.95	0.88
1:B:2:LEU:C	1:B:3:ASN:CG	2.29	0.88
1:B:3:ASN:HB3	1:B:236:ASP:H	1.38	0.88
1:B:182:ASN:O	1:B:183:ILE:CD1	2.23	0.87
1:B:38:THR:HB	1:B:65:ILE:HG13	1.55	0.87
1:B:4:LEU:HD22	1:B:31:LEU:HB3	1.57	0.87
1:A:59:GLU:H	1:A:60:ALA:CA	1.86	0.87
1:A:39:TYR:OH	1:A:64:GLN:HG3	1.74	0.87
1:A:4:LEU:CD1	1:A:236:ASP:OD2	2.22	0.87
1:A:167:LEU:HD13	1:A:187:ALA:HB1	1.57	0.86
1:A:166:SER:CB	1:A:169:ALA:HB3	2.05	0.86
1:A:57:GLN:OE1	1:A:58:PRO:HD2	1.75	0.86
1:B:193:ILE:HG12	1:B:222:ASP:HA	1.57	0.86
1:B:89:GLY:CA	1:B:136:MET:CE	2.51	0.86
1:A:170:ASN:ND2	1:A:170:ASN:N	2.24	0.86
1:B:34:LYS:NZ	1:B:34:LYS:CB	2.29	0.86
1:A:57:GLN:N	1:A:57:GLN:OE1	2.09	0.85
1:B:139:GLY:CA	1:B:183:ILE:HD11	2.06	0.85
1:B:123:TYR:CD2	1:B:123:TYR:O	2.29	0.85
1:A:11:ILE:HG22	1:A:12:MET:N	1.92	0.85
1:B:194:ARG:CZ	1:B:194:ARG:CB	2.52	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ALA:O	1:A:173:TYR:HD2	1.59	0.85
1:A:194:ARG:O	1:A:194:ARG:HD2	1.74	0.85
1:A:42:GLU:C	1:A:45:ARG:H	1.78	0.85
1:B:2:LEU:HB2	1:B:3:ASN:HD21	1.36	0.85
1:A:208:LEU:HB3	1:A:209:LYS:HD2	1.57	0.84
1:B:123:TYR:CE2	1:B:127:ILE:HG13	2.11	0.84
1:B:76:GLY:O	1:B:80:ILE:HG13	1.77	0.84
1:A:234:LEU:HD13	1:A:234:LEU:H	1.41	0.83
1:A:5:GLU:O	1:A:6:ASN:HB2	1.77	0.83
1:B:35:LEU:HB2	1:B:56:ASN:HD21	1.42	0.83
1:A:236:ASP:O	1:A:239:SER:HB2	1.79	0.83
1:B:4:LEU:CD2	1:B:31:LEU:HB3	2.07	0.83
1:A:38:THR:CG2	1:A:39:TYR:H	1.91	0.83
1:A:47:GLU:O	1:A:50:LYS:HB3	1.79	0.83
1:A:51:LEU:HB3	1:A:52:LEU:O	1.78	0.83
1:A:147:TYR:CD1	1:A:147:TYR:O	2.32	0.83
1:B:10:VAL:CG1	1:B:36:VAL:HG12	2.07	0.83
1:B:66:ASP:O	1:B:66:ASP:CG	2.17	0.83
1:A:146:THR:CG2	1:A:167:LEU:HD12	2.09	0.82
1:A:194:ARG:HB3	1:A:194:ARG:HH11	1.29	0.82
1:A:188:ILE:HG22	1:A:189:SER:N	1.95	0.82
1:B:59:GLU:HG3	1:B:61:HIS:CA	2.08	0.82
1:B:69:SER:O	1:B:70:ASP:C	2.15	0.82
1:A:5:GLU:CG	1:A:6:ASN:N	2.42	0.81
1:B:125:LEU:O	1:B:129:ALA:HB2	1.78	0.81
1:A:1:MET:HA	1:A:1:MET:CE	2.10	0.81
1:A:204:PHE:HA	1:A:207:ILE:HG13	1.62	0.81
1:A:39:TYR:CZ	1:A:42:GLU:HB3	2.14	0.81
1:A:39:TYR:CD1	1:A:39:TYR:O	2.33	0.81
1:A:204:PHE:HA	1:A:207:ILE:CG1	2.09	0.81
1:B:184:ARG:HD2	1:B:241:VAL:O	1.81	0.81
1:A:24:VAL:HG21	1:A:91:TYR:CE1	2.16	0.80
1:B:45:ARG:O	1:B:49:GLU:HG2	1.82	0.80
1:B:2:LEU:CB	1:B:3:ASN:OD1	2.30	0.80
1:B:60:ALA:O	1:B:62:LEU:HD13	1.82	0.80
1:B:169:ALA:O	1:B:173:TYR:HD2	1.64	0.80
1:B:5:GLU:O	1:B:6:ASN:CB	2.30	0.79
1:A:59:GLU:N	1:A:60:ALA:HA	1.97	0.79
1:A:81:GLY:O	1:A:85:GLY:HA2	1.81	0.79
1:A:254:ALA:O	1:A:255:ILE:HG22	1.82	0.79
1:B:43:ARG:O	1:B:46:LYS:CB	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASN:C	1:A:86:ASN:HD22	1.85	0.79
1:A:86:ASN:C	1:A:86:ASN:ND2	2.36	0.79
1:A:124:SER:O	1:A:128:VAL:CG2	2.30	0.79
1:A:194:ARG:O	1:A:194:ARG:CD	2.30	0.79
1:B:48:LEU:HA	1:B:51:LEU:HB2	1.64	0.79
1:B:52:LEU:C	1:B:54:GLN:HB3	2.03	0.78
1:B:45:ARG:CG	1:B:45:ARG:O	2.30	0.78
1:A:169:ALA:O	1:A:173:TYR:CD2	2.36	0.78
1:A:171:VAL:CG2	1:A:187:ALA:HB2	2.13	0.78
1:B:164:LYS:HB3	1:B:165:ALA:HB2	1.63	0.78
1:A:77:PHE:HA	1:A:80:ILE:HD12	1.65	0.78
1:B:254:ALA:C	1:B:255:ILE:CG2	2.52	0.77
1:B:6:ASN:HA	1:B:34:LYS:CD	2.15	0.77
1:B:59:GLU:N	1:B:60:ALA:CA	2.41	0.77
1:A:10:VAL:HG21	1:A:77:PHE:HE2	1.49	0.77
1:B:254:ALA:C	1:B:255:ILE:HG22	2.04	0.77
1:B:167:LEU:CD2	1:B:168:GLU:HB3	2.14	0.77
1:B:254:ALA:O	1:B:255:ILE:HG22	1.85	0.77
1:B:10:VAL:HG13	1:B:36:VAL:CG1	2.11	0.77
1:B:120:ILE:HA	1:B:121:SER:HB2	1.67	0.77
1:B:67:VAL:HG22	1:B:67:VAL:O	1.85	0.77
1:A:48:LEU:HG	1:A:62:LEU:HD22	1.67	0.77
1:B:59:GLU:H	1:B:60:ALA:HA	1.49	0.77
1:B:75:ASN:O	1:B:79:GLN:CB	2.26	0.77
1:A:92:HIS:CE1	1:A:124:SER:HG	2.03	0.76
1:A:24:VAL:HG11	1:A:91:TYR:CG	2.21	0.76
1:A:234:LEU:CD1	1:A:234:LEU:H	1.99	0.76
1:B:67:VAL:CG2	1:B:124:SER:HB2	2.15	0.76
1:B:54:GLN:CG	1:B:54:GLN:O	2.34	0.76
