



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:45 AM GMT

PDB ID : 2SBT  
Title : A COMPARISON OF THE THREE-DIMENSIONAL STRUCTURES OF  
SUBTILISIN BPN AND SUBTILISIN NOVO  
Authors : Drenth, J.; Hol, W.G.J.; Jansonius, J.N.; Koekoek, R.  
Deposited on : 1976-09-07  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

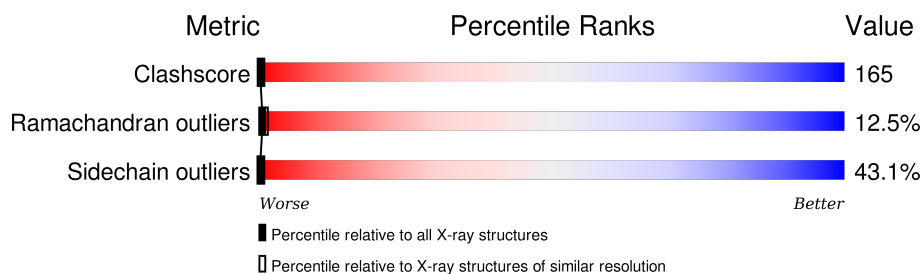
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.


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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACN	A	276	-	X	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1948 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.

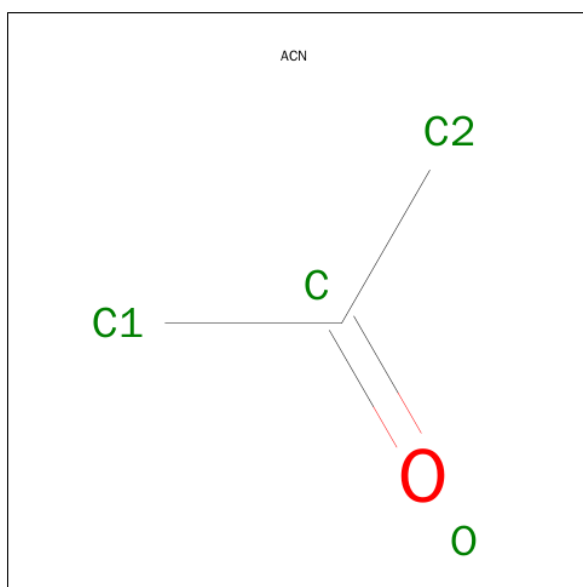
- Molecule 1 is a protein called SUBTILISIN NOVO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			1934	1202	335	392	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	PRO	ASN	CONFLICT	UNP P00782
A	57	ASN	PRO	CONFLICT	UNP P00782
A	61	ASP	ASN	CONFLICT	UNP P00782
A	88	SER	ALA	CONFLICT	UNP P00782
A	89	ALA	SER	CONFLICT	UNP P00782
A	98	ASP	ALA	CONFLICT	UNP P00782
A	99	ALA	ASP	CONFLICT	UNP P00782
A	158	SER	THR	CONFLICT	UNP P00782
A	159	THR	SER	CONFLICT	UNP P00782
A	251	GLN	GLU	CONFLICT	UNP P00782

- Molecule 2 is ACETONE (three-letter code: ACN) (formula: C<sub>3</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 3 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		

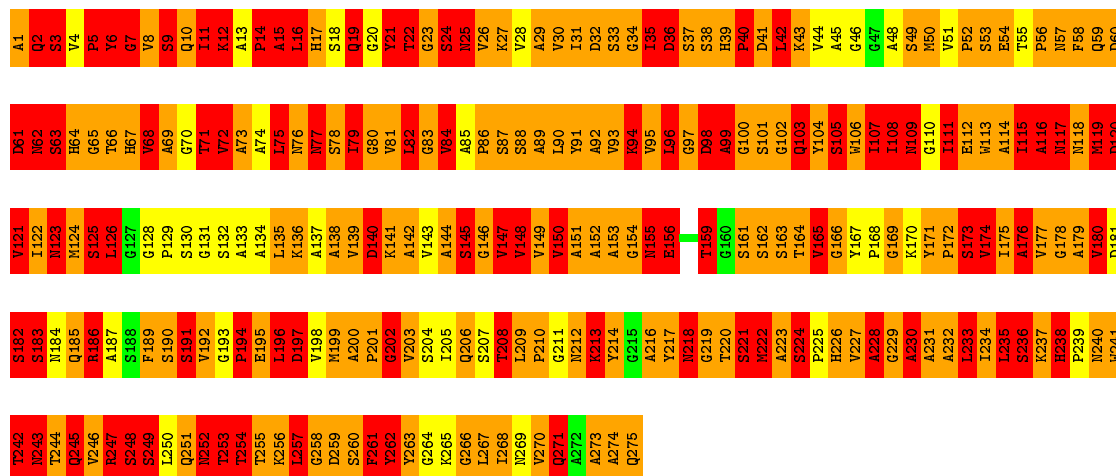
### 3 Residue-property plots

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

Note EDS was not executed.

