



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:14 am BST

PDB ID : 2Q4N  
Title : Ensemble refinement of the crystal structure of protein from Arabidopsis thaliana At1g79260  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 1.32 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

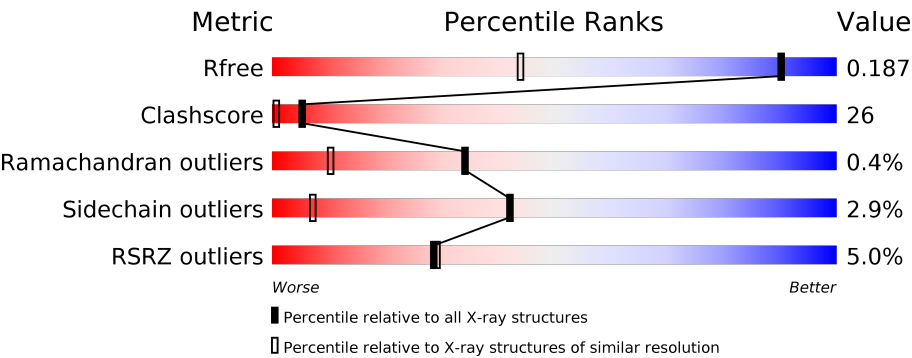
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.32 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	1611 (1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)
RSRZ outliers	127900	1580 (1.34-1.30)

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	1-A	166	<div><div>5%</div><div><div></div><div>47%</div><div>36%</div><div>8%</div><div>•</div><div>8%</div></div></div>
1	2-A	166	<div><div>5%</div><div><div></div><div>42%</div><div>35%</div><div>15%</div><div>•</div><div>8%</div></div></div>
1	3-A	166	<div><div>5%</div><div><div></div><div>42%</div><div>36%</div><div>11%</div><div>•</div><div>8%</div></div></div>
1	4-A	166	<div><div>5%</div><div><div></div><div>47%</div><div>34%</div><div>10%</div><div>•</div><div>8%</div></div></div>
1	5-A	166	<div><div>5%</div><div><div></div><div>53%</div><div>31%</div><div>7%</div><div>•</div><div>8%</div></div></div>
1	6-A	166	<div><div>5%</div><div><div></div><div>48%</div><div>34%</div><div>10%</div><div>•</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	7-A	166	<div><div></div><div>5%</div><div>57%</div><div>27%</div><div>7%</div><div>8%</div></div>
1	8-A	166	<div><div></div><div>5%</div><div>46%</div><div>37%</div><div>8%</div><div>8%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12256 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 Uncharacterized protein At1g79260.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	153	Total	C	N	O	Se	0	0	0
			1203	770	204	227	2			
1	2-A	153	Total	C	N	O	Se	0	0	0
			1203	770	204	227	2			
1	3-A	153	Total	C	N	O	Se	0	0	0
			1203	770	204	227	2			
1	4-A	153	Total	C	N	O	Se	0	0	0
			1203	770	204	227	2			
1	5-A	153	Total	C	N	O	Se	0	0	0
			1203	770	204	227	2			
1	6-A	153	Total	C	N	O	Se	0	0	0
			1203	770	204	227	2			
1	7-A	153	Total	C	N	O	Se	0	0	0
			1203	770	204	227	2			
1	8-A	153	Total	C	N	O	Se	0	0	0
			1203	770	204	227	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP O64527
A	75	MSE	MET	MODIFIED RESIDUE	UNP O64527
A	148	MSE	MET	MODIFIED RESIDUE	UNP O64527

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	329	Total	O	0	0
			329	329		
2	2-A	329	Total	O	0	0
			329	329		
2	3-A	329	Total	O	0	0
			329	329		

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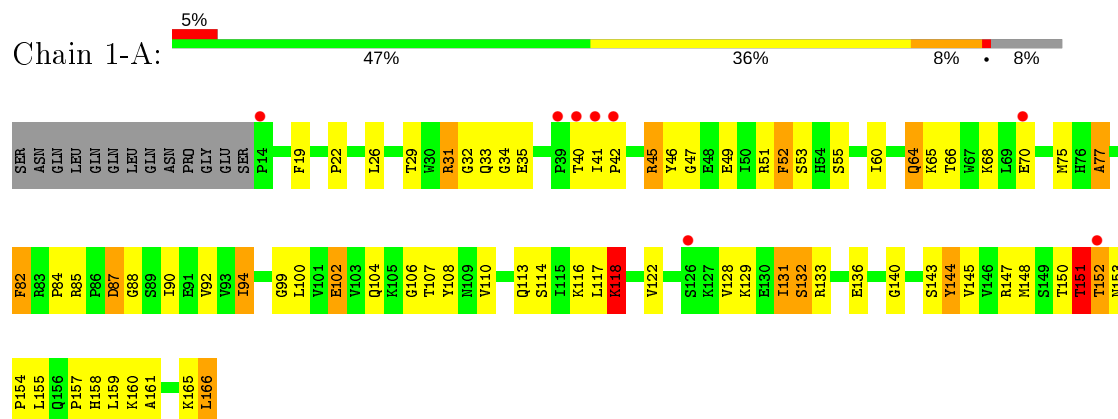
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	4-A	329	Total 329	O 329	0	0
2	5-A	329	Total 329	O 329	0	0
2	6-A	329	Total 329	O 329	0	0
2	7-A	329	Total 329	O 329	0	0
2	8-A	329	Total 329	O 329	0	0

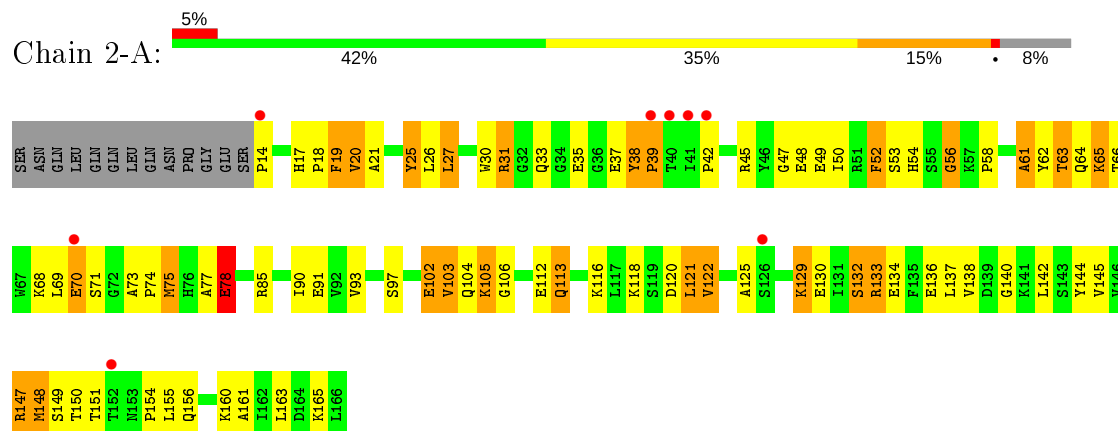
### 3 Residue-property plots [i](#)

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

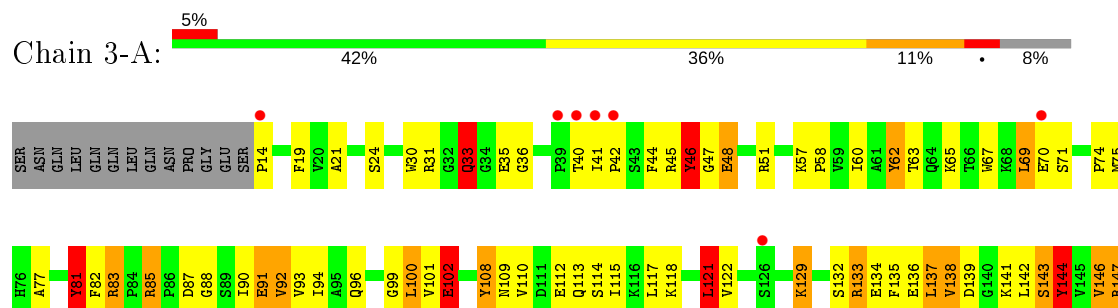
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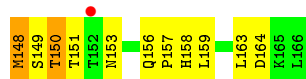


#### • Molecule 1: Uncharacterized protein At1g79260

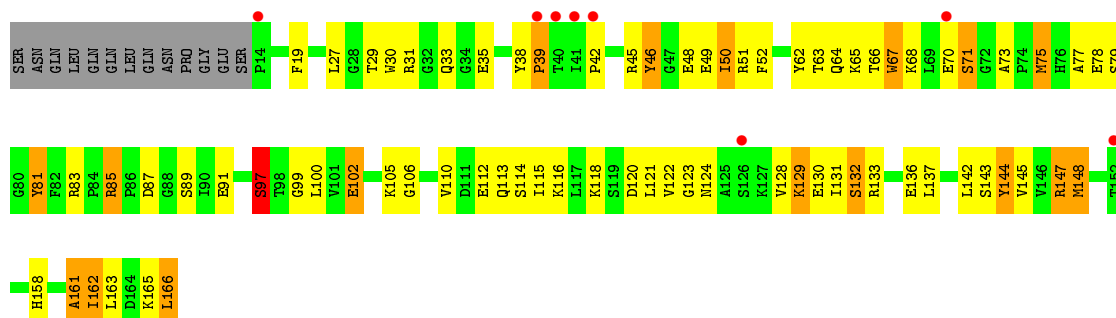


#### • Molecule 1: Uncharacterized protein At1g79260

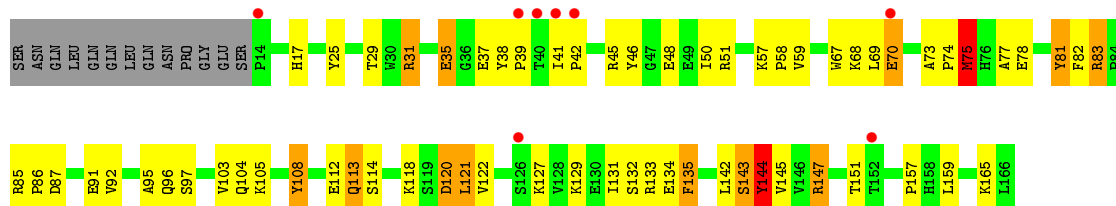




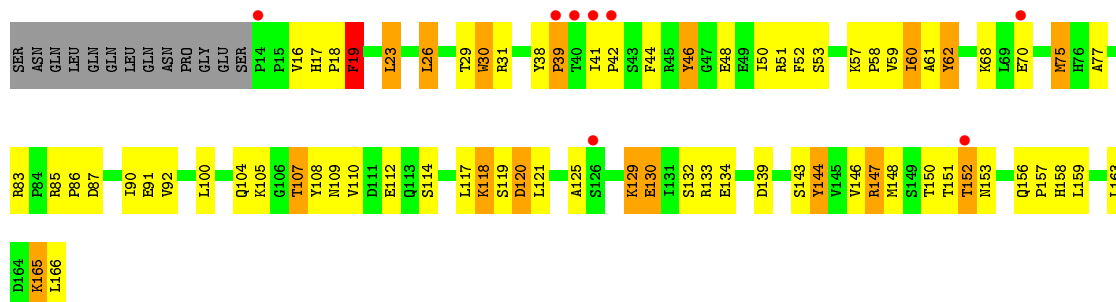
- Molecule 1: Uncharacterized protein At1g79260