1:B:86:ASN:CB	1:B:135:LEU:O	2.32	0.76
1:B:67:VAL:HG23	1:B:124:SER:HB2	1.67	0.76
1:B:39:TYR:CE2	1:B:45:ARG:NH1	2.54	0.76
1:B:2:LEU:HB2	1:B:3:ASN:CG	2.06	0.75
1:B:39:TYR:HE2	1:B:45:ARG:HH12	1.31	0.75
1:A:4:LEU:HD11	1:A:236:ASP:OD2	1.86	0.75
1:A:193:ILE:CG2	1:A:221:VAL:O	2.35	0.75
1:B:58:PRO:C	1:B:60:ALA:HA	2.07	0.75
1:A:193:ILE:HG21	1:A:221:VAL:O	1.86	0.75
1:A:29:ASP:CB	1:A:54:GLN:HE21	1.98	0.75
1:A:50:LYS:C	1:A:52:LEU:N	2.31	0.75
1:A:204:PHE:CA	1:A:207:ILE:HG13	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:TYR:HE2	1:B:45:ARG:NH1	1.82	0.75
1:A:211:ILE:HG23	1:A:215:ALA:HB2	1.68	0.74
1:B:171:VAL:HG21	1:B:187:ALA:HB2	1.68	0.74
1:B:187:ALA:O	1:B:245:ASN:HA	1.88	0.74
1:A:94:ILE:O	1:A:94:ILE:CG2	2.35	0.73
1:B:125:LEU:O	1:B:129:ALA:CB	2.35	0.73
1:A:29:ASP:HB2	1:A:54:GLN:HE21	1.53	0.73
1:A:93:SER:O	1:A:94:ILE:CB	2.27	0.73
1:A:221:VAL:HA	1:A:225:GLU:OE1	1.88	0.73
1:A:1:MET:HG3	1:A:1:MET:O	1.89	0.72
1:B:89:GLY:CA	1:B:136:MET:HE3	2.14	0.72
1:A:129:ALA:CB	1:A:174:LEU:HD11	2.19	0.72
1:A:211:ILE:H	1:A:211:ILE:HD12	1.52	0.72
1:A:35:LEU:HB2	1:A:56:ASN:ND2	2.05	0.72
1:A:193:ILE:HG21	1:A:222:ASP:HA	1.72	0.72
1:A:42:GLU:O	1:A:45:ARG:CB	2.37	0.71
1:B:66:ASP:O	1:B:66:ASP:OD2	2.08	0.71
1:A:178:LEU:N	1:A:178:LEU:HD13	2.05	0.71
1:A:39:TYR:CE1	1:A:64:GLN:CG	2.68	0.71
1:A:50:LYS:C	1:A:52:LEU:H	1.92	0.71
1:B:146:THR:HG23	1:B:147:TYR:N	2.05	0.71
1:B:147:TYR:CD1	1:B:147:TYR:O	2.42	0.71
1:B:48:LEU:O	1:B:51:LEU:HB2	1.90	0.71
1:A:171:VAL:HG21	1:A:187:ALA:CB	2.16	0.71
1:A:211:ILE:HD12	1:A:211:ILE:N	2.06	0.71
1:B:35:LEU:HB2	1:B:56:ASN:ND2	2.04	0.71
1:A:10:VAL:HG13	1:A:36:VAL:CG1	2.20	0.71
1:B:1:MET:CB	1:B:2:LEU:CD2	2.63	0.71
1:A:42:GLU:OE2	1:A:42:GLU:O	2.09	0.71
1:A:45:ARG:HD3	1:A:62:LEU:HD13	1.71	0.71
1:A:5:GLU:HB2	1:A:31:LEU:O	1.90	0.70
1:B:193:ILE:CG1	1:B:222:ASP:HA	2.20	0.70
1:A:1:MET:C	1:A:2:LEU:HG	2.12	0.70
1:B:24:VAL:O	1:B:28:LEU:HB2	1.92	0.70
1:B:86:ASN:HB2	1:B:135:LEU:O	1.91	0.70
1:B:167:LEU:CA	1:B:168:GLU:HB3	2.21	0.70
1:A:7:LYS:HG2	1:A:88:ASP:CG	2.12	0.69
1:A:16:ASN:HB3	1:A:47:GLU:OE1	1.91	0.69
1:B:65:ILE:HG22	1:B:73:VAL:HG13	1.72	0.69
1:B:59:GLU:CG	1:B:61:HIS:N	2.35	0.69
1:A:40:ARG:HH12	1:A:68:GLN:HE21	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG11	1:A:91:TYR:CD1	2.27	0.69
1:B:45:ARG:O	1:B:46:LYS:C	2.22	0.69
1:A:71:GLU:O	1:A:75:ASN:ND2	2.26	0.69
1:A:41:LYS:O	1:A:44:SER:HB2	1.93	0.69
1:A:70:ASP:O	1:A:74:ILE:HG13	1.92	0.69
1:B:124:SER:O	1:B:128:VAL:CG2	2.37	0.69
1:A:70:ASP:OD1	1:A:70:ASP:N	2.25	0.68
1:B:20:ILE:CG2	1:B:226:VAL:HG11	2.22	0.68
1:A:167:LEU:HD13	1:A:187:ALA:CB	2.23	0.68
1:B:86:ASN:H	1:B:86:ASN:ND2	1.88	0.68
1:A:166:SER:HB3	1:A:169:ALA:HB2	1.71	0.68
1:A:43:ARG:HA	1:A:46:LYS:HB2	1.74	0.68
1:B:139:GLY:CA	1:B:183:ILE:CD1	2.69	0.68
1:B:2:LEU:HB2	1:B:3:ASN:OD1	1.93	0.68
1:B:67:VAL:CG2	1:B:124:SER:CB	2.71	0.68
1:B:166:SER:OG	1:B:167:LEU:N	2.23	0.68
1:B:143:VAL:CG2	1:B:234:LEU:HD13	2.24	0.68
1:A:83:ASP:N	1:A:83:ASP:OD1	2.22	0.68
1:B:140:GLY:H	1:B:183:ILE:HD12	1.59	0.67
1:B:231:ALA:O	1:B:235:SER:HB3	1.94	0.67
1:A:129:ALA:CB	1:A:174:LEU:CD1	2.72	0.67
1:A:178:LEU:N	1:A:178:LEU:CD1	2.57	0.67
1:B:123:TYR:CE2	1:B:127:ILE:HG12	2.29	0.67
1:B:211:ILE:O	1:B:213:GLU:N	2.27	0.67
1:B:46:LYS:O	1:B:49:GLU:CG	2.42	0.67
1:A:43:ARG:HG2	1:A:43:ARG:O	1.94	0.67
1:A:51:LEU:HD13	1:A:53:GLU:HB2	1.76	0.66
1:B:66:ASP:O	1:B:67:VAL:HG12	1.94	0.66
1:B:23:GLY:O	1:B:27:VAL:HG23	1.95	0.66
1:B:27:VAL:O	1:B:30:GLN:HB3	1.95	0.66
1:A:231:ALA:O	1:A:235:SER:HB3	1.96	0.66
1:A:216:PRO:HG2	1:A:251:GLY:HA3	1.76	0.66
1:B:60:ALA:O	1:B:61:HIS:C	2.34	0.66
1:B:61:HIS:CD2	1:B:84:VAL:HG12	2.30	0.66
1:A:123:TYR:CD1	1:A:127:ILE:HD11	2.30	0.66
1:B:123:TYR:HD2	1:B:124:SER:N	1.94	0.66