#### • Molecule 1: SUBTILISIN NOVO

Chain A: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.20 Å 78.50 Å 37.10 Å 90.00° 114.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	4.34	423/1971 (21.5%)	3.37	285/2688 (10.6%)

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	20

All (423) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	SER	C-N	-25.47	0.75	1.34
1	A	34	GLY	C-N	24.07	1.89	1.34
1	A	70	GLY	N-CA	-20.64	1.15	1.46
1	A	214	TYR	CE2-CZ	19.04	1.63	1.38
1	A	195	GLU	C-N	17.39	1.74	1.34
1	A	59	GLN	C-N	16.73	1.72	1.34
1	A	113	TRP	NE1-CE2	16.34	1.58	1.37
1	A	6	TYR	CE2-CZ	16.31	1.59	1.38
1	A	21	TYR	CG-CD2	15.70	1.59	1.39
1	A	156	GLU	CD-OE1	-15.14	1.08	1.25
1	A	190	SER	CB-OG	14.30	1.60	1.42
1	A	101	SER	CB-OG	14.20	1.60	1.42
1	A	49	SER	CB-OG	13.96	1.60	1.42
1	A	34	GLY	C-O	-13.75	1.01	1.23
1	A	163	SER	CB-OG	13.74	1.60	1.42
1	A	131	GLY	N-CA	13.68	1.66	1.46
1	A	97	GLY	C-N	13.66	1.65	1.34
1	A	113	TRP	CG-CD1	13.63	1.55	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	GLY	CA-C	13.09	1.72	1.51
1	A	146	GLY	CA-C	12.98	1.72	1.51
1	A	211	GLY	CA-C	12.81	1.72	1.51
1	A	146	GLY	N-CA	-12.55	1.27	1.46
1	A	195	GLU	CD-OE1	12.55	1.39	1.25
1	A	145	SER	N-CA	12.42	1.71	1.46
1	A	106	TRP	NE1-CE2	12.16	1.53	1.37
1	A	80	GLY	C-O	-12.01	1.04	1.23
1	A	111	ILE	C-O	-11.63	1.01	1.23
1	A	113	TRP	CG-CD2	-11.48	1.24	1.43
1	A	91	TYR	CE2-CZ	11.47	1.53	1.38
1	A	91	TYR	CG-CD2	-11.47	1.24	1.39
1	A	236	SER	CB-OG	11.46	1.57	1.42
1	A	217	TYR	CG-CD2	-11.42	1.24	1.39
1	A	241	TRP	CG-CD1	11.36	1.52	1.36
1	A	129	PRO	N-CD	11.33	1.63	1.47
1	A	98	ASP	N-CA	-11.31	1.23	1.46
1	A	214	TYR	CD2-CE2	-11.30	1.22	1.39
1	A	23	GLY	CA-C	11.29	1.70	1.51
1	A	247	ARG	NE-CZ	11.28	1.47	1.33
1	A	186	ARG	CZ-NH2	11.14	1.47	1.33
1	A	213	LYS	N-CA	-11.02	1.24	1.46
1	A	91	TYR	CE1-CZ	-10.95	1.24	1.38
1	A	112	GLU	CD-OE2	10.85	1.37	1.25
1	A	123	ASN	C-N	10.83	1.58	1.34
1	A	242	THR	N-CA	10.81	1.68	1.46
1	A	59	GLN	N-CA	10.60	1.67	1.46
1	A	114	ALA	C-N	-10.42	1.10	1.34
1	A	183	SER	CB-OG	10.41	1.55	1.42
1	A	274	ALA	CA-CB	10.39	1.74	1.52
1	A	113	TRP	CD2-CE2	10.32	1.53	1.41
1	A	262	TYR	CD1-CE1	10.28	1.54	1.39
1	A	114	ALA	C-O	10.27	1.42	1.23
1	A	235	LEU	N-CA	10.26	1.66	1.46
1	A	262	TYR	CB-CG	10.24	1.67	1.51
1	A	59	GLN	CD-OE1	-10.15	1.01	1.24
1	A	190	SER	C-N	-10.06	1.10	1.34
1	A	217	TYR	CB-CG	10.06	1.66	1.51
1	A	52	PRO	N-CA	10.04	1.64	1.47
1	A	268	ILE	N-CA	10.04	1.66	1.46
1	A	259	ASP	N-CA	10.02	1.66	1.46
1	A	263	TYR	CD2-CE2	9.89	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ALA	C-N	9.85	1.50	1.33
1	A	229	GLY	C-O	-9.82	1.07	1.23
1	A	174	VAL	CB-CG2	9.81	1.73	1.52
1	A	248	SER	CA-CB	9.77	1.67	1.52
1	A	128	GLY	C-N	-9.69	1.15	1.34
1	A	26	VAL	CB-CG1	9.56	1.73	1.52
1	A	244	THR	N-CA	9.55	1.65	1.46
1	A	52	PRO	C-N	-9.53	1.12	1.34
1	A	145	SER	CB-OG	9.53	1.54	1.42
1	A	249	SER	CA-CB	9.49	1.67	1.52
1	A	73	ALA	C-N	-9.46	1.12	1.34
1	A	96	LEU	N-CA	-9.44	1.27	1.46
1	A	54	GLU	CD-OE2	-9.40	1.15	1.25
1	A	42	LEU	C-O	-9.39	1.05	1.23
1	A	233	LEU	CA-CB	9.38	1.75	1.53
1	A	264	GLY	N-CA	9.35	1.60	1.46
1	A	14	PRO	N-CD	-9.34	1.34	1.47
1	A	128	GLY	N-CA	9.26	1.59	1.46
1	A	214	TYR	CG-CD2	9.17	1.51	1.39
1	A	144	ALA	C-O	-9.12	1.06	1.23