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- Molecule 1: Uncharacterized protein At1g79260

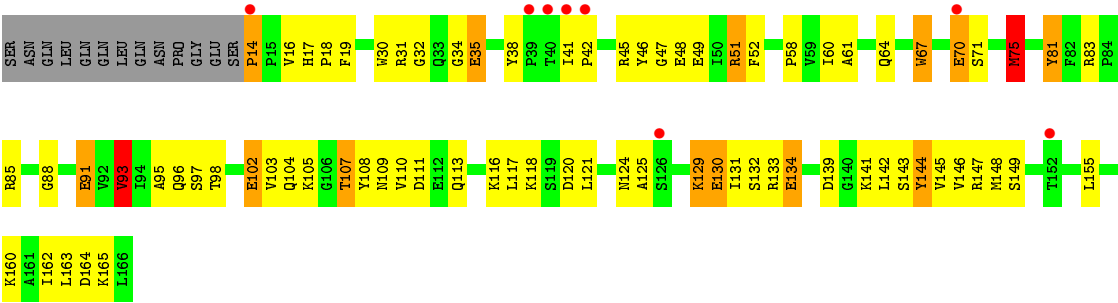


- Molecule 1: Uncharacterized protein At1g79260





● Molecule 1: Uncharacterized protein At1g79260





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.06 Å 80.03 Å 36.89 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.26 – 1.32 29.26 – 1.32	Depositor EDS
% Data completeness (in resolution range)	95.3 (29.26-1.32) 95.4 (29.26-1.32)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.32 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.152 , 0.195 0.145 , 0.187	Depositor DCC
$R_{free}$ test set	2068 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.2	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% 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	1-A	1.92	20/1232 (1.6%)	1.59	15/1666 (0.9%)
1	2-A	1.98	31/1232 (2.5%)	1.71	18/1666 (1.1%)
1	3-A	1.95	28/1232 (2.3%)	1.71	34/1666 (2.0%)
1	4-A	1.84	24/1232 (1.9%)	1.56	21/1666 (1.3%)
1	5-A	2.02	33/1232 (2.7%)	1.64	22/1666 (1.3%)
1	6-A	1.99	30/1232 (2.4%)	1.59	21/1666 (1.3%)
1	7-A	1.91	25/1232 (2.0%)	1.51	16/1666 (1.0%)
1	8-A	1.95	24/1232 (1.9%)	1.68	22/1666 (1.3%)
All	All	1.95	215/9856 (2.2%)	1.63	169/13328 (1.3%)

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	1-A	0	1
1	2-A	0	1
1	3-A	0	3
1	4-A	0	2
1	5-A	0	2
1	6-A	0	1
1	7-A	0	1
All	All	0	11

All (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	75	MSE	CG-SE	15.96	2.49	1.95
1	5-A	143	SER	CA-CB	13.96	1.73	1.52
1	6-A	143	SER	CA-CB	13.67	1.73	1.52
1	5-A	144	TYR	CE2-CZ	12.97	1.55	1.38
1	1-A	132	SER	CA-CB	12.47	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	81	TYR	CD1-CE1	11.98	1.57	1.39
1	7-A	91	GLU	CD-OE2	11.84	1.38	1.25
1	3-A	144	TYR	CD1-CE1	11.19	1.56	1.39
1	8-A	144	TYR	CD2-CE2	10.37	1.54	1.39
1	1-A	52	PHE	CE1-CZ	10.31	1.56	1.37
1	3-A	108	TYR	CD2-CE2	10.20	1.54	1.39
1	5-A	143	SER	CB-OG	10.09	1.55	1.42
1	6-A	144	TYR	CD2-CE2	10.01	1.54	1.39
1	6-A	16	VAL	CB-CG2	9.59	1.73	1.52
1	8-A	93	VAL	CB-CG1	9.58	1.73	1.52
1	1-A	143	SER	CB-OG	9.53	1.54	1.42
1	8-A	144	TYR	CD1-CE1	9.40	1.53	1.39
1	3-A	81	TYR	CD2-CE2	9.19	1.53	1.39
1	3-A	101	VAL	CB-CG1	9.09	1.72	1.52
1	8-A	91	GLU	CG-CD	8.90	1.65	1.51
1	8-A	97	SER	CB-OG	-8.67	1.30	1.42
1	2-A	132	SER	CA-CB	8.54	1.65	1.52
1	8-A	129	LYS	CE-NZ	8.49	1.70	1.49
1	5-A	144	TYR	CD1-CE1	8.27	1.51	1.39
1	1-A	102	GLU	CG-CD	8.27	1.64	1.51
1	7-A	152	THR	CB-CG2	8.16	1.79	1.52
1	5-A	82	PHE	CG-CD1	8.02	1.50	1.38
1	2-A	145	VAL	CB-CG2	7.98	1.69	1.52
1	6-A	119	SER	CB-OG	7.93	1.52	1.42
1	4-A	144	TYR	CE2-CZ	7.91	1.48	1.38
1	1-A	55	SER	CA-CB	7.85	1.64	1.52
1	3-A	144	TYR	CD2-CE2	-7.83	1.27	1.39
1	2-A	52	PHE	CE1-CZ	7.72	1.52	1.37
1	6-A	44	PHE	CD1-CE1	7.71	1.54	1.39
1	4-A	161	ALA	CA-CB	7.71	1.68	1.52
1	3-A	35	GLU	CG-CD	7.67	1.63	1.51
1	7-A	103	VAL	CB-CG1	7.61	1.68	1.52
1	2-A	61	ALA	CA-CB	7.51	1.68	1.52
1	3-A	144	TYR	CE1-CZ	7.40	1.48	1.38
1	2-A	25	TYR	CE1-CZ	7.36	1.48	1.38
1	2-A	20	VAL	CB-CG2	7.32	1.68	1.52
1	2-A	102	GLU	CG-CD	7.30	1.62	1.51
1	5-A	82	PHE	CD1-CE1	7.30	1.53	1.39
1	3-A	108	TYR	CG-CD1	7.28	1.48	1.39
1	5-A	92	VAL	CB-CG2	7.25	1.68	1.52
1	6-A	91	GLU	CD-OE2	7.20	1.33	1.25
1	2-A	31	ARG	CG-CD	7.14	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	20	VAL	CB-CG1	7.12	1.67	1.52
1	7-A	91	GLU	CD-OE1	7.12	1.33	1.25
1	4-A	77	ALA	CA-CB	7.12	1.67	1.52
1	5-A	108	TYR	CD2-CE2	7.08	1.50	1.39
1	2-A	161	ALA	CA-CB	7.07	1.67	1.52
1	5-A	144	TYR	CZ-OH	7.06	1.49	1.37
1	7-A	136	GLU	CB-CG	7.05	1.65	1.52
1	1-A	132	SER	CB-OG	7.04	1.51	1.42
1	2-A	144	TYR	CE2-CZ	6.96	1.47	1.38
1	4-A	97	SER	CA-CB	6.95	1.63	1.52
1	7-A	78	GLU	CB-CG	6.87	1.65	1.52
1	6-A	62	TYR	CD2-CE2	6.86	1.49	1.39
1	2-A	148	MSE	CG-SE	6.82	2.18	1.95
1	3-A	148	MSE	CG-SE	-6.80	1.72	1.95
1	3-A	91	GLU	CD-OE2	6.77	1.33	1.25
1	2-A	78	GLU	CD-OE2	-6.75	1.18	1.25
1	7-A	136	GLU	CA-CB	6.73	1.68	1.53
1	6-A	144	TYR	CD1-CE1	6.73	1.49	1.39
1	3-A	48	GLU	CD-OE1	-6.72	1.18	1.25
1	3-A	77	ALA	CA-CB	6.72	1.66	1.52
1	2-A	62	TYR	CE1-CZ	6.69	1.47	1.38
1	4-A	52	PHE	CE1-CZ	6.66	1.50	1.37
1	5-A	85	ARG	CB-CG	6.65	1.70	1.52
1	6-A	152	THR	C-O	6.60	1.35	1.23
1	8-A	91	GLU	CD-OE2	6.60	1.32	1.25
1	1-A	102	GLU	CD-OE1	6.59	1.32	1.25
1	4-A	50	ILE	CB-CG2	6.57	1.73	1.52
1	5-A	118	LYS	CD-CE	6.56	1.67	1.51
1	6-A	143	SER	CB-OG	6.56	1.50	1.42
1	6-A	77	ALA	CA-CB	6.54	1.66	1.52
1	4-A	132	SER	CA-CB	6.47	1.62	1.52
1	5-A	77	ALA	CA-CB	6.46	1.66	1.52
1	7-A	102	GLU	CD-OE1	6.42	1.32	1.25
1	5-A	91	GLU	CD-OE2	6.41	1.32	1.25
1	3-A	102	GLU	CG-CD	6.41	1.61	1.51
1	8-A	139	ASP	C-O	6.39	1.35	1.23
1	2-A	18	PRO	CG-CD	6.38	1.71	1.50
1	3-A	33	GLN	CA-CB	6.38	1.68	1.53
1	3-A	46	TYR	CG-CD1	6.37	1.47	1.39
1	8-A	134	GLU	CB-CG	6.35	1.64	1.52
1	3-A	136	GLU	CB-CG	6.34	1.64	1.52
1	1-A	151	THR	C-O	6.33	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	109	ASN	C-O	6.26	1.35	1.23
1	1-A	19	PHE	CE2-CZ	6.22	1.49	1.37
1	5-A	91	GLU	CD-OE1	6.21	1.32	1.25
1	1-A	60	ILE	CA-CB	6.19	1.69	1.54
1	1-A	144	TYR	CD2-CE2	6.18	1.48	1.39
1	5-A	35	GLU	CB-CG	-6.18	1.40	1.52
1	3-A	81	TYR	CG-CD1	6.17	1.47	1.39
1	6-A	121	LEU	CA-CB	6.17	1.68	1.53
1	6-A	31	ARG	CZ-NH1	6.17	1.41	1.33
1	2-A	113	GLN	CG-CD	6.16	1.65	1.51
1	3-A	46	TYR	CE2-CZ	6.12	1.46	1.38
1	8-A	81	TYR	CD1-CE1	6.11	1.48	1.39
1	8-A	132	SER	CA-CB	6.11	1.62	1.52
1	3-A	102	GLU	CD-OE1	6.06	1.32	1.25
1	6-A	107	THR	CA-CB	6.06	1.69	1.53
1	6-A	148	MSE	SE-CE	-5.99	1.60	1.95
1	2-A	62	TYR	CD2-CE2	5.98	1.48	1.39
1	4-A	52	PHE	C-O	5.97	1.34	1.23
1	4-A	62	TYR	CE1-CZ	5.96	1.46	1.38
1	5-A	135	PHE	CD2-CE2	5.96	1.51	1.39
1	5-A	129	LYS	CD-CE	-5.95	1.36	1.51
1	6-A	108	TYR	CB-CG	-5.92	1.42	1.51
1	4-A	136	GLU	CB-CG	5.92	1.63	1.52
1	8-A	120	ASP	CA-CB	5.91	1.67	1.53
1	7-A	85	ARG	CZ-NH2	5.90	1.40	1.33
1	4-A	81	TYR	CD2-CE2	-5.85	1.30	1.39
1	7-A	77	ALA	CA-CB	5.85	1.64	1.52
1	3-A	93	VAL	CB-CG2	5.85	1.65	1.52
1	1-A	77	ALA	CA-CB	5.84	1.64	1.52
1	6-A	29	THR	CB-CG2	5.81	1.71	1.52
1	8-A	35	GLU	CD-OE1	5.80	1.32	1.25
1	5-A	145	VAL	CA-CB	5.80	1.67	1.54
1	7-A	81	TYR	CE2-CZ	5.79	1.46	1.38
1	2-A	90	ILE	CB-CG2	5.78	1.70	1.52
1	8-A	95	ALA	CA-CB	5.76	1.64	1.52
1	5-A	92	VAL	CB-CG1	5.76	1.65	1.52
1	2-A	132	SER	N-CA	5.75	1.57	1.46
1	6-A	166	LEU	CG-CD2	5.73	1.73	1.51
1	5-A	38	TYR	CE1-CZ	5.71	1.46	1.38
1	6-A	119	SER	CA-CB	5.71	1.61	1.52
1	7-A	136	GLU	CG-CD	5.70	1.60	1.51
1	8-A	81	TYR	CE2-CZ	5.68	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	52	PHE	CG-CD2	5.68	1.47	1.38
1	4-A	52	PHE	CD2-CE2	5.66	1.50	1.39
1	6-A	118	LYS	CB-CG	-5.66	1.37	1.52
1	6-A	130	GLU	CD-OE2	5.65	1.31	1.25
1	3-A	143	SER	CA-CB	5.64	1.61	1.52
1	8-A	130	GLU	CD-OE2	5.64	1.31	1.25
1	2-A	103	VAL	CB-CG1	5.64	1.64	1.52
1	3-A	150	THR	C-O	-5.63	1.12	1.23
1	4-A	85	ARG	C-N	5.62	1.45	1.34
1	8-A	125	ALA	CA-CB	5.61	1.64	1.52
1	7-A	83	ARG	CG-CD	5.60	1.66	1.51
1	4-A	67	TRP	CB-CG	5.60	1.60	1.50
1	5-A	38	TYR	CG-CD1	5.58	1.46	1.39
1	3-A	148	MSE	CB-CG	-5.56	1.35	1.52
1	8-A	38	TYR	CG-CD1	5.55	1.46	1.39
1	4-A	62	TYR	CD2-CE2	5.54	1.47	1.39
1	6-A	30	TRP	CE3-CZ3	5.54	1.47	1.38
1	7-A	38	TYR	CG-CD1	5.53	1.46	1.39
1	4-A	62	TYR	CG-CD1	5.52	1.46	1.39
1	5-A	67	TRP	CZ3-CH2	5.50	1.48	1.40
1	7-A	144	TYR	CD1-CE1	5.50	1.47	1.39
1	6-A	30	TRP	CZ3-CH2	5.49	1.48	1.40
1	6-A	120	ASP	CB-CG	-5.47	1.40	1.51
1	5-A	38	TYR	CB-CG	5.47	1.59	1.51
1	1-A	32	GLY	N-CA	5.47	1.54	1.46
1	2-A	91	GLU	CD-OE2	5.46	1.31	1.25
1	5-A	142	LEU	C-O	5.46	1.33	1.23
1	3-A	46	TYR	CG-CD2	5.45	1.46	1.39
1	2-A	129	LYS	CB-CG	5.43	1.67	1.52
1	7-A	59	VAL	CB-CG2	5.42	1.64	1.52
1	2-A	122	VAL	C-O	5.41	1.33	1.23
1	7-A	145	VAL	CA-CB	5.40	1.66	1.54
1	4-A	145	VAL	CB-CG2	5.39	1.64	1.52
1	3-A	139	ASP	CB-CG	5.38	1.63	1.51
1	3-A	144	TYR	CG-CD1	5.38	1.46	1.39
1	6-A	91	GLU	CD-OE1	5.38	1.31	1.25
1	6-A	139	ASP	CB-CG	5.37	1.63	1.51
1	4-A	102	GLU	CB-CG	5.36	1.62	1.52
1	7-A	30	TRP	C-O	5.36	1.33	1.23
1	1-A	52	PHE	CD1-CE1	5.34	1.50	1.39
1	8-A	142	LEU	CG-CD2	5.34	1.71	1.51
1	2-A	25	TYR	CD2-CE2	5.33	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	129	LYS	CD-CE	-5.33	1.38	1.51
1	7-A	129	LYS	CE-NZ	5.32	1.62	1.49
1	5-A	82	PHE	CE2-CZ	5.32	1.47	1.37
1	1-A	94	ILE	CA-CB	5.30	1.67	1.54
1	7-A	14	PRO	CG-CD	5.30	1.68	1.50
1	7-A	129	LYS	CB-CG	5.30	1.66	1.52
1	6-A	129	LYS	CE-NZ	5.29	1.62	1.49
1	4-A	79	SER	CA-CB	5.28	1.60	1.52
1	8-A	143	SER	CB-OG	5.26	1.49	1.42
1	5-A	87	ASP	CG-OD1	5.25	1.37	1.25
1	2-A	62	TYR	CG-CD1	5.23	1.46	1.39
1	2-A	136	GLU	CG-CD	5.21	1.59	1.51
1	5-A	134	GLU	CB-CG	5.21	1.62	1.52
1	4-A	81	TYR	CD1-CE1	-5.19	1.31	1.39
1	5-A	118	LYS	CA-CB	5.19	1.65	1.53
1	1-A	166	LEU	C-OXT	5.19	1.33	1.23
1	1-A	129	LYS	CD-CE	-5.18	1.38	1.51
1	7-A	93	VAL	CB-CG1	5.17	1.63	1.52
1	1-A	118	LYS	CA-CB	5.17	1.65	1.53
1	2-A	56	GLY	C-O	5.16	1.31	1.23
1	4-A	114	SER	CB-OG	5.15	1.49	1.42
1	2-A	30	TRP	CE3-CZ3	5.14	1.47	1.38
1	5-A	48	GLU	CB-CG	5.14	1.61	1.52
1	5-A	132	SER	CA-CB	5.13	1.60	1.52
1	5-A	37	GLU	CG-CD	5.13	1.59	1.51
1	4-A	33	GLN	CG-CD	5.13	1.62	1.51
1	4-A	166	LEU	C-OXT	5.12	1.33	1.23
1	8-A	88	GLY	CA-C	5.12	1.60	1.51
1	3-A	146	VAL	CB-CG2	5.11	1.63	1.52
1	5-A	113	GLN	CB-CG	5.11	1.66	1.52
1	8-A	67	TRP	N-CA	5.10	1.56	1.46
1	6-A	114	SER	CB-OG	5.09	1.48	1.42
1	6-A	75	MSE	CB-CG	5.09	1.67	1.52
1	6-A	146	VAL	CB-CG2	5.09	1.63	1.52
1	2-A	129	LYS	CE-NZ	5.08	1.61	1.49
1	2-A	125	ALA	CA-CB	5.07	1.63	1.52
1	2-A	30	TRP	CG-CD1	5.06	1.43	1.36
1	7-A	101	VAL	CB-CG2	5.05	1.63	1.52
1	7-A	81	TYR	CD2-CE2	5.04	1.47	1.39
1	3-A	138	VAL	CB-CG2	5.03	1.63	1.52
1	1-A	131	ILE	CB-CG2	5.01	1.68	1.52
1	5-A	85	ARG	C-N	5.01	1.43	1.34