1:B:39:TYR:CE1	1:B:64:GLN:CB	2.79	0.66
1:A:10:VAL:HG13	1:A:36:VAL:HG12	1.78	0.66
1:B:146:THR:CG2	1:B:147:TYR:N	2.53	0.66
1:B:135:LEU:HD23	1:B:135:LEU:N	2.11	0.66
1:A:123:TYR:CD2	1:A:127:ILE:HD11	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:H	1:A:56:ASN:HD21	1.43	0.65
1:B:122:SER:OG	1:B:123:TYR:N	2.29	0.65
1:B:2:LEU:HB3	1:B:3:ASN:OD1	1.96	0.65
1:B:120:ILE:O	1:B:120:ILE:HG22	1.96	0.65
1:B:211:ILE:CG2	1:B:215:ALA:HB2	2.27	0.65
1:A:76:GLY:O	1:A:80:ILE:HG13	1.96	0.65
1:B:17:LYS:HE2	1:B:18:ARG:NH2	2.11	0.65
1:A:146:THR:OG1	1:A:147:TYR:N	2.23	0.65
1:B:57:GLN:OE1	1:B:58:PRO:HD3	1.97	0.65
1:B:17:LYS:O	1:B:17:LYS:CG	2.43	0.65
1:B:249:ASP:OD1	1:B:253:HIS:HD2	1.80	0.65
1:A:217:LEU:O	1:A:219:ARG:HG2	1.97	0.64
1:A:1:MET:CG	1:A:1:MET:O	2.45	0.64
1:B:43:ARG:C	1:B:45:ARG:N	2.47	0.64
1:A:29:ASP:OD1	1:A:54:GLN:HB3	1.98	0.64
1:B:43:ARG:O	1:B:46:LYS:N	2.31	0.64
1:B:120:ILE:HA	1:B:121:SER:CB	2.25	0.64
1:B:123:TYR:CE2	1:B:127:ILE:CD1	2.64	0.64
1:A:2:LEU:N	1:A:2:LEU:CD1	2.43	0.64
1:B:43:ARG:C	1:B:46:LYS:H	2.01	0.64
1:A:171:VAL:HG12	1:A:243:GLY:HA2	1.80	0.64
1:A:167:LEU:CD1	1:A:187:ALA:HB1	2.28	0.64
1:A:207:ILE:CD1	1:A:207:ILE:C	2.67	0.64
1:B:2:LEU:O	1:B:3:ASN:ND2	2.30	0.63
1:B:43:ARG:O	1:B:43:ARG:HG2	1.98	0.63
1:A:38:THR:HG23	1:A:39:TYR:N	2.00	0.63
1:B:122:SER:OG	1:B:123:TYR:C	2.37	0.63
1:B:1:MET:HB3	1:B:2:LEU:CG	2.28	0.63
1:B:52:LEU:HA	1:B:54:GLN:CB	2.28	0.63
1:B:70:ASP:O	1:B:74:ILE:HG13	1.99	0.63
1:B:86:ASN:HB3	1:B:135:LEU:O	1.96	0.63
1:A:137:PRO:HG2	1:A:138:GLU:HG2	1.80	0.63
1:A:39:TYR:CZ	1:A:64:GLN:CG	2.81	0.63
1:A:39:TYR:CE1	1:A:42:GLU:HB3	2.34	0.63
1:B:48:LEU:CA	1:B:51:LEU:HB2	2.28	0.63
1:B:52:LEU:HA	1:B:54:GLN:HG3	1.74	0.63
1:A:38:THR:HG22	1:A:39:TYR:N	2.08	0.63
1:A:193:ILE:HD12	1:A:222:ASP:HA	1.80	0.62
1:A:187:ALA:N	1:A:244:GLU:O	2.31	0.62
1:B:130:HIS:HE1	1:B:177:ASP:OD2	1.82	0.62
1:B:223:GLN:N	1:B:223:GLN:OE1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:HG3	1:B:61:HIS:H	0.69	0.62
1:A:208:LEU:HD13	1:A:209:LYS:NZ	2.15	0.62
1:A:2:LEU:H	1:A:2:LEU:HD12	1.63	0.62
1:A:170:ASN:C	1:A:172:LYS:N	2.45	0.62
1:A:140:GLY:O	1:A:184:ARG:N	2.33	0.62
1:A:147:TYR:CZ	1:A:192:PRO:HA	2.34	0.62
1:A:120:ILE:HG23	1:A:121:SER:N	2.14	0.62
1:A:170:ASN:C	1:A:172:LYS:H	2.03	0.62
1:A:170:ASN:O	1:A:171:VAL:C	2.34	0.62
1:A:228:LYS:O	1:A:231:ALA:HB3	2.00	0.61
1:B:135:LEU:C	1:B:137:PRO:HD3	2.17	0.61
1:B:164:LYS:CB	1:B:165:ALA:HB2	2.28	0.61
1:B:7:LYS:HD3	1:B:88:ASP:OD1	2.00	0.61
1:B:52:LEU:N	1:B:54:GLN:HG2	2.13	0.61
1:A:130:HIS:O	1:A:133:LYS:CD	2.48	0.61
1:A:169:ALA:C	1:A:170:ASN:HD22	2.03	0.61
1:A:188:ILE:HD11	1:A:229:THR:HG22	1.82	0.61
1:A:39:TYR:CZ	1:A:42:GLU:CB	2.83	0.61
1:B:143:VAL:HG21	1:B:234:LEU:HD13	1.82	0.61
1:A:25:ALA:HB1	1:A:35:LEU:CD1	2.30	0.61
1:A:42:GLU:O	1:A:45:ARG:HB2	2.01	0.61
1:B:146:THR:HG21	1:B:189:SER:HB2	1.82	0.61
1:B:77:PHE:HA	1:B:80:ILE:HG13	1.83	0.61
1:A:5:GLU:HG3	1:A:6:ASN:H	1.64	0.61
1:A:234:LEU:CD1	1:A:234:LEU:N	2.62	0.60
1:B:170:ASN:HA	1:B:173:TYR:HD2	1.66	0.60
1:A:3:ASN:HD21	1:A:236:ASP:HB2	1.66	0.60
1:B:235:SER:OG	1:B:237:LEU:HB2	2.02	0.60
1:A:89:GLY:HA2	1:A:136:MET:HE1	1.82	0.60
1:A:49:GLU:CG	1:A:49:GLU:O	2.21	0.60
1:B:2:LEU:CB	1:B:3:ASN:CG	2.70	0.60
1:B:123:TYR:HD2	1:B:124:SER:CA	2.14	0.60
1:A:210:GLU:HB3	1:A:211:ILE:HD12	1.85	0.59
1:A:45:ARG:O	1:A:45:ARG:HD2	2.02	0.59
1:B:64:GLN:C	1:B:65:ILE:HG12	2.21	0.59
1:B:22:PHE:O	1:B:23:GLY:C	2.37	0.59
1:B:84:VAL:HG23	1:B:85:GLY:N	2.17	0.59
1:A:207:ILE:HD12	1:A:207:ILE:O	2.00	0.59
1:B:3:ASN:HD21	1:B:237:LEU:HD13	1.68	0.59
1:A:7:LYS:HB3	1:A:9:TYR:CE2	2.38	0.59
1:B:164:LYS:HE2	1:B:164:LYS:CA	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ARG:HG2	1:B:194:ARG:NH1	1.90	0.59
1:A:94:ILE:O	1:A:94:ILE:HG22	2.03	0.59