1	A	243	ASN	CG-OD1	9.11	1.44	1.24
1	A	54	GLU	CA-CB	9.10	1.74	1.53
1	A	226	HIS	CE1-NE2	9.09	1.53	1.32
1	A	148	VAL	CB-CG1	9.07	1.72	1.52
1	A	83	GLY	C-O	9.01	1.38	1.23
1	A	113	TRP	CE3-CZ3	8.99	1.53	1.38
1	A	231	ALA	C-O	-8.93	1.06	1.23
1	A	3	SER	N-CA	8.83	1.64	1.46
1	A	149	VAL	N-CA	-8.81	1.28	1.46
1	A	202	GLY	N-CA	8.79	1.59	1.46
1	A	6	TYR	CD2-CE2	8.78	1.52	1.39
1	A	212	ASN	CB-CG	8.75	1.71	1.51
1	A	171	TYR	CG-CD2	8.73	1.50	1.39
1	A	142	ALA	N-CA	8.72	1.63	1.46
1	A	30	VAL	CA-C	8.70	1.75	1.52
1	A	87	SER	CA-CB	8.69	1.66	1.52
1	A	58	PHE	CG-CD2	8.68	1.51	1.38
1	A	241	TRP	C-N	-8.68	1.14	1.34
1	A	6	TYR	CZ-OH	8.65	1.52	1.37
1	A	57	ASN	C-O	-8.63	1.06	1.23
1	A	63	SER	N-CA	8.52	1.63	1.46
1	A	43	LYS	CA-CB	8.52	1.72	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	LEU	C-N	-8.51	1.18	1.34
1	A	172	PRO	N-CA	8.49	1.61	1.47
1	A	71	THR	C-N	-8.46	1.14	1.34
1	A	238	HIS	CG-CD2	8.42	1.50	1.35
1	A	43	LYS	C-O	-8.36	1.07	1.23
1	A	64	HIS	CA-CB	8.36	1.72	1.53
1	A	56	PRO	N-CA	-8.34	1.33	1.47
1	A	106	TRP	CD2-CE2	-8.33	1.31	1.41
1	A	210	PRO	CA-CB	8.33	1.70	1.53
1	A	54	GLU	CG-CD	-8.33	1.39	1.51
1	A	100	GLY	C-O	8.33	1.36	1.23
1	A	33	SER	N-CA	-8.28	1.29	1.46
1	A	112	GLU	C-N	-8.26	1.15	1.34
1	A	174	VAL	C-O	8.21	1.39	1.23
1	A	270	VAL	CB-CG2	8.17	1.70	1.52
1	A	79	ILE	C-N	-8.15	1.18	1.33
1	A	35	ILE	C-O	-8.14	1.07	1.23
1	A	60	ASP	CG-OD1	-8.12	1.06	1.25
1	A	258	GLY	C-O	-8.11	1.10	1.23
1	A	112	GLU	C-O	8.10	1.38	1.23
1	A	148	VAL	N-CA	-8.07	1.30	1.46
1	A	116	ALA	CA-CB	8.03	1.69	1.52
1	A	183	SER	CA-CB	-7.97	1.41	1.52
1	A	94	LYS	C-N	-7.97	1.15	1.34
1	A	148	VAL	C-O	-7.93	1.08	1.23
1	A	108	ILE	C-N	-7.91	1.15	1.34
1	A	125	SER	N-CA	7.88	1.62	1.46
1	A	195	GLU	CD-OE2	-7.88	1.17	1.25
1	A	241	TRP	CG-CD2	-7.88	1.30	1.43
1	A	102	GLY	CA-C	7.87	1.64	1.51
1	A	231	ALA	CA-C	7.86	1.73	1.52
1	A	150	VAL	CB-CG1	7.85	1.69	1.52
1	A	56	PRO	CA-C	7.83	1.68	1.52
1	A	38	SER	N-CA	-7.77	1.30	1.46
1	A	94	LYS	C-O	7.77	1.38	1.23
1	A	113	TRP	CD1-NE1	7.76	1.51	1.38
1	A	99	ALA	CA-CB	7.75	1.68	1.52
1	A	22	THR	CB-CG2	7.74	1.77	1.52
1	A	39	HIS	CG-CD2	-7.74	1.22	1.35
1	A	238	HIS	C-N	7.72	1.49	1.34
1	A	247	ARG	CZ-NH2	-7.66	1.23	1.33
1	A	74	ALA	CA-CB	7.65	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLY	CA-C	7.64	1.64	1.51
1	A	46	GLY	CA-C	-7.63	1.39	1.51
1	A	146	GLY	C-N	-7.63	1.16	1.34
1	A	206	GLN	C-O	7.62	1.37	1.23
1	A	43	LYS	CD-CE	7.61	1.70	1.51
1	A	234	ILE	CA-C	7.59	1.72	1.52
1	A	208	THR	CA-C	7.58	1.72	1.52
1	A	104	TYR	CA-C	7.58	1.72	1.52
1	A	260	SER	CA-CB	7.54	1.64	1.52
1	A	99	ALA	C-N	7.54	1.46	1.33
1	A	109	ASN	N-CA	7.52	1.61	1.46
1	A	95	VAL	C-O	7.51	1.37	1.23
1	A	112	GLU	CB-CG	7.48	1.66	1.52
1	A	58	PHE	CE1-CZ	7.48	1.51	1.37
1	A	249	SER	C-N	-7.46	1.16	1.34
1	A	211	GLY	C-N	-7.46	1.16	1.34
1	A	74	ALA	N-CA	7.45	1.61	1.46
1	A	19	GLN	C-O	-7.43	1.09	1.23
1	A	100	GLY	CA-C	-7.41	1.40	1.51
1	A	7	GLY	C-N	-7.41	1.17	1.34
1	A	89	ALA	CA-CB	7.32	1.67	1.52
1	A	217	TYR	CD2-CE2	-7.30	1.28	1.39
1	A	237	LYS	CE-NZ	7.29	1.67	1.49
1	A	202	GLY	CA-C	7.28	1.63	1.51
1	A	121	VAL	C-N	-7.27	1.17	1.34
1	A	48	ALA	C-O	7.27	1.37	1.23
1	A	252	ASN	N-CA	7.24	1.60	1.46
1	A	72	VAL	CA-C	7.24	1.71	1.52
1	A	86	PRO	N-CD	7.24	1.57	1.47
1	A	258	GLY	CA-C	7.22	1.63	1.51