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	83	ARG	NE-CZ-NH1	17.75	129.17	120.30
1	2-A	133	ARG	NE-CZ-NH1	16.96	128.78	120.30
1	2-A	31	ARG	NE-CZ-NH2	-14.24	113.18	120.30
1	2-A	85	ARG	NE-CZ-NH1	14.01	127.31	120.30
1	8-A	139	ASP	CB-CG-OD2	-13.29	106.33	118.30
1	2-A	133	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	8-A	85	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	3-A	85	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	4-A	85	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	2-A	20	VAL	CG1-CB-CG2	-11.24	92.92	110.90
1	7-A	85	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	8-A	31	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	2-A	105	LYS	CD-CE-NZ	10.93	136.84	111.70
1	3-A	144	TYR	CG-CD2-CE2	10.14	129.41	121.30
1	1-A	19	PHE	CB-CG-CD1	10.12	127.88	120.80
1	3-A	85	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	4-A	85	ARG	NE-CZ-NH2	-10.01	115.29	120.30
1	3-A	81	TYR	CB-CG-CD2	-9.94	115.03	121.00
1	2-A	31	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	3-A	133	ARG	NE-CZ-NH2	9.58	125.09	120.30
1	6-A	85	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	2-A	85	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	5-A	121	LEU	CB-CG-CD1	-9.40	95.02	111.00
1	2-A	75	MSE	CG-SE-CE	9.23	119.20	98.90
1	5-A	31	ARG	NE-CZ-NH2	9.21	124.91	120.30
1	8-A	139	ASP	CB-CG-OD1	9.18	126.56	118.30
1	4-A	148	MSE	CB-CG-SE	-9.12	85.34	112.70
1	8-A	85	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	1-A	19	PHE	CB-CG-CD2	-8.84	114.61	120.80
1	8-A	51	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	5-A	103	VAL	CG1-CB-CG2	-8.53	97.25	110.90
1	3-A	81	TYR	CG-CD2-CE2	-8.37	114.61	121.30
1	7-A	85	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	3-A	144	TYR	CB-CG-CD1	8.35	126.01	121.00
1	5-A	31	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	3-A	35	GLU	OE1-CD-OE2	-8.06	113.63	123.30
1	6-A	147	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	6-A	60	ILE	CB-CG1-CD1	-7.83	91.98	113.90
1	1-A	85	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	4-A	166	LEU	CB-CG-CD2	7.55	123.84	111.00
1	7-A	69	LEU	CB-CG-CD1	-7.53	98.20	111.00
1	4-A	133	ARG	NE-CZ-NH1	7.51	124.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	147	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	3-A	144	TYR	CB-CG-CD2	-7.13	116.72	121.00
1	6-A	121	LEU	CB-CG-CD2	-7.13	98.88	111.00
1	5-A	87	ASP	CB-CG-OD1	-7.13	111.89	118.30
1	7-A	152	THR	CA-CB-CG2	-7.07	102.50	112.40
1	3-A	121	LEU	CA-CB-CG	7.01	131.44	115.30
1	1-A	151	THR	N-CA-CB	7.01	123.62	110.30
1	5-A	143	SER	CA-CB-OG	-6.99	92.32	111.20
1	6-A	120	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	5-A	147	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	5-A	85	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	5-A	75	MSE	CB-CG-SE	6.92	133.47	112.70
1	1-A	52	PHE	CB-CG-CD2	6.89	125.62	120.80
1	8-A	31	ARG	NH1-CZ-NH2	6.86	126.94	119.40
1	4-A	91	GLU	OE1-CD-OE2	-6.86	115.07	123.30
1	5-A	121	LEU	CB-CG-CD2	6.83	122.60	111.00
1	8-A	144	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	3-A	83	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	7-A	83	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	6-A	87	ASP	C-N-CA	-6.79	108.03	122.30
1	8-A	83	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	8-A	108	TYR	CB-CG-CD1	6.77	125.06	121.00
1	7-A	59	VAL	CB-CA-C	-6.67	98.72	111.40
1	5-A	83	ARG	NH1-CZ-NH2	-6.64	112.09	119.40
1	3-A	92	VAL	CG1-CB-CG2	-6.61	100.32	110.90
1	8-A	142	LEU	CB-CG-CD2	6.60	122.22	111.00
1	4-A	31	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	2-A	65	LYS	CG-CD-CE	-6.56	92.21	111.90
1	6-A	147	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	4-A	147	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	1-A	151	THR	OG1-CB-CG2	-6.45	95.17	110.00
1	6-A	62	TYR	CB-CG-CD2	6.44	124.86	121.00
1	1-A	87	ASP	CB-CG-OD2	6.40	124.06	118.30
1	5-A	82	PHE	CB-CG-CD2	-6.36	116.35	120.80
1	6-A	83	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	2-A	27	LEU	CB-CG-CD1	6.35	121.79	111.00
1	4-A	50	ILE	CG1-CB-CG2	6.31	125.29	111.40
1	7-A	85	ARG	CG-CD-NE	6.26	124.94	111.80
1	4-A	97	SER	CA-CB-OG	-6.24	94.36	111.20
1	3-A	121	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	6-A	44	PHE	CB-CG-CD2	-6.22	116.45	120.80
1	4-A	83	ARG	NE-CZ-NH1	-6.22	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	85	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	7-A	59	VAL	N-CA-C	-6.21	94.23	111.00
1	8-A	35	GLU	CA-CB-CG	6.19	127.02	113.40
1	6-A	46	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	8-A	91	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	1-A	165	LYS	CD-CE-NZ	-6.12	97.61	111.70
1	4-A	83	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	8-A	165	LYS	CD-CE-NZ	-6.08	97.72	111.70
1	4-A	148	MSE	CA-CB-CG	6.07	123.62	113.30
1	4-A	166	LEU	CB-CG-CD1	-6.06	100.69	111.00
1	6-A	143	SER	CA-CB-OG	-6.05	94.87	111.20
1	5-A	120	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	7-A	73	ALA	C-N-CD	6.01	141.02	128.40
1	5-A	59	VAL	CG1-CB-CG2	-6.00	101.31	110.90
1	3-A	62	TYR	CB-CG-CD2	-5.94	117.43	121.00
1	2-A	75	MSE	CB-CG-SE	-5.94	94.89	112.70
1	3-A	133	ARG	NE-CZ-NH1	-5.93	117.34	120.30
1	7-A	147	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	5-A	120	ASP	CB-CG-OD1	5.89	123.60	118.30
1	1-A	52	PHE	CD1-CE1-CZ	-5.88	113.04	120.10
1	4-A	31	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	7-A	143	SER	C-N-CA	-5.84	107.10	121.70
1	8-A	16	VAL	CG1-CB-CG2	-5.83	101.58	110.90
1	1-A	45	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	6-A	26	LEU	CB-CG-CD1	-5.76	101.21	111.00
1	8-A	19	PHE	CB-CG-CD1	5.74	124.82	120.80
1	2-A	147	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	2-A	148	MSE	CA-CB-CG	5.71	123.01	113.30
1	6-A	62	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	3-A	31	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	3-A	69	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	3-A	19	PHE	CB-CG-CD1	5.65	124.75	120.80
1	3-A	147	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	1-A	31	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	3-A	33	GLN	N-CA-C	-5.61	95.87	111.00
1	2-A	19	PHE	CB-CG-CD1	5.59	124.72	120.80
1	6-A	165	LYS	CD-CE-NZ	-5.59	98.85	111.70
1	5-A	25	TYR	CB-CG-CD2	5.55	124.33	121.00
1	3-A	62	TYR	CG-CD1-CE1	-5.55	116.86	121.30
1	5-A	57	LYS	CD-CE-NZ	-5.55	98.94	111.70
1	8-A	118	LYS	CD-CE-NZ	-5.54	98.95	111.70
1	3-A	87	ASP	CB-CG-OD1	5.53	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	93	VAL	CA-CB-CG2	5.52	119.18	110.90
1	3-A	101	VAL	CG1-CB-CG2	-5.51	102.08	110.90
1	1-A	82	PHE	CB-CG-CD1	5.50	124.65	120.80
1	4-A	147	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	4-A	162	ILE	CB-CG1-CD1	-5.48	98.55	113.90
1	3-A	91	GLU	OE1-CD-OE2	5.47	129.86	123.30
1	2-A	21	ALA	N-CA-CB	-5.46	102.46	110.10
1	3-A	122	VAL	CG1-CB-CG2	5.46	119.63	110.90
1	3-A	83	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	5-A	83	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	4-A	133	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	2-A	31	ARG	CD-NE-CZ	5.40	131.16	123.60
1	8-A	18	PRO	N-CD-CG	-5.40	95.11	103.20
1	3-A	137	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	8-A	81	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	5-A	159	LEU	CA-CB-CG	5.36	127.63	115.30
1	2-A	105	LYS	CG-CD-CE	-5.35	95.85	111.90
1	5-A	87	ASP	OD1-CG-OD2	5.34	133.44	123.30
1	3-A	148	MSE	CA-CB-CG	-5.34	104.23	113.30
1	6-A	117	LEU	N-CA-C	-5.34	96.59	111.00
1	8-A	108	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	3-A	108	TYR	CB-CG-CD1	5.29	124.17	121.00
1	7-A	133	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	4-A	27	LEU	CB-CG-CD2	-5.27	102.05	111.00
1	7-A	75	MSE	CA-CB-CG	-5.26	104.35	113.30
1	6-A	133	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	1-A	52	PHE	CG-CD1-CE1	5.22	126.55	120.80
1	1-A	152	THR	N-CA-CB	-5.22	100.38	110.30
1	6-A	148	MSE	CA-CB-CG	5.21	122.16	113.30
1	3-A	144	TYR	CG-CD1-CE1	-5.19	117.15	121.30
1	4-A	75	MSE	CA-CB-CG	-5.18	104.50	113.30
1	5-A	81	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	3-A	31	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	7-A	53	SER	N-CA-CB	-5.17	102.75	110.50
1	7-A	75	MSE	CG-SE-CE	5.16	110.25	98.90
1	6-A	16	VAL	CA-CB-CG1	-5.14	103.20	110.90
1	3-A	164	ASP	CB-CG-OD1	5.11	122.90	118.30
1	4-A	19	PHE	CB-CG-CD1	5.11	124.37	120.80
1	8-A	14	PRO	N-CA-CB	5.10	109.42	103.30
1	6-A	23	LEU	CB-CG-CD2	5.09	119.66	111.00
1	6-A	19	PHE	CB-CG-CD1	5.07	124.35	120.80
1	8-A	102	GLU	OE1-CD-OE2	-5.05	117.23	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	3-A	48	GLU	OE1-CD-OE2	-5.01	117.29	123.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	151	THR	Mainchain
1	2-A	38	TYR	Sidechain
1	3-A	46	TYR	Sidechain
1	3-A	62	TYR	Sidechain
1	3-A	81	TYR	Sidechain
1	4-A	46	TYR	Sidechain
1	4-A	81	TYR	Sidechain
1	5-A	144	TYR	Sidechain
1	5-A	81	TYR	Sidechain
1	6-A	19	PHE	Sidechain
1	7-A	81	TYR	Sidechain