1:B:143:VAL:HG23	1:B:234:LEU:CD1	2.33	0.59
1:A:207:ILE:O	1:A:211:ILE:HD13	2.02	0.58
1:A:5:GLU:O	1:A:6:ASN:CB	2.49	0.58
1:B:211:ILE:HG22	1:B:215:ALA:HB2	1.85	0.58
1:A:42:GLU:HB2	1:A:45:ARG:HB2	1.86	0.58
1:B:146:THR:HG23	1:B:147:TYR:CA	2.33	0.58
1:B:35:LEU:HD13	1:B:37:PHE:CZ	2.38	0.58
1:A:136:MET:O	1:A:139:GLY:N	2.30	0.58
1:A:58:PRO:HB2	1:A:59:GLU:HB2	1.86	0.58
1:A:10:VAL:CG1	1:A:36:VAL:HG12	2.34	0.57
1:A:170:ASN:O	1:A:172:LYS:N	2.37	0.57
1:B:127:ILE:C	1:B:129:ALA:H	2.08	0.57
1:B:38:THR:HA	1:B:63:TYR:O	2.03	0.57
1:B:24:VAL:HG22	1:B:227:GLY:HA2	1.86	0.57
1:A:130:HIS:O	1:A:133:LYS:HD3	2.04	0.57
1:B:194:ARG:CZ	1:B:194:ARG:HB3	2.25	0.57
1:B:9:TYR:O	1:B:36:VAL:N	2.34	0.57
1:A:129:ALA:HB1	1:A:174:LEU:HD13	1.86	0.57
1:A:215:ALA:O	1:A:218:LYS:HD3	2.03	0.57
1:B:20:ILE:HA	1:B:223:GLN:HG3	1.86	0.57
1:B:2:LEU:C	1:B:3:ASN:ND2	2.57	0.57
1:A:188:ILE:HG23	1:A:189:SER:N	2.20	0.57
1:A:89:GLY:HA2	1:A:136:MET:CE	2.35	0.57
1:A:29:ASP:CB	1:A:54:GLN:NE2	2.55	0.57
1:A:94:ILE:O	1:A:94:ILE:HG23	2.04	0.57
1:A:78:GLU:O	1:A:79:GLN:C	2.41	0.57
1:A:147:TYR:CD1	1:A:147:TYR:C	2.71	0.56
1:A:41:LYS:O	1:A:44:SER:CB	2.52	0.56
1:B:14:ILE:HG21	1:B:48:LEU:HD11	1.86	0.56
1:B:140:GLY:H	1:B:183:ILE:CD1	2.18	0.56
1:B:45:ARG:O	1:B:49:GLU:CG	2.53	0.56
1:A:2:LEU:O	1:A:3:ASN:O	2.22	0.56
1:A:16:ASN:CB	1:A:47:GLU:OE1	2.53	0.56
1:B:74:ILE:C	1:B:76:GLY:H	2.05	0.56
1:A:205:ASN:O	1:A:209:LYS:HD3	2.05	0.56
1:A:7:LYS:CG	1:A:88:ASP:CG	2.74	0.56
1:B:43:ARG:C	1:B:45:ARG:H	2.08	0.56
1:A:40:ARG:HH12	1:A:68:GLN:NE2	2.04	0.56
1:A:184:ARG:HG2	1:B:217:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:N	1:B:36:VAL:O	2.38	0.56
1:A:24:VAL:HG21	1:A:91:TYR:CZ	2.40	0.56
1:B:236:ASP:C	1:B:238:SER:H	2.09	0.56
1:A:136:MET:O	1:A:138:GLU:N	2.39	0.56
1:A:29:ASP:HB2	1:A:54:GLN:HE22	1.66	0.56
1:A:8:THR:HA	1:A:34:LYS:O	2.05	0.56
1:A:193:ILE:HD13	1:A:221:VAL:HG23	1.88	0.55
1:A:206:THR:O	1:A:209:LYS:N	2.35	0.55
1:B:244:GLU:OE1	1:B:245:ASN:N	2.37	0.55
1:A:146:THR:CG2	1:A:167:LEU:CD1	2.83	0.55
1:A:50:LYS:HG3	1:A:51:LEU:H	1.71	0.55
1:B:52:LEU:CA	1:B:54:GLN:CG	2.48	0.55
1:A:57:GLN:OE1	1:A:58:PRO:CD	2.52	0.55
1:B:139:GLY:C	1:B:183:ILE:HD11	2.26	0.55
1:A:90:VAL:HG23	1:A:142:ILE:HG12	1.89	0.55
1:A:45:ARG:CD	1:A:45:ARG:C	2.74	0.54
1:B:44:SER:O	1:B:48:LEU:CD2	2.52	0.54
1:B:92:HIS:N	1:B:143:VAL:O	2.40	0.54
1:B:164:LYS:HE2	1:B:164:LYS:N	2.21	0.54
1:A:11:ILE:CG2	1:A:12:MET:N	2.62	0.54
1:A:46:LYS:HD2	1:A:46:LYS:O	2.06	0.54
1:A:185:VAL:O	1:A:243:GLY:N	2.40	0.54
1:B:193:ILE:HD12	1:B:193:ILE:N	2.22	0.54
1:B:28:LEU:O	1:B:33:ALA:HB3	2.07	0.54
1:A:42:GLU:C	1:A:44:SER:N	2.61	0.54
1:B:48:LEU:C	1:B:51:LEU:HB2	2.28	0.54
1:B:140:GLY:N	1:B:183:ILE:CD1	2.71	0.54
1:A:14:ILE:HD12	1:A:37:PHE:HD1	1.73	0.54
1:A:211:ILE:CD1	1:A:211:ILE:H	2.19	0.54
1:B:168:GLU:O	1:B:169:ALA:HB2	2.07	0.54
1:A:60:ALA:C	1:A:61:HIS:CG	2.75	0.53
1:B:27:VAL:HG21	1:B:227:GLY:HA3	1.91	0.53
1:B:141:SER:C	1:B:142:ILE:HG13	2.29	0.53
1:B:10:VAL:HA	1:B:36:VAL:O	2.08	0.53
1:A:123:TYR:O	1:A:127:ILE:CG1	2.43	0.53
1:A:217:LEU:HD23	1:A:250:SER:O	2.08	0.53
1:A:230:ALA:O	1:A:233:LEU:N	2.41	0.53
1:A:35:LEU:N	1:A:56:ASN:HD21	2.05	0.53
1:B:3:ASN:ND2	1:B:237:LEU:HD13	2.23	0.53
1:B:2:LEU:O	1:B:3:ASN:CG	2.47	0.53
1:A:204:PHE:O	1:A:208:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:O	1:B:129:ALA:N	2.41	0.53
1:B:23:GLY:O	1:B:26:LYS:HB3	2.09	0.53
1:A:9:TYR:N	1:A:34:LYS:O	2.37	0.53
1:B:178:LEU:O	1:B:179:GLY:C	2.45	0.53
1:B:211:ILE:O	1:B:212:GLU:C	2.45	0.53
1:A:120:ILE:HG23	1:A:121:SER:H	1.74	0.53
1:A:91:TYR:CE2	1:A:93:SER:HB3	2.44	0.53
1:A:61:HIS:HB3	1:A:63:TYR:HE2	1.73	0.53
1:B:86:ASN:HB3	1:B:135:LEU:HB2	1.90	0.53
1:B:45:ARG:C	1:B:47:GLU:N	2.58	0.53
1:B:76:GLY:O	1:B:80:ILE:CG1	2.55	0.53
1:B:86:ASN:N	1:B:86:ASN:ND2	2.49	0.53