1	A	164	THR	C-O	7.20	1.37	1.23
1	A	260	SER	CB-OG	7.19	1.51	1.42
1	A	123	ASN	CB-CG	7.19	1.67	1.51
1	A	55	THR	N-CA	7.16	1.60	1.46
1	A	144	ALA	CA-C	7.16	1.71	1.52
1	A	250	LEU	N-CA	7.13	1.60	1.46
1	A	253	THR	C-N	7.09	1.50	1.34
1	A	84	VAL	CB-CG2	-7.08	1.38	1.52
1	A	58	PHE	N-CA	7.07	1.60	1.46
1	A	217	TYR	CG-CD1	7.06	1.48	1.39
1	A	249	SER	CB-OG	-7.05	1.33	1.42
1	A	53	SER	CA-CB	7.04	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	ASN	C-O	7.04	1.36	1.23
1	A	123	ASN	N-CA	7.02	1.60	1.46
1	A	17	HIS	C-N	-6.99	1.18	1.34
1	A	178	GLY	CA-C	6.96	1.62	1.51
1	A	196	LEU	CG-CD2	6.95	1.77	1.51
1	A	54	GLU	CD-OE1	-6.94	1.18	1.25
1	A	113	TRP	C-O	-6.94	1.10	1.23
1	A	183	SER	N-CA	6.92	1.60	1.46
1	A	174	VAL	C-N	-6.92	1.18	1.34
1	A	71	THR	CA-CB	6.91	1.71	1.53
1	A	132	SER	C-O	6.90	1.36	1.23
1	A	111	ILE	CA-C	6.84	1.70	1.52
1	A	163	SER	CA-CB	6.82	1.63	1.52
1	A	261	PHE	CB-CG	6.81	1.62	1.51
1	A	136	LYS	CA-C	6.80	1.70	1.52
1	A	241	TRP	CD1-NE1	-6.76	1.26	1.38
1	A	112	GLU	CD-OE1	-6.75	1.18	1.25
1	A	154	GLY	C-O	-6.75	1.12	1.23
1	A	130	SER	CB-OG	-6.75	1.33	1.42
1	A	255	THR	C-O	6.73	1.36	1.23
1	A	99	ALA	C-O	-6.72	1.10	1.23
1	A	165	VAL	CB-CG1	6.70	1.67	1.52
1	A	59	GLN	C-O	-6.67	1.10	1.23
1	A	139	VAL	C-O	6.67	1.36	1.23
1	A	146	GLY	C-O	6.64	1.34	1.23
1	A	126	LEU	C-N	-6.63	1.21	1.33
1	A	177	VAL	CB-CG1	-6.62	1.39	1.52
1	A	93	VAL	CB-CG1	6.61	1.66	1.52
1	A	61	ASP	N-CA	6.60	1.59	1.46
1	A	267	LEU	C-O	-6.60	1.10	1.23
1	A	182	SER	N-CA	6.58	1.59	1.46
1	A	22	THR	CA-C	-6.57	1.35	1.52
1	A	230	ALA	N-CA	6.55	1.59	1.46
1	A	240	ASN	CB-CG	6.55	1.66	1.51
1	A	92	ALA	CA-CB	6.53	1.66	1.52
1	A	130	SER	C-N	6.52	1.44	1.33
1	A	113	TRP	CB-CG	-6.50	1.38	1.50
1	A	134	ALA	C-O	-6.49	1.11	1.23
1	A	107	ILE	N-CA	-6.48	1.33	1.46
1	A	19	GLN	CD-OE1	6.46	1.38	1.24
1	A	62	ASN	C-N	-6.45	1.19	1.34
1	A	194	PRO	CG-CD	6.45	1.72	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	TYR	CE2-CZ	6.43	1.47	1.38
1	A	61	ASP	C-N	6.42	1.48	1.34
1	A	15	ALA	CA-C	6.40	1.69	1.52
1	A	91	TYR	CG-CD1	6.38	1.47	1.39
1	A	180	VAL	CB-CG1	6.36	1.66	1.52
1	A	132	SER	N-CA	6.36	1.59	1.46
1	A	144	ALA	N-CA	6.35	1.59	1.46
1	A	1	ALA	C-N	-6.35	1.19	1.34
1	A	131	GLY	C-O	6.34	1.33	1.23
1	A	209	LEU	C-O	6.33	1.35	1.23
1	A	36	ASP	N-CA	6.32	1.58	1.46
1	A	147	VAL	C-N	6.32	1.48	1.34
1	A	175	ILE	CB-CG1	6.31	1.71	1.54
1	A	265	LYS	N-CA	-6.30	1.33	1.46
1	A	210	PRO	N-CD	6.30	1.56	1.47
1	A	40	PRO	N-CD	6.30	1.56	1.47
1	A	241	TRP	NE1-CE2	6.30	1.45	1.37
1	A	5	PRO	C-N	6.29	1.48	1.34
1	A	156	GLU	CD-OE2	6.28	1.32	1.25
1	A	213	LYS	CA-C	-6.28	1.36	1.52
1	A	64	HIS	C-N	-6.26	1.21	1.33
1	A	23	GLY	C-O	-6.26	1.13	1.23
1	A	220	THR	C-O	-6.26	1.11	1.23
1	A	185	GLN	C-O	-6.25	1.11	1.23
1	A	217	TYR	C-N	-6.24	1.19	1.34
1	A	208	THR	C-N	6.23	1.48	1.34
1	A	197	ASP	CA-CB	6.22	1.67	1.53
1	A	49	SER	CA-CB	-6.21	1.43	1.52
1	A	82	LEU	CA-CB	6.20	1.68	1.53
1	A	99	ALA	N-CA	-6.20	1.33	1.46
1	A	221	SER	C-N	-6.19	1.19	1.34
1	A	214	TYR	CG-CD1	6.19	1.47	1.39
1	A	175	ILE	C-N	-6.18	1.19	1.34
1	A	140	ASP	CA-C	6.17	1.69	1.52
1	A	175	ILE	CA-CB	6.17	1.69	1.54
1	A	227	VAL	CB-CG1	6.16	1.65	1.52
1	A	41	ASP	CB-CG	6.15	1.64	1.51
1	A	120	ASP	N-CA	6.12	1.58	1.46
1	A	206	GLN	CB-CG	6.12	1.69	1.52
1	A	126	LEU	C-O	-6.11	1.11	1.23