## 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	1-A	1203	0	1205	79	0
1	2-A	1203	0	1205	88	0
1	3-A	1203	0	1205	70	0
1	4-A	1203	0	1205	59	0
1	5-A	1203	0	1205	41	0
1	6-A	1203	0	1205	71	0
1	7-A	1203	0	1205	40	0
1	8-A	1203	0	1205	60	0
2	1-A	329	0	0	33	0
2	2-A	329	0	0	25	0
2	3-A	329	0	0	18	0
2	4-A	329	0	0	14	0
2	5-A	329	0	0	18	0
2	6-A	329	0	0	17	0
2	7-A	329	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	8-A	329	0	0	24	0
All	All	12256	0	9640	508	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:CG2	1:A:152:THR:CB	1.79	1.59
1:A:115:ILE:CG1	1:A:115:ILE:CD1	1.79	1.55
1:A:129:LYS:CE	1:A:129:LYS:NZ	1.70	1.54
1:A:148:MSE:SE	1:A:148:MSE:CG	2.18	1.41
1:A:151:THR:HB	2:A:306:HOH:O	1.15	1.32
1:A:41:ILE:O	2:A:271:HOH:O	1.59	1.18
1:A:41:ILE:O	2:A:271:HOH:O	1.61	1.17
1:A:60:ILE:N	1:A:60:ILE:HD12	1.56	1.16
1:A:118:LYS:HE3	2:A:228:HOH:O	1.41	1.15
1:A:118:LYS:HE3	2:A:228:HOH:O	1.50	1.10
1:A:75:MSE:SE	1:A:75:MSE:CG	2.49	1.10
1:A:113:GLN:NE2	2:A:443:HOH:O	1.84	1.08
1:A:68:LYS:HD2	1:A:73:ALA:HB3	1.34	1.06
1:A:51:ARG:NH2	2:A:342:HOH:O	1.92	1.02
1:A:41:ILE:HG13	1:A:41:ILE:O	1.55	1.02
1:A:68:LYS:CG	1:A:75:MSE:HE3	1.90	1.00
1:A:118:LYS:HB2	1:A:118:LYS:NZ	1.76	0.99
1:A:120:ASP:HB3	1:A:121:LEU:HD12	1.43	0.98
1:A:113:GLN:OE1	2:A:335:HOH:O	1.81	0.98
1:A:17:HIS:HB2	1:A:56:GLY:O	1.62	0.98
1:A:68:LYS:HG3	1:A:75:MSE:CE	1.94	0.97
1:A:68:LYS:HG3	1:A:75:MSE:HE3	0.99	0.97
1:A:105:LYS:HE3	2:A:284:HOH:O	1.63	0.96
1:A:145:VAL:HG12	1:A:145:VAL:O	1.64	0.95
1:A:65:LYS:NZ	2:A:260:HOH:O	1.95	0.94
1:A:82:PHE:HA	1:A:92:VAL:HG22	1.50	0.94
1:A:111:ASP:OD2	2:A:259:HOH:O	1.86	0.93
1:A:51:ARG:HD3	2:A:307:HOH:O	1.67	0.93
1:A:134:GLU:OE1	1:A:147:ARG:NH1	2.04	0.91
1:A:157:PRO:HB3	2:A:268:HOH:O	1.69	0.91
1:A:118:LYS:HG2	1:A:132:SER:OG	1.71	0.91
1:A:128:VAL:HG22	1:A:148:MSE:HE1	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:O	1:A:153:ASN:OD1	1.90	0.89
1:A:137:LEU:HD11	1:A:140:GLY:HA2	1.52	0.89
1:A:75:MSE:HE2	2:A:261:HOH:O	1.72	0.89
1:A:150:THR:OG1	1:A:153:ASN:OD1	1.92	0.87
1:A:102:GLU:OE2	1:A:131:ILE:HD13	1.74	0.87
1:A:105:LYS:HD2	2:A:435:HOH:O	1.74	0.86
1:A:152:THR:C	1:A:153:ASN:OD1	2.14	0.86
1:A:51:ARG:NH2	2:A:342:HOH:O	1.85	0.86
1:A:41:ILE:HG13	1:A:41:ILE:O	1.76	0.85
1:A:70:GLU:H	1:A:70:GLU:CD	1.78	0.85
1:A:60:ILE:HB	1:A:82:PHE:HB2	1.59	0.85
1:A:120:ASP:HB3	1:A:121:LEU:CD1	2.07	0.84
1:A:137:LEU:HD11	1:A:140:GLY:CA	2.07	0.84
1:A:42:PRO:O	2:A:286:HOH:O	1.95	0.84
1:A:48:GLU:OE2	1:A:144:TYR:CE2	2.31	0.84
1:A:51:ARG:NH2	2:A:342:HOH:O	2.08	0.84
1:A:60:ILE:HD12	1:A:60:ILE:H	1.43	0.83
1:A:94:ILE:HB	1:A:102:GLU:HG3	1.59	0.83
1:A:64:GLN:NE2	1:A:78:GLU:OE2	2.11	0.83
1:A:151:THR:N	2:A:258:HOH:O	2.11	0.82
1:A:50:ILE:HG23	1:A:63:THR:O	1.77	0.82
1:A:102:GLU:OE1	1:A:133:ARG:NE	2.11	0.82
1:A:131:ILE:HG12	1:A:148:MSE:HG2	1.61	0.82
1:A:141:LYS:HD3	1:A:164:ASP:OD1	1.79	0.81
1:A:154:PRO:HD2	2:A:240:HOH:O	1.81	0.80
1:A:27:LEU:HD13	1:A:54:HIS:CD2	2.17	0.80
1:A:129:LYS:CD	1:A:129:LYS:NZ	2.45	0.80
1:A:118:LYS:HB2	1:A:118:LYS:HZ3	1.45	0.79
1:A:64:GLN:CD	1:A:78:GLU:OE2	2.21	0.79
1:A:70:GLU:CD	1:A:70:GLU:H	1.84	0.79
1:A:124:ASN:OD1	2:A:217:HOH:O	2.00	0.79
1:A:75:MSE:HE2	1:A:75:MSE:HA	1.64	0.79
1:A:69:LEU:O	2:A:325:HOH:O	2.00	0.79
1:A:147:ARG:NH2	2:A:431:HOH:O	2.16	0.79
1:A:118:LYS:HB2	1:A:118:LYS:NZ	1.98	0.79
1:A:118:LYS:HD3	2:A:278:HOH:O	1.82	0.78
1:A:152:THR:CA	1:A:152:THR:CG2	2.60	0.78
1:A:64:GLN:O	2:A:194:HOH:O	2.00	0.78
1:A:84:PRO:HB3	1:A:90:ILE:HD12	1.65	0.78
1:A:151:THR:HG23	2:A:469:HOH:O	1.82	0.78
1:A:113:GLN:OE1	2:A:335:HOH:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HG	1:A:125:ALA:HB2	1.67	0.77
1:A:128:VAL:HG23	2:A:219:HOH:O	1.84	0.76
1:A:148:MSE:CE	2:A:386:HOH:O	2.32	0.76
1:A:48:GLU:CD	1:A:144:TYR:HE2	1.89	0.76
1:A:48:GLU:OE2	1:A:144:TYR:HE2	1.68	0.76
1:A:41:ILE:O	2:A:271:HOH:O	2.03	0.76
1:A:153:ASN:ND2	2:A:240:HOH:O	1.96	0.75
1:A:70:GLU:CD	1:A:70:GLU:H	1.91	0.74
1:A:45:ARG:NE	2:A:439:HOH:O	2.20	0.74
1:A:68:LYS:HD3	2:A:299:HOH:O	1.87	0.74
1:A:96:GLN:NE2	2:A:265:HOH:O	2.14	0.74
1:A:105:LYS:CD	2:A:435:HOH:O	2.32	0.74
1:A:129:LYS:NZ	2:A:233:HOH:O	2.19	0.74
1:A:51:ARG:HH12	1:A:53:SER:HB3	1.53	0.74
1:A:32:GLY:HA3	1:A:163:LEU:HA	1.69	0.74
1:A:113:GLN:OE1	2:A:335:HOH:O	2.05	0.74
1:A:132:SER:HB2	1:A:147:ARG:HB2	1.69	0.73
1:A:96:GLN:OE1	2:A:265:HOH:O	2.05	0.73
1:A:151:THR:CB	2:A:258:HOH:O	2.36	0.73
1:A:120:ASP:OD1	2:A:421:HOH:O	2.07	0.73
1:A:42:PRO:HG2	2:A:286:HOH:O	1.88	0.72
1:A:75:MSE:CE	1:A:75:MSE:HA	2.18	0.72
1:A:70:GLU:OE2	2:A:304:HOH:O	2.07	0.72
1:A:51:ARG:NH1	1:A:53:SER:OG	2.22	0.72
1:A:68:LYS:HD2	1:A:73:ALA:HB3	1.70	0.72
1:A:148:MSE:HE3	2:A:386:HOH:O	1.89	0.72
1:A:77:ALA:HB3	1:A:97:SER:HB3	1.71	0.72
1:A:33:GLN:HG2	2:A:289:HOH:O	1.90	0.72
1:A:147:ARG:HD3	2:A:290:HOH:O	1.90	0.71
1:A:75:MSE:CE	2:A:261:HOH:O	2.33	0.71
1:A:42:PRO:HG2	2:A:286:HOH:O	1.90	0.71
1:A:130:GLU:OE2	2:A:349:HOH:O	2.08	0.71
1:A:137:LEU:HA	1:A:141:LYS:O	1.91	0.71
1:A:48:GLU:OE1	1:A:144:TYR:OH	2.03	0.71
1:A:35:GLU:CG	1:A:45:ARG:HG2	2.20	0.71
1:A:45:ARG:NE	2:A:439:HOH:O	2.23	0.71
1:A:41:ILE:O	2:A:271:HOH:O	2.08	0.70
1:A:148:MSE:SE	1:A:148:MSE:CB	2.89	0.70
1:A:42:PRO:CB	2:A:348:HOH:O	2.39	0.70
1:A:33:GLN:HG2	2:A:293:HOH:O	1.92	0.70
1:A:51:ARG:NH1	1:A:53:SER:HB3	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NE	2:A:439:HOH:O	2.20	0.69
1:A:106:GLY:HA3	1:A:116:LYS:O	1.92	0.69
1:A:45:ARG:NH1	2:A:400:HOH:O	2.25	0.69
1:A:145:VAL:O	1:A:145:VAL:CG1	2.27	0.69
1:A:41:ILE:HD11	1:A:158:HIS:HE1	1.58	0.69
1:A:133:ARG:HG2	1:A:146:VAL:HG22	1.73	0.69
1:A:51:ARG:HB3	1:A:63:THR:OG1	1.93	0.69
1:A:118:LYS:HG2	1:A:132:SER:CB	2.22	0.69
1:A:42:PRO:CB	2:A:348:HOH:O	2.41	0.69
1:A:87:ASP:OD2	2:A:396:HOH:O	2.11	0.69
1:A:35:GLU:OE1	2:A:406:HOH:O	2.11	0.69