1:A:60:ALA:O	1:A:61:HIS:CB	2.57	0.53
1:B:127:ILE:C	1:B:129:ALA:N	2.62	0.53
1:B:86:ASN:CB	1:B:135:LEU:HB2	2.39	0.52
1:B:172:LYS:O	1:B:175:ALA:HB3	2.10	0.52
1:B:5:GLU:HB3	1:B:32:GLY:HA3	1.92	0.52
1:A:125:LEU:O	1:A:129:ALA:N	2.35	0.52
1:A:207:ILE:HD12	1:A:208:LEU:N	2.25	0.52
1:A:27:VAL:HG21	1:A:227:GLY:HA3	1.91	0.52
1:B:169:ALA:O	1:B:173:TYR:CE2	2.63	0.52
1:B:194:ARG:CZ	1:B:194:ARG:HB2	2.39	0.52
1:A:253:HIS:HE1	1:B:243:GLY:O	1.93	0.52
1:A:244:GLU:OE2	1:B:247:HIS:ND1	2.41	0.52
1:A:147:TYR:HD1	1:A:147:TYR:O	1.86	0.52
1:A:176:LEU:O	1:A:180:PRO:HD3	2.09	0.52
1:A:224:VAL:O	1:A:228:LYS:HG3	2.10	0.52
1:A:39:TYR:CZ	1:A:64:GLN:HG3	2.42	0.52
1:B:178:LEU:O	1:B:181:ASP:N	2.43	0.52
1:A:145:THR:HG22	1:A:146:THR:N	2.25	0.51
1:B:146:THR:CG2	1:B:189:SER:HB2	2.39	0.51
1:A:3:ASN:OD1	1:A:4:LEU:N	2.43	0.51
1:A:69:SER:O	1:A:70:ASP:C	2.48	0.51
1:B:167:LEU:CB	1:B:168:GLU:HB3	2.40	0.51
1:B:229:THR:HB	1:B:248:VAL:HG21	1.91	0.51
1:B:211:ILE:HG22	1:B:215:ALA:CB	2.40	0.51
1:A:45:ARG:O	1:A:48:LEU:N	2.44	0.51
1:A:89:GLY:HA3	1:A:141:SER:O	2.11	0.51
1:A:228:LYS:HE3	1:B:236:ASP:O	2.11	0.51
1:B:46:LYS:O	1:B:49:GLU:HG3	2.11	0.51
1:B:52:LEU:O	1:B:54:GLN:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:O	1:B:212:GLU:HG3	2.10	0.51
1:A:20:ILE:HA	1:A:223:GLN:HG2	1.93	0.51
1:A:10:VAL:HG22	1:A:87:ILE:HD11	1.92	0.51
1:B:19:SER:O	1:B:22:PHE:N	2.44	0.51
1:A:194:ARG:CG	1:A:194:ARG:NH1	2.68	0.51
1:B:86:ASN:HA	1:B:135:LEU:HB2	1.91	0.51
1:B:92:HIS:O	1:B:144:ALA:HA	2.10	0.51
1:B:2:LEU:O	1:B:3:ASN:CB	2.56	0.51
1:A:7:LYS:HG2	1:A:88:ASP:CB	2.41	0.51
1:B:46:LYS:O	1:B:49:GLU:HG2	2.11	0.51
1:A:188:ILE:HG23	1:A:189:SER:H	1.76	0.50
1:A:211:ILE:CG2	1:A:215:ALA:HB2	2.38	0.50
1:A:253:HIS:NE2	1:B:242:THR:O	2.43	0.50
1:B:69:SER:HB2	1:B:72:GLU:HB2	1.93	0.50
1:A:167:LEU:C	1:A:169:ALA:H	2.14	0.50
1:A:237:LEU:HG	1:B:228:LYS:HB3	1.92	0.50
1:B:211:ILE:HG23	1:B:215:ALA:HB2	1.92	0.50
1:A:37:PHE:CD2	1:A:37:PHE:N	2.79	0.50
1:B:78:GLU:OE2	1:B:82:LYS:HE2	2.11	0.50
1:A:165:ALA:C	1:A:166:SER:HG	2.14	0.50
1:A:34:LYS:NZ	1:A:58:PRO:HG2	2.26	0.50
1:B:69:SER:O	1:B:70:ASP:O	2.30	0.50
1:A:237:LEU:CD1	1:B:228:LYS:HB3	2.42	0.50
1:B:39:TYR:CE1	1:B:64:GLN:CG	2.95	0.50
1:A:167:LEU:C	1:A:169:ALA:N	2.58	0.50
1:A:184:ARG:HB3	1:A:242:THR:HB	1.92	0.50
1:A:39:TYR:HD1	1:A:40:ARG:N	2.06	0.50
1:B:75:ASN:ND2	1:B:78:GLU:OE1	2.45	0.50
1:A:19:SER:O	1:A:20:ILE:C	2.49	0.50
1:A:208:LEU:HB3	1:A:209:LYS:CD	2.36	0.50
1:A:42:GLU:CD	1:A:42:GLU:O	2.50	0.50
1:A:62:LEU:O	1:A:63:TYR:CD2	2.65	0.50
1:B:143:VAL:HG23	1:B:234:LEU:HD13	1.92	0.50
1:B:44:SER:C	1:B:47:GLU:H	2.15	0.50
1:A:70:ASP:O	1:A:74:ILE:CG1	2.60	0.49
1:B:141:SER:O	1:B:142:ILE:HG13	2.12	0.49
1:B:241:VAL:O	1:B:242:THR:HB	2.11	0.49
1:A:129:ALA:HB3	1:A:174:LEU:HD11	1.94	0.49
1:A:185:VAL:O	1:A:243:GLY:HA2	2.12	0.49
1:A:11:ILE:O	1:A:37:PHE:HA	2.13	0.49
1:A:4:LEU:HD12	1:A:236:ASP:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:MET:HE3	1:B:77:PHE:HZ	1.76	0.49
1:A:194:ARG:CA	1:A:194:ARG:HH11	2.25	0.49
1:A:219:ARG:NH2	1:A:225:GLU:OE2	2.46	0.49
1:B:20:ILE:O	1:B:23:GLY:N	2.45	0.49
1:B:127:ILE:O	1:B:128:VAL:C	2.51	0.49
1:B:66:ASP:C	1:B:67:VAL:HG12	2.31	0.49
1:B:238:SER:O	1:B:241:VAL:HB	2.13	0.49
1:B:36:VAL:HG22	1:B:61:HIS:CB	2.43	0.49
1:B:67:VAL:CG2	1:B:67:VAL:O	2.57	0.49
1:B:75:ASN:HA	1:B:78:GLU:HB3	1.95	0.49
1:A:25:ALA:CB	1:A:35:LEU:CD1	2.91	0.49
1:B:58:PRO:HD2	1:B:58:PRO:O	2.12	0.49
1:A:42:GLU:O	1:A:45:ARG:HB3	2.13	0.49
1:A:77:PHE:HB3	1:A:135:LEU:HD11	1.94	0.48
1:B:8:THR:O	1:B:88:ASP:N	2.46	0.48
1:B:9:TYR:O	1:B:35:LEU:HA	2.13	0.48
1:A:10:VAL:HG21	1:A:77:PHE:CE2	2.38	0.48
1:A:121:SER:O	1:A:121:SER:OG	2.28	0.48
1:A:204:PHE:C	1:A:207:ILE:HG13	2.34	0.48
1:B:236:ASP:C	1:B:238:SER:N	2.66	0.48