1	A	151	ALA	C-N	-6.10	1.20	1.34
1	A	197	ASP	CB-CG	6.10	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	GLN	C-O	-6.09	1.11	1.23
1	A	270	VAL	CB-CG1	-6.06	1.40	1.52
1	A	217	TYR	CE2-CZ	6.06	1.46	1.38
1	A	139	VAL	N-CA	-6.04	1.34	1.46
1	A	115	ILE	C-O	6.02	1.34	1.23
1	A	184	ASN	N-CA	-6.01	1.34	1.46
1	A	227	VAL	CA-C	5.99	1.68	1.52
1	A	185	GLN	C-N	-5.99	1.20	1.34
1	A	139	VAL	C-N	-5.97	1.20	1.34
1	A	268	ILE	C-N	-5.96	1.20	1.34
1	A	58	PHE	CB-CG	-5.95	1.41	1.51
1	A	219	GLY	C-O	5.92	1.33	1.23
1	A	65	GLY	CA-C	5.92	1.61	1.51
1	A	186	ARG	N-CA	5.92	1.58	1.46
1	A	263	TYR	C-O	5.90	1.34	1.23
1	A	246	VAL	CB-CG2	5.88	1.65	1.52
1	A	76	ASN	N-CA	-5.88	1.34	1.46
1	A	113	TRP	N-CA	-5.88	1.34	1.46
1	A	184	ASN	CG-OD1	5.88	1.36	1.24
1	A	117	ASN	N-CA	5.88	1.58	1.46
1	A	221	SER	C-O	5.88	1.34	1.23
1	A	189	PHE	CB-CG	5.85	1.61	1.51
1	A	186	ARG	CD-NE	-5.85	1.36	1.46
1	A	40	PRO	N-CA	5.84	1.57	1.47
1	A	56	PRO	C-O	-5.84	1.11	1.23
1	A	241	TRP	CD2-CE2	5.84	1.48	1.41
1	A	103	GLN	CG-CD	5.81	1.64	1.51
1	A	10	GLN	CG-CD	5.81	1.64	1.51
1	A	209	LEU	CA-C	5.81	1.68	1.52
1	A	113	TRP	CA-C	5.80	1.68	1.52
1	A	5	PRO	CG-CD	5.79	1.69	1.50
1	A	25	ASN	CA-CB	-5.78	1.38	1.53
1	A	261	PHE	CE1-CZ	5.77	1.48	1.37
1	A	183	SER	CA-C	5.76	1.68	1.52
1	A	223	ALA	C-N	-5.76	1.20	1.34
1	A	136	LYS	N-CA	-5.75	1.34	1.46
1	A	251	GLN	CA-C	5.75	1.68	1.52
1	A	251	GLN	C-N	-5.74	1.20	1.34
1	A	228	ALA	CA-C	5.73	1.67	1.52
1	A	98	ASP	CG-OD2	5.73	1.38	1.25
1	A	53	SER	N-CA	5.72	1.57	1.46
1	A	143	VAL	CB-CG2	5.72	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	TYR	C-N	-5.71	1.21	1.34
1	A	66	THR	CB-OG1	-5.67	1.31	1.43
1	A	106	TRP	N-CA	5.67	1.57	1.46
1	A	98	ASP	C-N	-5.67	1.21	1.34
1	A	109	ASN	C-O	-5.67	1.12	1.23
1	A	252	ASN	CG-OD1	5.66	1.36	1.24
1	A	265	LYS	C-N	5.65	1.43	1.33
1	A	21	TYR	CE1-CZ	5.65	1.45	1.38
1	A	133	ALA	C-N	5.64	1.47	1.34
1	A	6	TYR	CD1-CE1	5.64	1.47	1.39
1	A	114	ALA	CA-C	5.63	1.67	1.52
1	A	2	GLN	C-O	5.63	1.34	1.23
1	A	140	ASP	CB-CG	5.63	1.63	1.51
1	A	247	ARG	CA-C	5.63	1.67	1.52
1	A	30	VAL	CA-CB	-5.61	1.43	1.54
1	A	229	GLY	CA-C	5.61	1.60	1.51
1	A	239	PRO	CA-C	5.61	1.64	1.52
1	A	266	GLY	CA-C	5.61	1.60	1.51
1	A	240	ASN	CG-ND2	-5.61	1.18	1.32
1	A	128	GLY	CA-C	5.60	1.60	1.51
1	A	189	PHE	CD1-CE1	5.60	1.50	1.39
1	A	59	GLN	CG-CD	5.59	1.64	1.51
1	A	24	SER	CA-CB	5.59	1.61	1.52
1	A	179	ALA	C-O	5.59	1.33	1.23
1	A	23	GLY	N-CA	5.59	1.54	1.46
1	A	136	LYS	CG-CD	5.58	1.71	1.52
1	A	218	ASN	C-N	5.58	1.43	1.33
1	A	76	ASN	CA-C	5.57	1.67	1.52
1	A	239	PRO	C-O	5.57	1.34	1.23
1	A	86	PRO	CG-CD	5.57	1.69	1.50
1	A	254	THR	N-CA	5.57	1.57	1.46
1	A	261	PHE	CG-CD2	5.54	1.47	1.38
1	A	141	LYS	C-O	-5.54	1.12	1.23
1	A	190	SER	C-O	5.53	1.33	1.23
1	A	6	TYR	CG-CD1	-5.51	1.31	1.39
1	A	35	ILE	C-N	5.51	1.46	1.34
1	A	30	VAL	CB-CG2	5.51	1.64	1.52
1	A	176	ALA	C-O	5.50	1.33	1.23
1	A	240	ASN	CG-OD1	-5.50	1.11	1.24
1	A	177	VAL	N-CA	-5.50	1.35	1.46
1	A	263	TYR	C-N	-5.49	1.23	1.33
1	A	118	ASN	N-CA	5.49	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	ILE	CA-CB	-5.48	1.42	1.54
1	A	247	ARG	CG-CD	-5.47	1.38	1.51
1	A	3	SER	CA-CB	5.46	1.61	1.52
1	A	141	LYS	CA-C	5.44	1.67	1.52
1	A	87	SER	CA-C	-5.43	1.38	1.52
1	A	237	LYS	CA-C	5.43	1.67	1.52