1:A:112:GLU:OE1	2:A:455:HOH:O	2.11	0.69
1:A:109:ASN:CG	1:A:112:GLU:HG3	2.14	0.68
1:A:35:GLU:HG2	1:A:45:ARG:HG2	1.75	0.68
1:A:152:THR:OG1	2:A:394:HOH:O	2.10	0.68
1:A:57:LYS:HB3	1:A:58:PRO:HD2	1.75	0.68
1:A:63:THR:HG21	2:A:307:HOH:O	1.94	0.68
1:A:102:GLU:OE2	1:A:133:ARG:NH2	2.26	0.68
1:A:81:TYR:O	1:A:92:VAL:HA	1.94	0.68
1:A:152:THR:N	2:A:394:HOH:O	2.22	0.67
1:A:38:TYR:CZ	1:A:148:MSE:HE3	2.29	0.67
1:A:37:GLU:OE1	2:A:346:HOH:O	2.12	0.67
1:A:41:ILE:O	2:A:271:HOH:O	2.13	0.66
1:A:46:TYR:OH	1:A:144:TYR:OH	2.14	0.66
1:A:109:ASN:OD1	1:A:112:GLU:HG3	1.95	0.66
1:A:35:GLU:HG2	1:A:45:ARG:NH1	2.11	0.66
1:A:68:LYS:HE3	2:A:205:HOH:O	1.95	0.66
1:A:145:VAL:HG13	2:A:268:HOH:O	1.95	0.66
1:A:81:TYR:OH	2:A:206:HOH:O	2.13	0.66
1:A:151:THR:CA	2:A:258:HOH:O	2.44	0.65
1:A:51:ARG:NH1	1:A:53:SER:CB	2.58	0.65
1:A:115:ILE:CB	1:A:115:ILE:CD1	2.72	0.65
1:A:102:GLU:OE1	1:A:131:ILE:HB	1.96	0.65
1:A:39:PRO:HG3	2:A:330:HOH:O	1.96	0.65
1:A:160:LYS:HE2	2:A:288:HOH:O	1.94	0.65
1:A:131:ILE:HG12	1:A:148:MSE:HG2	1.78	0.65
1:A:48:GLU:CD	1:A:144:TYR:CE2	2.70	0.65
1:A:51:ARG:NH2	2:A:342:HOH:O	2.29	0.65
1:A:132:SER:OG	1:A:155:LEU:HD21	1.97	0.65
1:A:64:GLN:OE1	1:A:78:GLU:HG2	1.97	0.64
1:A:33:GLN:HB3	1:A:69:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HB3	1:A:69:LEU:HD11	1.80	0.64
1:A:122:VAL:HG22	1:A:131:ILE:HD12	1.79	0.63
1:A:156:GLN:HB2	1:A:157:PRO:HD2	1.80	0.63
1:A:134:GLU:CD	2:A:401:HOH:O	2.36	0.63
1:A:109:ASN:ND2	2:A:451:HOH:O	2.27	0.63
1:A:165:LYS:O	2:A:404:HOH:O	2.15	0.62
1:A:48:GLU:OE1	1:A:144:TYR:OH	2.14	0.62
1:A:151:THR:OG1	2:A:258:HOH:O	2.16	0.62
1:A:133:ARG:HG2	1:A:146:VAL:HG22	1.82	0.62
1:A:106:GLY:HA3	1:A:116:LYS:O	1.99	0.62
1:A:39:PRO:HG3	2:A:330:HOH:O	1.99	0.62
1:A:92:VAL:HB	1:A:104:GLN:HB2	1.80	0.62
1:A:63:THR:HG21	2:A:385:HOH:O	1.99	0.62
1:A:105:LYS:HE2	1:A:120:ASP:OD2	1.99	0.62
1:A:14:PRO:HD3	2:A:474:HOH:O	1.99	0.62
1:A:134:GLU:O	1:A:144:TYR:HA	2.00	0.62
1:A:48:GLU:OE1	1:A:144:TYR:OH	2.18	0.61
1:A:98:THR:HG21	2:A:265:HOH:O	2.00	0.61
1:A:107:THR:HG23	2:A:376:HOH:O	1.99	0.61
1:A:68:LYS:HB3	1:A:70:GLU:OE2	2.01	0.61
1:A:118:LYS:HB2	1:A:118:LYS:HZ2	1.62	0.60
1:A:57:LYS:HB3	1:A:58:PRO:HD2	1.83	0.60
1:A:51:ARG:HD2	2:A:256:HOH:O	2.00	0.60
1:A:112:GLU:OE2	2:A:451:HOH:O	2.16	0.60
1:A:46:TYR:HE2	1:A:48:GLU:OE1	1.85	0.60
1:A:137:LEU:HG	2:A:201:HOH:O	2.00	0.60
1:A:105:LYS:NZ	2:A:284:HOH:O	2.33	0.60
1:A:152:THR:O	1:A:153:ASN:CG	2.41	0.59
1:A:118:LYS:HA	1:A:132:SER:HA	1.85	0.59
1:A:91:GLU:HG3	1:A:105:LYS:HE3	1.81	0.59
1:A:64:GLN:HB3	1:A:78:GLU:HG3	1.82	0.59
1:A:49:GLU:O	1:A:64:GLN:HA	2.02	0.59
1:A:96:GLN:NE2	2:A:265:HOH:O	2.35	0.59
1:A:90:ILE:HG23	1:A:117:LEU:HD21	1.84	0.59
1:A:14:PRO:N	2:A:474:HOH:O	2.34	0.59
1:A:74:PRO:HD2	2:A:343:HOH:O	2.03	0.58
1:A:39:PRO:HG3	2:A:330:HOH:O	2.03	0.58
1:A:148:MSE:HE1	2:A:386:HOH:O	1.96	0.58
1:A:109:ASN:ND2	1:A:112:GLU:HG3	2.18	0.58
1:A:42:PRO:HG2	2:A:286:HOH:O	2.03	0.58
1:A:142:LEU:HB3	1:A:163:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLN:NE2	2:A:443:HOH:O	2.23	0.58
1:A:122:VAL:CG2	1:A:131:ILE:HD12	2.34	0.58
1:A:42:PRO:HG2	2:A:286:HOH:O	2.04	0.57
1:A:51:ARG:NH1	1:A:53:SER:HB3	2.19	0.57
1:A:42:PRO:HG2	2:A:286:HOH:O	2.04	0.57
1:A:114:SER:HB3	1:A:136:GLU:HG3	1.86	0.57
1:A:148:MSE:HE1	2:A:383:HOH:O	2.04	0.57
1:A:14:PRO:N	2:A:474:HOH:O	2.36	0.57
1:A:131:ILE:HD11	1:A:148:MSE:HE3	1.87	0.57
1:A:83:ARG:HB2	1:A:91:GLU:HG2	1.86	0.57
1:A:99:GLY:O	1:A:124:ASN:ND2	2.29	0.57
1:A:29:THR:HG22	1:A:166:LEU:HD12	1.86	0.57
1:A:109:ASN:ND2	1:A:112:GLU:OE2	2.38	0.57
1:A:41:ILE:CG1	1:A:41:ILE:O	2.49	0.56
1:A:129:LYS:HB3	1:A:130:GLU:OE2	2.06	0.56
1:A:147:ARG:HD2	2:A:203:HOH:O	2.05	0.56
1:A:104:GLN:HG3	1:A:133:ARG:HD2	1.86	0.56
1:A:100:LEU:HD12	1:A:100:LEU:N	2.20	0.56
1:A:42:PRO:HG2	2:A:286:HOH:O	2.06	0.56
1:A:113:GLN:HB3	1:A:137:LEU:HB3	1.87	0.56
1:A:38:TYR:CD2	1:A:39:PRO:HD2	2.41	0.56
1:A:68:LYS:HB3	1:A:70:GLU:OE2	2.06	0.56
1:A:133:ARG:HD3	1:A:146:VAL:HG22	1.88	0.56
1:A:156:GLN:HB2	1:A:157:PRO:HD2	1.88	0.56
1:A:97:SER:HB3	2:A:210:HOH:O	2.05	0.56
1:A:42:PRO:HG2	2:A:286:HOH:O	2.05	0.55
1:A:118:LYS:HZ1	1:A:118:LYS:HB2	1.68	0.55
1:A:105:LYS:HE3	1:A:120:ASP:OD2	2.07	0.55
1:A:68:LYS:HG3	1:A:75:MSE:SE	2.56	0.55
1:A:105:LYS:CE	1:A:120:ASP:OD2	2.54	0.55
1:A:41:ILE:HD11	1:A:158:HIS:CE1	2.41	0.55
1:A:69:LEU:O	1:A:71:SER:N	2.39	0.55
1:A:35:GLU:HG2	1:A:45:ARG:CG	2.37	0.55
1:A:91:GLU:HG2	2:A:171:HOH:O	2.07	0.55
1:A:148:MSE:HG2	1:A:149:SER:N	2.22	0.55
1:A:68:LYS:CD	1:A:73:ALA:HB3	2.21	0.55
1:A:131:ILE:HG12	1:A:148:MSE:CG	2.36	0.55
1:A:48:GLU:OE1	1:A:144:TYR:CE2	2.60	0.55
1:A:39:PRO:CG	2:A:330:HOH:O	2.54	0.55
1:A:111:ASP:OD2	2:A:259:HOH:O	2.18	0.54
1:A:135:PHE:HA	1:A:143:SER:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLN:HB3	1:A:78:GLU:HG2	1.88	0.54
1:A:20:VAL:HG23	1:A:58:PRO:HA	1.90	0.54
1:A:70:GLU:O	1:A:71:SER:HB3	2.08	0.54
1:A:147:ARG:NH2	2:A:431:HOH:O	2.40	0.54
1:A:105:LYS:O	1:A:118:LYS:N	2.33	0.54
1:A:129:LYS:HG3	1:A:151:THR:N	2.22	0.54
1:A:14:PRO:CD	2:A:474:HOH:O	2.54	0.53
1:A:131:ILE:HA	1:A:147:ARG:O	2.08	0.53
1:A:60:ILE:N	1:A:60:ILE:CD1	2.43	0.53
1:A:113:GLN:OE1	1:A:137:LEU:HD23	2.09	0.53
1:A:110:VAL:HG23	2:A:345:HOH:O	2.08	0.53
1:A:63:THR:HG21	2:A:307:HOH:O	2.08	0.53
1:A:42:PRO:CA	2:A:348:HOH:O	2.57	0.53
1:A:113:GLN:HG3	2:A:335:HOH:O	2.08	0.53
1:A:83:ARG:HB2	1:A:91:GLU:O	2.08	0.53
1:A:38:TYR:O	1:A:39:PRO:C	2.47	0.53
1:A:65:LYS:HA	1:A:77:ALA:HA	1.91	0.53
1:A:29:THR:HG22	1:A:166:LEU:HD12	1.91	0.53
1:A:49:GLU:OE2	1:A:65:LYS:CE	2.57	0.53
1:A:59:VAL:HG13	1:A:83:ARG:HG2	1.90	0.53
1:A:143:SER:OG	2:A:248:HOH:O	1.90	0.53
1:A:132:SER:HB2	1:A:147:ARG:HB2	1.91	0.53
1:A:17:HIS:CD2	1:A:58:PRO:HD3	2.44	0.53
1:A:132:SER:OG	1:A:147:ARG:HB2	2.09	0.52