1:A:208:LEU:HD13	1:A:209:LYS:HZ3	1.78	0.48
1:A:20:ILE:HA	1:A:223:GLN:CG	2.44	0.48
1:A:185:VAL:N	1:A:242:THR:OG1	2.45	0.48
1:A:84:VAL:HG23	1:A:85:GLY:N	2.29	0.48
1:B:164:LYS:CA	1:B:165:ALA:HB2	2.43	0.48
1:A:11:ILE:HG22	1:A:12:MET:H	1.74	0.48
1:A:28:LEU:O	1:A:29:ASP:C	2.49	0.48
1:A:146:THR:HG23	1:A:167:LEU:HD12	1.94	0.48
1:B:146:THR:CG2	1:B:147:TYR:HA	2.43	0.48
1:B:178:LEU:O	1:B:181:ASP:HB2	2.14	0.48
1:A:26:LYS:C	1:A:28:LEU:H	2.17	0.48
1:B:34:LYS:HG2	1:B:34:LYS:H	1.52	0.48
1:B:5:GLU:HB3	1:B:31:LEU:O	2.13	0.48
1:B:146:THR:CG2	1:B:147:TYR:CA	2.91	0.47
1:B:36:VAL:HG22	1:B:61:HIS:HB3	1.95	0.47
1:A:89:GLY:CA	1:A:141:SER:O	2.62	0.47
1:B:80:ILE:O	1:B:84:VAL:HG22	2.14	0.47
1:B:123:TYR:CD2	1:B:124:SER:HA	2.49	0.47
1:B:125:LEU:HA	1:B:128:VAL:HB	1.96	0.47
1:B:193:ILE:HG12	1:B:222:ASP:CA	2.38	0.47
1:B:229:THR:O	1:B:232:TYR:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ALA:O	1:A:166:SER:OG	2.30	0.47
1:A:39:TYR:O	1:A:39:TYR:HD1	1.80	0.47
1:A:171:VAL:HG13	1:A:185:VAL:O	2.13	0.47
1:B:182:ASN:O	1:B:183:ILE:HD13	2.12	0.47
1:A:25:ALA:O	1:A:29:ASP:N	2.34	0.47
1:A:57:GLN:CA	1:A:57:GLN:OE1	2.62	0.47
1:A:92:HIS:ND1	1:A:92:HIS:O	2.47	0.47
1:B:218:LYS:HD3	1:B:218:LYS:HA	1.44	0.47
1:B:52:LEU:HD21	1:B:56:ASN:O	2.14	0.47
1:A:173:TYR:CD2	1:A:173:TYR:N	2.79	0.47
1:A:2:LEU:HD12	1:A:2:LEU:C	2.21	0.47
1:B:18:ARG:HG2	1:B:194:ARG:NH2	2.30	0.47
1:A:204:PHE:HA	1:A:207:ILE:HG12	1.95	0.47
1:A:57:GLN:N	1:A:58:PRO:O	2.48	0.47
1:B:3:ASN:HB3	1:B:236:ASP:N	2.18	0.47
1:A:48:LEU:O	1:A:50:LYS:O	2.32	0.47
1:B:247:HIS:CD2	1:B:253:HIS:HB3	2.50	0.47
1:B:18:ARG:HG2	1:B:194:ARG:HH21	1.80	0.47
1:B:25:ALA:HA	1:B:35:LEU:HD11	1.96	0.47
1:A:45:ARG:CD	1:A:45:ARG:O	2.62	0.46
1:A:47:GLU:O	1:A:50:LYS:CB	2.56	0.46
1:A:39:TYR:CE1	1:A:64:GLN:HA	2.50	0.46
1:B:146:THR:HG22	1:B:147:TYR:HA	1.98	0.46
1:A:168:GLU:HG3	1:A:172:LYS:HZ3	1.78	0.46
1:B:8:THR:N	1:B:88:ASP:HB2	2.30	0.46
1:A:66:ASP:OD1	1:A:66:ASP:C	2.54	0.46
1:B:17:LYS:HE2	1:B:18:ARG:HH21	1.81	0.46
1:A:123:TYR:CG	1:A:127:ILE:CD1	2.79	0.45
1:A:50:LYS:CG	1:A:51:LEU:N	2.66	0.45
1:B:11:ILE:HD13	1:B:37:PHE:CE1	2.51	0.45
1:B:66:ASP:O	1:B:67:VAL:CG1	2.62	0.45
1:A:140:GLY:O	1:A:183:ILE:HA	2.17	0.45
1:B:67:VAL:HG22	1:B:124:SER:CB	2.45	0.45
1:B:89:GLY:CA	1:B:136:MET:HE2	2.29	0.45
1:A:123:TYR:CD2	1:A:127:ILE:CD1	2.98	0.45
1:A:175:ALA:HA	1:A:185:VAL:HG13	1.97	0.45
1:A:91:TYR:HE2	1:A:93:SER:HB3	1.81	0.45
1:A:171:VAL:O	1:A:175:ALA:HB2	2.16	0.45
1:A:77:PHE:CD2	1:A:80:ILE:HD12	2.51	0.45
1:A:90:VAL:CG2	1:A:142:ILE:HG12	2.46	0.45
1:A:62:LEU:H	1:A:62:LEU:HG	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HB3	1:B:209:LYS:HD2	1.99	0.45
1:B:121:SER:H	1:B:122:SER:HA	1.82	0.45
1:A:178:LEU:HD13	1:A:178:LEU:H	1.77	0.45
1:A:255:ILE:HD13	1:A:255:ILE:HG21	1.48	0.45
1:B:123:TYR:HD2	1:B:124:SER:HA	1.81	0.45
1:B:16:ASN:OD1	1:B:19:SER:OG	2.33	0.45
1:A:127:ILE:H	1:A:127:ILE:HG13	1.67	0.45
1:B:180:PRO:C	1:B:182:ASN:H	2.20	0.45
1:B:143:VAL:HG22	1:B:233:LEU:HB3	1.97	0.45
1:A:189:SER:HB3	1:A:245:ASN:HD21	1.82	0.44
1:B:164:LYS:HE2	1:B:164:LYS:HA	1.99	0.44
1:B:211:ILE:C	1:B:213:GLU:N	2.71	0.44
1:B:25:ALA:O	1:B:29:ASP:N	2.47	0.44
1:A:167:LEU:O	1:A:168:GLU:C	2.51	0.44
1:A:78:GLU:C	1:A:80:ILE:N	2.68	0.44
1:B:52:LEU:CA	1:B:54:GLN:HB3	2.47	0.44
1:B:143:VAL:CG2	1:B:234:LEU:CD1	2.91	0.44
1:B:49:GLU:C	1:B:51:LEU:H	2.20	0.44
1:A:146:THR:HG21	1:A:167:LEU:HD12	1.98	0.44
1:A:168:GLU:HG3	1:A:172:LYS:NZ	2.32	0.44
1:A:26:LYS:C	1:A:28:LEU:N	2.68	0.44
1:A:89:GLY:CA	1:A:136:MET:HE1	2.46	0.44
1:B:16:ASN:OD1	1:B:16:ASN:N	2.50	0.44
1:B:48:LEU:HA	1:B:51:LEU:CB	2.43	0.44
1:A:87:ILE:HD13	1:A:87:ILE:HG21	1.61	0.44
1:B:78:GLU:O	1:B:79:GLN:C	2.55	0.44
1:A:45:ARG:CZ	1:A:49:GLU:HB2	2.47	0.44
1:B:1:MET:HB3	1:B:2:LEU:HD21	1.86	0.44