1	A	9	SER	CA-C	5.43	1.67	1.52
1	A	202	GLY	C-N	-5.43	1.21	1.34
1	A	262	TYR	CG-CD1	-5.43	1.32	1.39
1	A	224	SER	C-O	5.41	1.33	1.23
1	A	257	LEU	C-N	5.41	1.42	1.33
1	A	60	ASP	CA-CB	5.40	1.65	1.53
1	A	74	ALA	C-O	-5.40	1.13	1.23
1	A	120	ASP	CA-CB	5.40	1.65	1.53
1	A	95	VAL	CB-CG2	-5.39	1.41	1.52
1	A	119	MET	CG-SD	5.39	1.95	1.81
1	A	77	ASN	C-O	-5.39	1.13	1.23
1	A	201	PRO	C-O	-5.39	1.12	1.23
1	A	60	ASP	CG-OD2	5.37	1.37	1.25
1	A	19	GLN	CA-CB	5.37	1.65	1.53
1	A	167	TYR	CG-CD1	5.37	1.46	1.39
1	A	221	SER	CB-OG	-5.36	1.35	1.42
1	A	119	MET	C-O	5.35	1.33	1.23
1	A	143	VAL	CA-C	5.35	1.66	1.52
1	A	235	LEU	C-N	-5.34	1.21	1.34
1	A	256	LYS	C-N	5.34	1.46	1.34
1	A	135	LEU	CG-CD2	5.33	1.71	1.51
1	A	67	HIS	CB-CG	-5.32	1.40	1.50
1	A	262	TYR	CE2-CZ	5.29	1.45	1.38
1	A	21	TYR	CZ-OH	5.28	1.46	1.37
1	A	96	LEU	CG-CD2	5.28	1.71	1.51
1	A	174	VAL	CA-C	5.26	1.66	1.52
1	A	19	GLN	CB-CG	-5.26	1.38	1.52
1	A	171	TYR	CA-CB	-5.26	1.42	1.53
1	A	238	HIS	CE1-NE2	5.24	1.44	1.32
1	A	58	PHE	C-N	-5.23	1.22	1.34
1	A	59	GLN	CD-NE2	-5.22	1.19	1.32
1	A	210	PRO	C-N	5.21	1.42	1.33
1	A	251	GLN	CG-CD	5.21	1.63	1.51
1	A	106	TRP	CZ3-CH2	-5.20	1.31	1.40
1	A	105	SER	C-N	-5.20	1.22	1.34
1	A	244	THR	C-N	-5.19	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	TRP	CZ3-CH2	5.19	1.48	1.40
1	A	167	TYR	CD2-CE2	-5.19	1.31	1.39
1	A	149	VAL	CA-CB	5.19	1.65	1.54
1	A	161	SER	C-N	5.19	1.46	1.34
1	A	208	THR	C-O	-5.17	1.13	1.23
1	A	34	GLY	CA-C	5.16	1.60	1.51
1	A	266	GLY	C-N	-5.16	1.22	1.34
1	A	226	HIS	C-N	-5.16	1.22	1.34
1	A	76	ASN	CB-CG	5.15	1.62	1.51
1	A	148	VAL	C-N	5.14	1.45	1.34
1	A	129	PRO	N-CA	5.14	1.55	1.47
1	A	273	ALA	C-N	-5.14	1.22	1.34
1	A	180	VAL	CA-CB	-5.13	1.44	1.54
1	A	245	GLN	CG-CD	5.11	1.62	1.51
1	A	103	GLN	CA-C	-5.11	1.39	1.52
1	A	105	SER	CB-OG	-5.10	1.35	1.42
1	A	228	ALA	CA-CB	5.10	1.63	1.52
1	A	200	ALA	N-CA	5.08	1.56	1.46
1	A	191	SER	CB-OG	-5.08	1.35	1.42
1	A	61	ASP	CG-OD1	-5.07	1.13	1.25
1	A	239	PRO	CG-CD	5.06	1.67	1.50
1	A	10	GLN	N-CA	5.03	1.56	1.46
1	A	167	TYR	CD1-CE1	-5.01	1.31	1.39
1	A	91	TYR	C-N	-5.01	1.22	1.34
1	A	235	LEU	CG-CD2	-5.01	1.33	1.51
1	A	103	GLN	N-CA	5.00	1.56	1.46
1	A	140	ASP	N-CA	5.00	1.56	1.46

All (285) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	NE-CZ-NH1	26.75	133.68	120.30
1	A	214	TYR	CG-CD2-CE2	20.16	137.43	121.30
1	A	247	ARG	NE-CZ-NH1	-18.20	111.20	120.30
1	A	52	PRO	O-C-N	16.05	148.39	122.70
1	A	186	ARG	NE-CZ-NH2	-15.68	112.46	120.30
1	A	217	TYR	CB-CG-CD1	-15.17	111.89	121.00
1	A	60	ASP	CB-CG-OD1	15.16	131.94	118.30
1	A	241	TRP	CH2-CZ2-CE2	14.34	131.74	117.40
1	A	34	GLY	CA-C-O	13.88	145.58	120.60
1	A	101	SER	O-C-N	-13.85	99.66	123.20
1	A	92	ALA	CB-CA-C	-13.25	90.23	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	VAL	CG1-CB-CG2	-13.18	89.82	110.90
1	A	262	TYR	CB-CG-CD1	-13.05	113.17	121.00
1	A	56	PRO	N-CA-CB	12.92	118.81	103.30
1	A	34	GLY	O-C-N	-12.87	102.12	122.70
1	A	214	TYR	CB-CG-CD1	12.86	128.72	121.00
1	A	49	SER	CB-CA-C	12.46	133.77	110.10
1	A	21	TYR	CB-CG-CD1	12.20	128.32	121.00
1	A	60	ASP	N-CA-CB	-12.09	88.85	110.60
1	A	144	ALA	O-C-N	11.99	141.88	122.70
1	A	5	PRO	N-CA-CB	11.68	117.31	103.30
1	A	111	ILE	O-C-N	11.65	141.35	122.70
1	A	274	ALA	N-CA-CB	11.62	126.37	110.10