1:A:102:GLU:OE2	1:A:131:ILE:CD1	2.52	0.52
1:A:148:MSE:SE	1:A:158:HIS:CD2	3.12	0.52
1:A:134:GLU:O	2:A:250:HOH:O	2.19	0.52
1:A:47:GLY:HA3	1:A:67:TRP:CE2	2.44	0.52
1:A:121:LEU:HG	2:A:215:HOH:O	2.08	0.52
1:A:53:SER:O	1:A:60:ILE:HG23	2.09	0.52
1:A:85:ARG:HB2	1:A:89:SER:OG	2.09	0.52
1:A:102:GLU:OE1	1:A:133:ARG:NE	2.42	0.52
1:A:68:LYS:CE	1:A:75:MSE:HE3	2.39	0.52
1:A:70:GLU:CD	1:A:70:GLU:N	2.60	0.52
1:A:74:PRO:O	1:A:75:MSE:HE2	2.10	0.52
1:A:134:GLU:OE1	1:A:147:ARG:NH1	2.42	0.52
1:A:129:LYS:HG2	1:A:150:THR:HA	1.92	0.52
1:A:38:TYR:CE1	1:A:148:MSE:HE3	2.45	0.52
1:A:33:GLN:CG	2:A:293:HOH:O	2.55	0.52
1:A:42:PRO:O	2:A:286:HOH:O	2.19	0.52
1:A:48:GLU:OE2	1:A:50:ILE:HD11	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PRO:N	2:A:474:HOH:O	2.44	0.51
1:A:68:LYS:HD3	2:A:304:HOH:O	2.09	0.51
1:A:70:GLU:N	1:A:70:GLU:CD	2.57	0.51
1:A:29:THR:CG2	1:A:166:LEU:HD12	2.40	0.51
1:A:64:GLN:HG2	1:A:65:LYS:H	1.75	0.51
1:A:151:THR:HA	2:A:469:HOH:O	2.09	0.51
1:A:31:ARG:HB2	1:A:166:LEU:HD11	1.92	0.51
1:A:34:GLY:HA3	1:A:46:TYR:CZ	2.46	0.51
1:A:113:GLN:OE1	1:A:137:LEU:HD23	2.10	0.51
1:A:104:GLN:O	1:A:105:LYS:HD3	2.09	0.51
1:A:147:ARG:NH2	2:A:431:HOH:O	2.43	0.51
1:A:46:TYR:HA	1:A:67:TRP:O	2.11	0.51
1:A:45:ARG:HD3	2:A:198:HOH:O	2.11	0.51
1:A:35:GLU:OE2	1:A:160:LYS:HE3	2.11	0.51
1:A:156:GLN:HB2	1:A:157:PRO:CD	2.40	0.51
1:A:147:ARG:HD3	2:A:290:HOH:O	2.11	0.50
1:A:121:LEU:C	1:A:121:LEU:HD23	2.31	0.50
1:A:159:LEU:HD13	2:A:390:HOH:O	2.10	0.50
1:A:30:TRP:O	1:A:49:GLU:HA	2.12	0.50
1:A:116:LYS:HD2	2:A:477:HOH:O	2.11	0.50
1:A:118:LYS:CB	1:A:118:LYS:NZ	2.63	0.50
1:A:19:PHE:HB2	1:A:58:PRO:HB3	1.94	0.50
1:A:144:TYR:O	1:A:160:LYS:HA	2.12	0.50
1:A:19:PHE:CD1	1:A:86:PRO:HD3	2.47	0.49
1:A:34:GLY:HA3	1:A:46:TYR:CZ	2.47	0.49
1:A:53:SER:O	1:A:60:ILE:CG2	2.60	0.49
1:A:151:THR:O	1:A:151:THR:CG2	2.60	0.49
1:A:154:PRO:O	1:A:155:LEU:C	2.51	0.49
1:A:60:ILE:O	1:A:81:TYR:HA	2.12	0.49
1:A:90:ILE:HG12	1:A:91:GLU:N	2.26	0.49
1:A:49:GLU:OE2	1:A:65:LYS:HE3	2.13	0.49
1:A:138:VAL:CG2	1:A:143:SER:OG	2.60	0.49
1:A:105:LYS:HD2	2:A:354:HOH:O	2.12	0.49
1:A:63:THR:HG23	2:A:177:HOH:O	2.12	0.49
1:A:31:ARG:HA	1:A:48:GLU:O	2.13	0.49
1:A:36:GLY:HA3	1:A:44:PHE:CZ	2.48	0.49
1:A:30:TRP:CZ3	1:A:165:LYS:HB2	2.48	0.49
1:A:46:TYR:HH	1:A:144:TYR:HH	1.51	0.49
1:A:82:PHE:HA	1:A:92:VAL:CG2	2.33	0.49
1:A:51:ARG:CZ	2:A:195:HOH:O	2.60	0.49
1:A:112:GLU:OE2	2:A:451:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:CE2	1:A:161:ALA:HB3	2.48	0.48
1:A:33:GLN:HB2	1:A:46:TYR:O	2.14	0.48
1:A:52:PHE:HA	1:A:61:ALA:O	2.13	0.48
1:A:110:VAL:HG23	2:A:345:HOH:O	2.13	0.48
1:A:121:LEU:C	1:A:121:LEU:HD23	2.34	0.48
1:A:51:ARG:NH2	2:A:195:HOH:O	2.45	0.48
1:A:52:PHE:HE1	1:A:82:PHE:CE1	2.31	0.48
1:A:118:LYS:HA	1:A:132:SER:HA	1.96	0.48
1:A:36:GLY:HA2	1:A:158:HIS:O	2.14	0.48
1:A:70:GLU:HG3	1:A:71:SER:N	2.29	0.48
1:A:129:LYS:NZ	2:A:363:HOH:O	2.08	0.48
1:A:33:GLN:NE2	2:A:400:HOH:O	2.44	0.48
1:A:48:GLU:OE1	1:A:144:TYR:CZ	2.66	0.48
1:A:70:GLU:O	1:A:71:SER:CB	2.62	0.48
1:A:85:ARG:HB3	1:A:87:ASP:OD1	2.13	0.48
1:A:23:LEU:HD13	1:A:26:LEU:CD1	2.44	0.48
1:A:42:PRO:HG2	2:A:286:HOH:O	2.13	0.48
1:A:50:ILE:HD12	1:A:163:LEU:HD22	1.96	0.48
1:A:19:PHE:HB2	1:A:58:PRO:CB	2.43	0.48
1:A:74:PRO:HG2	2:A:343:HOH:O	2.13	0.48
1:A:118:LYS:HG2	1:A:132:SER:HB3	1.95	0.47
1:A:30:TRP:CZ3	1:A:142:LEU:HB2	2.49	0.47
1:A:99:GLY:C	1:A:100:LEU:HD12	2.35	0.47
1:A:129:LYS:CG	1:A:150:THR:HA	2.45	0.47
1:A:99:GLY:O	1:A:124:ASN:HB3	2.13	0.47
1:A:148:MSE:SE	1:A:148:MSE:HB3	2.65	0.47
1:A:68:LYS:HB3	1:A:70:GLU:OE2	2.15	0.47
1:A:38:TYR:CD2	1:A:39:PRO:HD2	2.49	0.47
1:A:69:LEU:C	1:A:71:SER:H	2.17	0.47
1:A:35:GLU:HG2	1:A:45:ARG:HG2	1.96	0.47
1:A:90:ILE:HG23	1:A:117:LEU:CD2	2.45	0.47
1:A:67:TRP:HB2	1:A:73:ALA:O	2.14	0.47
1:A:23:LEU:HD13	1:A:26:LEU:HD11	1.96	0.47
1:A:38:TYR:O	1:A:39:PRO:C	2.52	0.47
1:A:42:PRO:CA	2:A:348:HOH:O	2.60	0.47
1:A:35:GLU:HG2	1:A:45:ARG:HG2	1.97	0.47
1:A:48:GLU:HG2	1:A:163:LEU:HD21	1.96	0.47
1:A:147:ARG:HG2	1:A:157:PRO:HA	1.97	0.47
1:A:42:PRO:CB	2:A:348:HOH:O	2.62	0.47
1:A:105:LYS:HE2	2:A:209:HOH:O	2.15	0.46
1:A:25:TYR:HE2	2:A:235:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:O	1:A:148:MSE:HA	2.15	0.46
1:A:145:VAL:HG13	2:A:268:HOH:O	2.16	0.46
1:A:144:TYR:CZ	1:A:161:ALA:HB3	2.50	0.46
1:A:14:PRO:CD	2:A:474:HOH:O	2.64	0.46
1:A:17:HIS:CD2	1:A:58:PRO:HD3	2.51	0.46
1:A:60:ILE:O	1:A:81:TYR:HA	2.16	0.46
1:A:148:MSE:C	1:A:155:LEU:HD12	2.37	0.46
1:A:118:LYS:CG	1:A:132:SER:OG	2.56	0.46
1:A:32:GLY:HA3	1:A:162:ILE:O	2.16	0.46
1:A:70:GLU:H	1:A:70:GLU:CD	2.18	0.46
1:A:138:VAL:O	1:A:138:VAL:HG23	2.16	0.46
1:A:16:VAL:HG22	1:A:54:HIS:NE2	2.30	0.46
1:A:37:GLU:O	1:A:38:TYR:HB2	2.16	0.45
1:A:109:ASN:ND2	1:A:112:GLU:OE2	2.49	0.45
1:A:144:TYR:C	1:A:144:TYR:CD1	2.90	0.45
1:A:48:GLU:HB3	1:A:163:LEU:HD21	1.98	0.45
1:A:105:LYS:HD2	1:A:120:ASP:OD2	2.15	0.45
1:A:150:THR:OG1	1:A:153:ASN:HB2	2.16	0.45
1:A:41:ILE:CG1	1:A:41:ILE:O	2.43	0.45
1:A:133:ARG:HH11	1:A:133:ARG:HD3	1.60	0.45
1:A:14:PRO:N	2:A:474:HOH:O	2.49	0.45
1:A:48:GLU:HG3	1:A:65:LYS:O	2.17	0.45
1:A:38:TYR:CG	1:A:39:PRO:HD2	2.52	0.45
1:A:23:LEU:HB3	1:A:26:LEU:HD12	1.97	0.45
1:A:99:GLY:C	1:A:100:LEU:HD12	2.36	0.45
1:A:132:SER:OG	1:A:155:LEU:HD21	2.17	0.45
1:A:103:VAL:HG23	1:A:121:LEU:HD22	1.99	0.45
1:A:57:LYS:HB3	1:A:58:PRO:CD	2.43	0.45
1:A:59:VAL:CG1	1:A:81:TYR:HB3	2.47	0.45
1:A:151:THR:HG22	1:A:152:THR:HG23	1.98	0.45
1:A:129:LYS:HG3	1:A:150:THR:C	2.37	0.45
1:A:38:TYR:CG	1:A:39:PRO:HD2	2.53	0.44
1:A:105:LYS:HB2	2:A:182:HOH:O	2.16	0.44
1:A:93:VAL:HG12	1:A:103:VAL:HG22	1.99	0.44
1:A:110:VAL:O	1:A:110:VAL:CG1	2.64	0.44
1:A:150:THR:OG1	1:A:153:ASN:HB2	2.16	0.44
1:A:116:LYS:HG2	1:A:134:GLU:HG2	1.98	0.44
1:A:35:GLU:CG	1:A:45:ARG:NH1	2.79	0.44