1:B:58:PRO:CB	1:B:59:GLU:HA	2.48	0.44
1:B:8:THR:H	1:B:88:ASP:HB2	1.83	0.44
1:A:215:ALA:HB1	1:A:250:SER:HB3	2.00	0.44
1:A:50:LYS:O	1:A:52:LEU:N	2.30	0.44
1:B:183:ILE:HG23	1:B:184:ARG:N	2.32	0.44
1:A:129:ALA:CB	1:A:174:LEU:HD13	2.43	0.44
1:A:34:LYS:HZ3	1:A:58:PRO:HG2	1.81	0.44
1:B:86:ASN:HB3	1:B:135:LEU:CB	2.48	0.44
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.62	0.43
1:B:28:LEU:HA	1:B:28:LEU:HD23	1.59	0.43
1:A:146:THR:O	1:A:189:SER:HA	2.17	0.43
1:A:57:GLN:C	1:A:58:PRO:O	2.56	0.43
1:A:40:ARG:NH1	1:A:68:GLN:HE21	2.10	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASP:C	1:A:74:ILE:HG13	2.38	0.43
1:B:179:GLY:N	1:B:180:PRO:HD3	2.33	0.43
1:B:20:ILE:HG23	1:B:226:VAL:HG11	1.98	0.43
1:A:178:LEU:HB3	1:A:183:ILE:HD12	2.00	0.43
1:B:234:LEU:HD13	1:B:234:LEU:N	2.32	0.43
1:B:41:LYS:O	1:B:43:ARG:N	2.50	0.43
1:A:233:LEU:O	1:A:238:SER:OG	2.31	0.43
1:A:185:VAL:O	1:A:243:GLY:CA	2.67	0.43
1:B:86:ASN:CA	1:B:135:LEU:HB2	2.48	0.43
1:B:249:ASP:OD1	1:B:253:HIS:CD2	2.66	0.43
1:A:39:TYR:OH	1:A:42:GLU:HB3	2.17	0.43
1:A:58:PRO:CB	1:A:59:GLU:HB2	2.48	0.43
1:B:208:LEU:HB3	1:B:209:LYS:CD	2.48	0.43
1:B:39:TYR:CE1	1:B:64:GLN:HG3	2.54	0.43
1:B:49:GLU:HG2	1:B:49:GLU:H	1.61	0.43
1:B:4:LEU:HD22	1:B:31:LEU:O	2.19	0.43
1:A:143:VAL:HG21	1:A:233:LEU:HB2	2.01	0.43
1:B:140:GLY:N	1:B:183:ILE:HD11	2.33	0.43
1:B:12:MET:CE	1:B:77:PHE:HZ	2.30	0.43
1:A:123:TYR:O	1:A:124:SER:C	2.57	0.43
1:A:254:ALA:O	1:A:255:ILE:CG2	2.58	0.43
1:B:210:GLU:HG2	1:B:210:GLU:O	2.11	0.43
1:B:251:GLY:O	1:B:252:PHE:C	2.57	0.43
1:A:123:TYR:CD1	1:A:127:ILE:CD1	3.02	0.42
1:B:1:MET:CB	1:B:2:LEU:HG	2.48	0.42
1:A:65:ILE:HD13	1:A:65:ILE:HG21	1.63	0.42
1:A:176:LEU:HA	1:B:216:PRO:HB3	2.01	0.42
1:B:2:LEU:CB	1:B:3:ASN:ND2	2.68	0.42
1:B:84:VAL:CG2	1:B:85:GLY:N	2.83	0.42
1:A:168:GLU:CG	1:A:168:GLU:O	2.67	0.42
1:A:208:LEU:HD13	1:A:209:LYS:HZ2	1.84	0.42
1:A:209:LYS:HD2	1:A:209:LYS:N	2.34	0.42
1:B:183:ILE:HD12	1:B:183:ILE:HA	1.86	0.42
1:B:1:MET:CB	1:B:2:LEU:CG	2.97	0.42
1:B:52:LEU:CA	1:B:54:GLN:CB	2.95	0.42
1:B:5:GLU:HB2	1:B:32:GLY:O	2.18	0.42
1:A:210:GLU:HG3	1:A:214:ARG:HD2	2.01	0.42
1:B:176:LEU:HA	1:B:176:LEU:HD13	1.43	0.42
1:B:214:ARG:O	1:B:255:ILE:CD1	2.68	0.42
1:A:16:ASN:C	1:A:18:ARG:H	2.22	0.42
1:B:60:ALA:O	1:B:62:LEU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:O	1:A:30:GLN:HB3	2.20	0.42
1:A:42:GLU:O	1:A:45:ARG:N	2.49	0.42
1:A:130:HIS:ND1	1:A:133:LYS:CD	2.83	0.42
1:A:146:THR:HG22	1:A:167:LEU:CD1	2.49	0.42
1:A:167:LEU:HD22	1:A:171:VAL:HG23	2.01	0.42
1:A:186:ASN:OD1	1:A:242:THR:HA	2.20	0.42
1:A:143:VAL:CG2	1:A:233:LEU:HB2	2.50	0.42
1:A:184:ARG:HB3	1:A:242:THR:CB	2.50	0.42
1:A:31:LEU:N	1:A:31:LEU:HD13	2.33	0.42
1:B:219:ARG:NH2	1:B:225:GLU:OE2	2.53	0.42
1:B:43:ARG:O	1:B:46:LYS:CA	2.67	0.42
1:B:179:GLY:O	1:B:182:ASN:N	2.48	0.42
1:B:237:LEU:HA	1:B:237:LEU:HD12	1.95	0.42
1:B:34:LYS:HZ2	1:B:34:LYS:CB	2.27	0.42
1:B:45:ARG:O	1:B:49:GLU:CD	2.58	0.42
1:B:80:ILE:HG22	1:B:84:VAL:HG22	2.02	0.42
1:A:249:ASP:OD2	1:A:253:HIS:N	2.53	0.41
1:A:14:ILE:HD12	1:A:37:PHE:CD1	2.53	0.41
1:A:178:LEU:O	1:A:179:GLY:C	2.56	0.41
1:B:134:LYS:C	1:B:135:LEU:HD23	2.40	0.41
1:A:39:TYR:OH	1:A:64:GLN:CG	2.54	0.41
1:B:58:PRO:HB2	1:B:59:GLU:HA	2.02	0.41
1:A:194:ARG:C	1:A:195:THR:HG22	2.41	0.41
1:A:45:ARG:NE	1:A:45:ARG:O	2.54	0.41
1:B:254:ALA:HB3	1:B:255:ILE:CG2	2.50	0.41
1:A:185:VAL:HG22	1:A:185:VAL:O	2.18	0.41
1:B:74:ILE:O	1:B:78:GLU:HB2	2.19	0.41
1:A:1:MET:O	1:A:1:MET:HE2	2.20	0.41
1:A:35:LEU:HB2	1:A:56:ASN:HD21	1.82	0.41
1:A:140:GLY:H	1:A:183:ILE:HA	1.85	0.41
1:A:254:ALA:C	1:A:255:ILE:CG2	2.89	0.41
1:A:232:TYR:O	1:A:238:SER:HB3	2.20	0.41
1:B:221:VAL:HG22	1:B:221:VAL:H	1.48	0.41
1:B:90:VAL:CG1	1:B:91:TYR:N	2.84	0.41
1:B:241:VAL:HG12	1:B:242:THR:N	2.36	0.41