1	A	36	ASP	CB-CG-OD1	11.59	128.73	118.30
1	A	120	ASP	CB-CG-OD2	11.59	128.73	118.30
1	A	59	GLN	C-N-CA	-11.57	92.78	121.70
1	A	97	GLY	O-C-N	-11.49	104.31	122.70
1	A	49	SER	N-CA-CB	-11.49	93.26	110.50
1	A	113	TRP	CE2-CD2-CG	11.25	116.30	107.30
1	A	104	TYR	CD1-CE1-CZ	11.09	129.78	119.80
1	A	167	TYR	CZ-CE2-CD2	11.05	129.75	119.80
1	A	69	ALA	O-C-N	-10.92	104.63	123.20
1	A	89	ALA	O-C-N	-10.85	105.34	122.70
1	A	91	TYR	CB-CG-CD1	-10.58	114.65	121.00
1	A	167	TYR	CB-CG-CD1	10.47	127.28	121.00
1	A	35	ILE	CA-C-O	10.47	142.09	120.10
1	A	214	TYR	CD1-CE1-CZ	10.43	129.19	119.80
1	A	59	GLN	CA-C-O	10.25	141.62	120.10
1	A	95	VAL	CA-CB-CG2	10.23	126.24	110.90
1	A	106	TRP	CE2-CD2-CG	10.06	115.35	107.30
1	A	106	TRP	CD1-NE1-CE2	-9.96	100.03	109.00
1	A	92	ALA	N-CA-CB	-9.83	96.33	110.10
1	A	52	PRO	C-N-CA	-9.78	97.26	121.70
1	A	6	TYR	CZ-CE2-CD2	-9.66	111.10	119.80
1	A	195	GLU	N-CA-CB	-9.65	93.22	110.60
1	A	208	THR	CA-C-N	-9.59	96.09	117.20
1	A	91	TYR	CZ-CE2-CD2	-9.57	111.19	119.80
1	A	232	ALA	O-C-N	9.57	138.01	122.70
1	A	263	TYR	CB-CG-CD1	-9.43	115.34	121.00
1	A	69	ALA	C-N-CA	9.12	141.46	122.30
1	A	247	ARG	CD-NE-CZ	-9.08	110.89	123.60
1	A	101	SER	CA-C-O	8.96	138.92	120.10
1	A	82	LEU	CA-CB-CG	-8.90	94.82	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	THR	O-C-N	-8.78	108.65	122.70
1	A	106	TRP	O-C-N	-8.71	108.77	122.70
1	A	29	ALA	O-C-N	8.69	136.60	122.70
1	A	190	SER	C-N-CA	8.65	143.32	121.70
1	A	103	GLN	CB-CA-C	8.63	127.65	110.40
1	A	58	PHE	CB-CG-CD2	-8.50	114.85	120.80
1	A	58	PHE	O-C-N	8.47	136.26	122.70
1	A	243	ASN	CA-C-N	-8.46	98.59	117.20
1	A	123	ASN	CA-C-O	8.40	137.74	120.10
1	A	241	TRP	CZ3-CH2-CZ2	-8.40	111.52	121.60
1	A	214	TYR	CD1-CG-CD2	-8.35	108.71	117.90
1	A	263	TYR	N-CA-CB	8.34	125.61	110.60
1	A	214	TYR	N-CA-CB	-8.30	95.66	110.60
1	A	99	ALA	CA-C-O	8.29	137.52	120.10
1	A	54	GLU	O-C-N	8.27	135.93	122.70
1	A	217	TYR	CB-CG-CD2	8.24	125.95	121.00
1	A	9	SER	N-CA-CB	8.24	122.86	110.50
1	A	250	LEU	CB-CG-CD1	-8.16	97.12	111.00
1	A	144	ALA	CA-C-N	-8.13	99.31	117.20
1	A	113	TRP	NE1-CE2-CD2	-8.10	99.20	107.30
1	A	270	VAL	CA-C-O	8.09	137.09	120.10
1	A	144	ALA	C-N-CA	-8.07	101.53	121.70
1	A	143	VAL	CA-CB-CG2	-8.03	98.86	110.90
1	A	123	ASN	O-C-N	-8.01	109.88	122.70
1	A	79	ILE	CA-C-N	7.97	132.14	116.20
1	A	214	TYR	CZ-CE2-CD2	-7.96	112.63	119.80
1	A	66	THR	CA-C-O	7.95	136.79	120.10
1	A	217	TYR	C-N-CA	7.82	141.25	121.70
1	A	5	PRO	O-C-N	-7.80	110.22	122.70
1	A	106	TRP	CG-CD2-CE3	-7.75	126.93	133.90
1	A	167	TYR	CG-CD2-CE2	-7.74	115.11	121.30
1	A	192	VAL	CA-C-N	7.67	131.54	116.20
1	A	190	SER	O-C-N	-7.63	110.49	122.70
1	A	270	VAL	CA-CB-CG2	-7.60	99.50	110.90
1	A	59	GLN	CA-C-N	-7.58	100.52	117.20
1	A	217	TYR	CG-CD1-CE1	-7.56	115.25	121.30
1	A	232	ALA	CA-C-N	-7.55	100.59	117.20
1	A	82	LEU	C-N-CA	-7.54	106.46	122.30
1	A	196	LEU	CA-CB-CG	-7.51	98.02	115.30
1	A	106	TRP	CA-CB-CG	-7.50	99.44	113.70
1	A	229	GLY	CA-C-N	-7.49	100.72	117.20
1	A	230	ALA	CB-CA-C	7.39	121.19	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASN	OD1-CG-ND2	7.38	138.87	121.90
1	A	91	TYR	CB-CG-CD2	7.37	125.42	121.00
1	A	120	ASP	OD1-CG-OD2	-7.37	109.30	123.30
1	A	113	TRP	CG-CD1-NE1	-7.36	102.74	110.10