1:A:50:ILE:HG22	1:A:51:ARG:N	2.33	0.44
1:A:163:LEU:N	1:A:163:LEU:HD12	2.32	0.44
1:A:104:GLN:HB3	1:A:117:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD23	1:A:121:LEU:C	2.38	0.44
1:A:142:LEU:O	1:A:162:ILE:HA	2.18	0.44
1:A:33:GLN:CB	1:A:46:TYR:O	2.65	0.44
1:A:127:LYS:HE2	2:A:300:HOH:O	2.17	0.44
1:A:31:ARG:HD2	1:A:31:ARG:HH11	1.62	0.44
1:A:51:ARG:HH12	1:A:53:SER:CB	2.27	0.44
1:A:104:GLN:HB3	1:A:117:LEU:HB3	1.99	0.44
1:A:109:ASN:HB3	1:A:114:SER:OG	2.18	0.43
1:A:30:TRP:O	1:A:49:GLU:HA	2.18	0.43
1:A:51:ARG:HH11	1:A:51:ARG:HG2	1.83	0.43
1:A:150:THR:OG1	1:A:153:ASN:HB2	2.18	0.43
1:A:102:GLU:HG2	1:A:122:VAL:HG22	2.01	0.43
1:A:148:MSE:HE2	1:A:148:MSE:HB3	1.08	0.43
1:A:83:ARG:NH1	2:A:249:HOH:O	2.04	0.43
1:A:165:LYS:NZ	2:A:183:HOH:O	2.51	0.43
1:A:151:THR:HA	2:A:469:HOH:O	2.17	0.43
1:A:144:TYR:C	1:A:144:TYR:CD1	2.91	0.43
1:A:156:GLN:HB2	1:A:157:PRO:CD	2.48	0.43
1:A:68:LYS:CG	1:A:75:MSE:SE	3.17	0.43
1:A:85:ARG:C	2:A:170:HOH:O	2.56	0.42
1:A:108:TYR:HA	1:A:114:SER:O	2.18	0.42
1:A:130:GLU:HB2	1:A:149:SER:OG	2.18	0.42
1:A:105:LYS:HD2	1:A:120:ASP:CG	2.40	0.42
1:A:138:VAL:HG22	1:A:143:SER:OG	2.18	0.42
1:A:47:GLY:HA3	1:A:67:TRP:NE1	2.34	0.42
1:A:143:SER:HB2	1:A:162:ILE:HG12	2.01	0.42
1:A:33:GLN:HA	1:A:47:GLY:HA2	2.01	0.42
1:A:92:VAL:HG21	1:A:117:LEU:HD11	2.01	0.42
1:A:88:GLY:HA3	2:A:270:HOH:O	2.20	0.42
1:A:74:PRO:O	1:A:75:MSE:HE3	2.19	0.42
1:A:78:GLU:HB2	1:A:95:ALA:O	2.19	0.42
1:A:112:GLU:CD	2:A:451:HOH:O	2.57	0.42
1:A:68:LYS:HE2	1:A:75:MSE:HE3	2.01	0.42
1:A:148:MSE:HG3	1:A:158:HIS:CB	2.50	0.42
1:A:122:VAL:O	2:A:213:HOH:O	2.21	0.42
1:A:90:ILE:CG2	1:A:117:LEU:HD21	2.49	0.42
1:A:40:THR:HG21	2:A:428:HOH:O	2.19	0.42
1:A:26:LEU:O	1:A:52:PHE:HB2	2.19	0.42
1:A:48:GLU:HG3	1:A:66:THR:HG22	2.02	0.42
1:A:158:HIS:O	1:A:159:LEU:HD23	2.20	0.42
1:A:22:PRO:HB2	1:A:108:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:CD1	1:A:144:TYR:C	2.93	0.42
1:A:88:GLY:HA2	1:A:108:TYR:CZ	2.55	0.42
1:A:129:LYS:HA	1:A:129:LYS:HD2	1.73	0.42
1:A:40:THR:HG23	2:A:428:HOH:O	2.20	0.42
1:A:100:LEU:HD12	1:A:100:LEU:N	2.35	0.42
1:A:59:VAL:C	1:A:60:ILE:HD12	2.32	0.42
1:A:42:PRO:HA	2:A:348:HOH:O	2.20	0.42
1:A:48:GLU:HG2	1:A:163:LEU:HD21	2.02	0.42
1:A:129:LYS:HE3	2:A:380:HOH:O	2.20	0.41
1:A:93:VAL:HG12	1:A:103:VAL:HA	2.02	0.41
1:A:105:LYS:HD3	2:A:435:HOH:O	2.11	0.41
1:A:106:GLY:HA3	1:A:116:LYS:O	2.20	0.41
1:A:17:HIS:ND1	1:A:18:PRO:N	2.68	0.41
1:A:51:ARG:NH2	2:A:342:HOH:O	2.39	0.41
1:A:70:GLU:N	1:A:70:GLU:CD	2.74	0.41
1:A:133:ARG:HH11	1:A:133:ARG:HD3	1.73	0.41
1:A:110:VAL:HA	2:A:235:HOH:O	2.19	0.41
1:A:35:GLU:HG2	1:A:45:ARG:NH1	2.36	0.41
1:A:32:GLY:CA	1:A:163:LEU:HA	2.45	0.41
1:A:27:LEU:HD13	1:A:54:HIS:HD2	1.80	0.41
1:A:51:ARG:CZ	1:A:53:SER:HB3	2.50	0.41
1:A:47:GLY:HA3	1:A:67:TRP:CE2	2.55	0.41
1:A:49:GLU:OE2	1:A:65:LYS:HE2	2.20	0.41
1:A:70:GLU:N	1:A:70:GLU:OE1	2.47	0.41
1:A:107:THR:OG1	2:A:489:HOH:O	2.22	0.41
1:A:144:TYR:C	1:A:144:TYR:CD1	2.94	0.41
1:A:110:VAL:HA	2:A:235:HOH:O	2.20	0.41
1:A:129:LYS:HB3	1:A:130:GLU:OE2	2.21	0.41
1:A:29:THR:HA	1:A:50:ILE:O	2.20	0.41
1:A:64:GLN:NE2	1:A:66:THR:HG23	2.36	0.41
1:A:78:GLU:HG2	2:A:484:HOH:O	2.21	0.41
1:A:100:LEU:HA	1:A:123:GLY:O	2.20	0.41
1:A:92:VAL:HG12	1:A:94:ILE:HD12	2.01	0.41
1:A:140:GLY:O	2:A:178:HOH:O	2.22	0.41
1:A:158:HIS:CD2	1:A:159:LEU:HG	2.56	0.41
1:A:68:LYS:HD2	1:A:75:MSE:HE3	2.01	0.41
1:A:151:THR:HA	2:A:469:HOH:O	2.20	0.41
1:A:122:VAL:HG21	1:A:131:ILE:HG13	2.02	0.41
1:A:42:PRO:CA	2:A:348:HOH:O	2.69	0.41
1:A:110:VAL:O	1:A:111:ASP:C	2.58	0.41
1:A:39:PRO:CD	1:A:156:GLN:OE1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLN:OE1	1:A:78:GLU:CG	2.69	0.41
1:A:69:LEU:C	1:A:71:SER:N	2.73	0.41
1:A:70:GLU:H	1:A:70:GLU:CD	2.24	0.41
1:A:68:LYS:HE3	1:A:75:MSE:HE3	2.03	0.41
1:A:34:GLY:HA2	1:A:160:LYS:O	2.20	0.41
1:A:47:GLY:O	1:A:66:THR:HA	2.20	0.41
1:A:26:LEU:HB3	1:A:52:PHE:CD2	2.56	0.41
1:A:21:ALA:HA	1:A:24:SER:HB3	2.03	0.41
1:A:35:GLU:OE2	1:A:45:ARG:NH1	2.54	0.41
1:A:17:HIS:CE1	1:A:19:PHE:H	2.39	0.41
1:A:100:LEU:CD1	1:A:100:LEU:N	2.83	0.41
1:A:86:PRO:C	1:A:88:GLY:H	2.23	0.41
1:A:68:LYS:CD	1:A:75:MSE:HE3	2.51	0.40
1:A:52:PHE:HA	1:A:61:ALA:O	2.21	0.40
1:A:149:SER:HB2	1:A:155:LEU:N	2.35	0.40
1:A:100:LEU:HD12	1:A:100:LEU:N	2.36	0.40
1:A:155:LEU:HA	1:A:155:LEU:HD12	1.76	0.40
1:A:165:LYS:NZ	2:A:183:HOH:O	2.53	0.40
1:A:64:GLN:HB3	1:A:78:GLU:CG	2.51	0.40
1:A:104:GLN:O	1:A:105:LYS:HG2	2.22	0.40
1:A:90:ILE:HG22	1:A:107:THR:HA	2.04	0.40
1:A:120:ASP:C	1:A:121:LEU:HG	2.42	0.40
1:A:83:ARG:HA	1:A:84:PRO:HD2	1.96	0.40
1:A:115:ILE:HB	1:A:135:PHE:HB2	2.04	0.40
1:A:53:SER:OG	1:A:61:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	151/166 (91%)	145 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-A	151/166 (91%)	142 (94%)	8 (5%)	1 (1%)	22	3
1	3-A	151/166 (91%)	139 (92%)	11 (7%)	1 (1%)	22	3
1	4-A	151/166 (91%)	143 (95%)	7 (5%)	1 (1%)	22	3
1	5-A	151/166 (91%)	147 (97%)	4 (3%)	0	100	100
1	6-A	151/166 (91%)	141 (93%)	10 (7%)	0	100	100
1	7-A	151/166 (91%)	144 (95%)	6 (4%)	1 (1%)	22	3
1	8-A	151/166 (91%)	143 (95%)	7 (5%)	1 (1%)	22	3
All	All	1208/1328 (91%)	1144 (95%)	59 (5%)	5 (0%)	34	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	4-A	71	SER
1	8-A	71	SER
1	3-A	151	THR
1	7-A	71	SER
1	2-A	39	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	133/143 (93%)	131 (98%)	2 (2%)	65	31
1	2-A	133/143 (93%)	128 (96%)	5 (4%)	33	3
1	3-A	133/143 (93%)	127 (96%)	6 (4%)	27	2
1	4-A	133/143 (93%)	131 (98%)	2 (2%)	65	31
1	5-A	133/143 (93%)	128 (96%)	5 (4%)	33	3
1	6-A	133/143 (93%)	130 (98%)	3 (2%)	50	13
1	7-A	133/143 (93%)	130 (98%)	3 (2%)	50	13
1	8-A	133/143 (93%)	128 (96%)	5 (4%)	33	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1064/1144 (93%)	1033 (97%)	31 (3%)	42 7