1:B:65:ILE:HG23	1:B:73:VAL:HA	2.02	0.41
1:B:77:PHE:O	1:B:81:GLY:N	2.54	0.41
1:A:166:SER:C	1:A:169:ALA:H	2.24	0.41
1:A:29:ASP:CG	1:A:54:GLN:HE21	2.24	0.41
1:B:49:GLU:C	1:B:51:LEU:N	2.75	0.40
1:B:61:HIS:CD2	1:B:84:VAL:CG1	3.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:NH2	1:A:256:LYS:HE2	2.37	0.40
1:B:214:ARG:O	1:B:255:ILE:HD11	2.21	0.40
1:B:59:GLU:CG	1:B:61:HIS:CA	2.91	0.40
1:B:211:ILE:O	1:B:214:ARG:N	2.54	0.40
1:B:9:TYR:HA	1:B:89:GLY:O	2.21	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	199/256 (78%)	147 (74%)	41 (21%)	11 (6%)	2	2
1	B	192/256 (75%)	150 (78%)	30 (16%)	12 (6%)	1	1
All	All	391/512 (76%)	297 (76%)	71 (18%)	23 (6%)	1	1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	B	3	ASN
1	B	52	LEU
1	B	54	GLN
1	B	58	PRO
1	B	168	GLU
1	B	169	ALA
1	B	128	VAL
1	B	212	GLU
1	A	3	ASN
1	A	6	ASN
1	A	17	LYS
1	B	53	GLU

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Mol	Chain	Res	Type
1	A	57	GLN
1	B	167	LEU
1	A	2	LEU
1	A	128	VAL
1	A	216	PRO
1	B	176	LEU
1	B	165	ALA
1	A	74	ILE
1	A	207	ILE
1	A	13	GLY

### 5.3.2 Protein sidechains [i](#)

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	175/210 (83%)	108 (62%)	67 (38%)	0	0
1	B	168/210 (80%)	114 (68%)	54 (32%)	0	0
All	All	343/420 (82%)	222 (65%)	121 (35%)	0	0

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LEU
1	A	5	GLU
1	A	10	VAL
1	A	11	ILE
1	A	14	ILE
1	A	16	ASN
1	A	17	LYS
1	A	19	SER
1	A	20	ILE
1	A	26	LYS
1	A	31	LEU
1	A	34	LYS

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Mol	Chain	Res	Type
1	A	35	LEU
1	A	39	TYR
1	A	41	LYS
1	A	42	GLU
1	A	43	ARG
1	A	45	ARG
1	A	46	LYS
1	A	51	LEU
1	A	52	LEU
1	A	55	LEU
1	A	57	GLN
1	A	62	LEU
1	A	64	GLN
1	A	67	VAL
1	A	68	GLN
1	A	69	SER
1	A	70	ASP
1	A	74	ILE
1	A	86	ASN
1	A	87	ILE
1	A	90	VAL
1	A	94	ILE
1	A	121	SER
1	A	127	ILE
1	A	133	LYS
1	A	137	PRO
1	A	146	THR
1	A	164	LYS
1	A	167	LEU
1	A	170	ASN
1	A	178	LEU
1	A	181	ASP
1	A	185	VAL
1	A	188	ILE
1	A	189	SER
1	A	193	ILE
1	A	194	ARG
1	A	195	THR
1	A	204	PHE
1	A	206	THR
1	A	207	ILE
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	209	LYS
1	A	213	GLU
1	A	214	ARG
1	A	219	ARG
1	A	234	LEU
1	A	235	SER
1	A	245	ASN
1	A	246	ILE
1	A	249	ASP
1	A	250	SER
1	A	255	ILE
1	A	256	LYS
1	B	1	MET
1	B	3	ASN
1	B	7	LYS
1	B	18	ARG
1	B	31	LEU
1	B	34	LYS
1	B	35	LEU
1	B	39	TYR
1	B	42	GLU
1	B	43	ARG
1	B	45	ARG
1	B	46	LYS
1	B	47	GLU
1	B	50	LYS
1	B	51	LEU
1	B	52	LEU
1	B	54	GLN
1	B	55	LEU
1	B	56	ASN
1	B	57	GLN
1	B	59	GLU
1	B	62	LEU
1	B	65	ILE
1	B	66	ASP
1	B	68	GLN
1	B	69	SER
1	B	71	GLU
1	B	79	GLN
1	B	86	ASN
1	B	87	ILE

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Mol	Chain	Res	Type
1	B	93	SER
1	B	120	ILE
1	B	123	TYR
1	B	124	SER
1	B	125	LEU
1	B	127	ILE
1	B	133	LYS
1	B	135	LEU
1	B	141	SER
1	B	146	THR
1	B	147	TYR
1	B	167	LEU
1	B	170	ASN
1	B	176	LEU
1	B	178	LEU
1	B	183	ILE
1	B	185	VAL
1	B	194	ARG
1	B	217	LEU
1	B	218	LYS
1	B	219	ARG
1	B	234	LEU
1	B	235	SER
1	B	255	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	54	GLN
1	A	56	ASN
1	A	68	GLN
1	A	75	ASN
1	A	86	ASN
1	A	170	ASN
1	A	245	ASN
1	B	6	ASN
1	B	54	GLN
1	B	56	ASN
1	B	68	GLN
1	B	75	ASN
1	B	86	ASN

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Mol	Chain	Res	Type
1	B	130	HIS
1	B	253	HIS

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	207/256 (80%)	-0.05	10 (4%) 30 36	12, 34, 63, 73	0
1	B	200/256 (78%)	-0.19	2 (1%) 82 87	8, 33, 56, 63	0
All	All	407/512 (79%)	-0.12	12 (2%) 51 61	8, 34, 59, 73	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	SER	5.4
1	A	60	ALA	4.3
1	A	207	ILE	3.4
1	B	6	ASN	3.3
1	A	173	TYR	3.0
1	A	41	LYS	2.9
1	A	72	GLU	2.9
1	B	208	LEU	2.7
1	A	195	THR	2.7
1	A	43	ARG	2.6
1	A	6	ASN	2.4
1	A	176	LEU	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.