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	64	GLN
1	1-A	118	LYS
1	2-A	63	THR
1	2-A	70	GLU
1	2-A	78	GLU
1	2-A	121	LEU
1	2-A	154	PRO
1	3-A	33	GLN
1	3-A	100	LEU
1	3-A	102	GLU
1	3-A	121	LEU
1	3-A	129	LYS
1	3-A	144	TYR
1	4-A	39	PRO
1	4-A	97	SER
1	5-A	70	GLU
1	5-A	75	MSE
1	5-A	86	PRO
1	5-A	97	SER
1	5-A	121	LEU
1	6-A	39	PRO
1	6-A	62	TYR
1	6-A	75	MSE
1	7-A	14	PRO
1	7-A	64	GLN
1	7-A	101	VAL
1	8-A	64	GLN
1	8-A	70	GLU
1	8-A	75	MSE
1	8-A	93	VAL
1	8-A	107	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	2-A	54	HIS

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Mol	Chain	Res	Type
1	3-A	96	GLN
1	3-A	158	HIS
1	8-A	96	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

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	1-A	151/166 (90%)	0.13	8 (5%)	26	26	5, 9, 21, 34	151 (100%)
1	2-A	151/166 (90%)	0.13	8 (5%)	26	26	5, 9, 21, 34	151 (100%)
1	3-A	151/166 (90%)	0.13	8 (5%)	26	26	5, 9, 21, 34	151 (100%)
1	4-A	151/166 (90%)	0.13	8 (5%)	26	26	5, 9, 21, 34	151 (100%)
1	5-A	151/166 (90%)	0.13	8 (5%)	26	26	5, 9, 21, 34	151 (100%)
1	6-A	151/166 (90%)	0.13	8 (5%)	26	26	5, 9, 21, 34	151 (100%)
1	7-A	151/166 (90%)	0.13	8 (5%)	26	26	5, 9, 21, 34	151 (100%)
1	8-A	151/166 (90%)	0.13	8 (5%)	26	26	5, 9, 21, 34	151 (100%)
All	All	1208/1328 (90%)	0.13	64 (5%)	28	26	5, 9, 22, 34	1208 (100%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	41	ILE	7.5
1	2-A	41	ILE	7.5
1	3-A	41	ILE	7.5
1	4-A	41	ILE	7.5
1	5-A	41	ILE	7.5
1	6-A	41	ILE	7.5
1	7-A	41	ILE	7.5
1	8-A	41	ILE	7.5
1	1-A	40	THR	6.6
1	2-A	40	THR	6.6
1	3-A	40	THR	6.6
1	4-A	40	THR	6.6
1	5-A	40	THR	6.6
1	6-A	40	THR	6.6
1	7-A	40	THR	6.6
1	8-A	40	THR	6.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1-A	70	GLU	4.8
1	2-A	70	GLU	4.8
1	3-A	70	GLU	4.8
1	4-A	70	GLU	4.8
1	5-A	70	GLU	4.8
1	6-A	70	GLU	4.8
1	7-A	70	GLU	4.8
1	8-A	70	GLU	4.8
1	1-A	126	SER	3.1
1	2-A	126	SER	3.1
1	3-A	126	SER	3.1
1	4-A	126	SER	3.1
1	5-A	126	SER	3.1
1	6-A	126	SER	3.1
1	7-A	126	SER	3.1
1	8-A	126	SER	3.1
1	1-A	39	PRO	2.5
1	2-A	39	PRO	2.5
1	3-A	39	PRO	2.5
1	4-A	39	PRO	2.5
1	5-A	39	PRO	2.5
1	6-A	39	PRO	2.5
1	7-A	39	PRO	2.5
1	8-A	39	PRO	2.5
1	1-A	42	PRO	2.4
1	2-A	42	PRO	2.4
1	3-A	42	PRO	2.4
1	4-A	42	PRO	2.4
1	5-A	42	PRO	2.4
1	6-A	42	PRO	2.4
1	7-A	42	PRO	2.4
1	8-A	42	PRO	2.4
1	1-A	14	PRO	2.3
1	2-A	14	PRO	2.3
1	3-A	14	PRO	2.3
1	4-A	14	PRO	2.3
1	5-A	14	PRO	2.3
1	6-A	14	PRO	2.3
1	7-A	14	PRO	2.3
1	8-A	14	PRO	2.3
1	1-A	152	THR	2.2
1	2-A	152	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	3-A	152	THR	2.2
1	4-A	152	THR	2.2
1	5-A	152	THR	2.2
1	6-A	152	THR	2.2
1	7-A	152	THR	2.2
1	8-A	152	THR	2.2

## 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.