1	A	257	LEU	N-CA-C	-7.33	91.22	111.00
1	A	21	TYR	CD1-CG-CD2	-7.27	109.90	117.90
1	A	172	PRO	N-CD-CG	7.24	114.06	103.20
1	A	148	VAL	CA-CB-CG1	7.24	121.75	110.90
1	A	106	TRP	CG-CD1-NE1	7.21	117.31	110.10
1	A	263	TYR	CG-CD2-CE2	-7.19	115.55	121.30
1	A	99	ALA	O-C-N	-7.18	110.99	123.20
1	A	39	HIS	ND1-CG-CD2	7.17	118.84	108.80
1	A	108	ILE	O-C-N	7.17	134.16	122.70
1	A	6	TYR	CB-CG-CD1	-7.16	116.70	121.00
1	A	167	TYR	CB-CG-CD2	-7.16	116.70	121.00
1	A	104	TYR	CE1-CZ-CE2	-7.15	108.36	119.80
1	A	68	VAL	CA-CB-CG1	-7.13	100.21	110.90
1	A	129	PRO	CA-N-CD	-7.12	101.53	111.50
1	A	87	SER	CA-C-O	7.10	135.00	120.10
1	A	227	VAL	CA-C-N	-7.07	101.64	117.20
1	A	113	TRP	CE2-CD2-CE3	-7.04	110.25	118.70
1	A	138	ALA	CB-CA-C	-7.03	99.56	110.10
1	A	189	PHE	CG-CD2-CE2	-6.98	113.12	120.80
1	A	243	ASN	O-C-N	6.97	133.86	122.70
1	A	6	TYR	N-CA-CB	-6.95	98.09	110.60
1	A	97	GLY	CA-C-O	6.94	133.09	120.60
1	A	201	PRO	O-C-N	6.87	134.88	123.20
1	A	213	LYS	CA-C-N	6.85	132.28	117.20
1	A	60	ASP	OD1-CG-OD2	-6.83	110.33	123.30
1	A	175	ILE	CA-CB-CG1	-6.83	98.03	111.00
1	A	227	VAL	O-C-N	6.81	133.59	122.70
1	A	125	SER	N-CA-CB	-6.80	100.30	110.50
1	A	235	LEU	CA-C-N	6.78	132.11	117.20
1	A	36	ASP	N-CA-CB	-6.76	98.42	110.60
1	A	254	THR	CA-CB-CG2	-6.76	102.94	112.40
1	A	113	TRP	CD1-CG-CD2	6.67	111.63	106.30
1	A	235	LEU	N-CA-CB	-6.64	97.11	110.40
1	A	79	ILE	O-C-N	-6.62	111.95	123.20
1	A	149	VAL	CA-C-N	-6.60	102.68	117.20
1	A	68	VAL	O-C-N	6.60	133.26	122.70
1	A	58	PHE	CD1-CE1-CZ	-6.59	112.19	120.10
1	A	275	GLN	OE1-CD-NE2	-6.59	106.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	THR	O-C-N	6.58	133.22	122.70
1	A	190	SER	CA-C-N	6.56	131.64	117.20
1	A	275	GLN	CG-CD-OE1	6.56	134.73	121.60
1	A	263	TYR	CD1-CG-CD2	6.49	125.04	117.90
1	A	89	ALA	N-CA-CB	-6.45	101.07	110.10
1	A	93	VAL	CG1-CB-CG2	-6.45	100.58	110.90
1	A	21	TYR	CG-CD1-CE1	6.43	126.45	121.30
1	A	87	SER	O-C-N	-6.40	112.46	122.70
1	A	210	PRO	CA-N-CD	-6.36	102.59	111.50
1	A	118	ASN	N-CA-CB	-6.36	99.16	110.60
1	A	233	LEU	CB-CG-CD2	-6.35	100.21	111.00
1	A	64	HIS	ND1-CG-CD2	-6.33	97.13	106.00
1	A	79	ILE	C-N-CA	6.33	135.60	122.30
1	A	58	PHE	CB-CG-CD1	6.32	125.22	120.80
1	A	113	TRP	CA-C-N	-6.32	103.30	117.20
1	A	115	ILE	CB-CG1-CD1	-6.30	96.25	113.90
1	A	195	GLU	O-C-N	-6.28	112.66	122.70
1	A	35	ILE	O-C-N	-6.27	112.67	122.70
1	A	189	PHE	CB-CG-CD2	-6.27	116.41	120.80
1	A	201	PRO	CA-C-N	-6.26	103.68	116.20
1	A	216	ALA	O-C-N	-6.26	112.68	122.70
1	A	31	ILE	CB-CG1-CD1	-6.26	96.38	113.90
1	A	29	ALA	CA-C-N	-6.24	103.47	117.20
1	A	164	THR	CA-CB-CG2	-6.23	103.67	112.40
1	A	210	PRO	N-CA-CB	6.22	110.77	103.30
1	A	52	PRO	CA-C-O	-6.22	105.28	120.20
1	A	159	THR	CA-CB-CG2	-6.22	103.70	112.40
1	A	145	SER	N-CA-CB	-6.20	101.20	110.50
1	A	148	VAL	O-C-N	-6.16	112.85	122.70
1	A	208	THR	CB-CA-C	-6.15	94.99	111.60
1	A	94	LYS	N-CA-CB	-6.15	99.53	110.60
1	A	192	VAL	O-C-N	-6.12	112.79	123.20
1	A	116	ALA	N-CA-CB	-6.11	101.55	110.10
1	A	253	THR	C-N-CA	-6.08	106.50	121.70
1	A	212	ASN	C-N-CA	6.07	136.88	121.70
1	A	113	TRP	CE3-CZ3-CH2	-6.06	114.54	121.20
1	A	108	ILE	CA-C-O	-6.05	107.40	120.10
1	A	255	THR	CA-CB-CG2	-6.05	103.94	112.40
1	A	195	GLU	CB-CA-C	6.02	122.44	110.40
1	A	6	TYR	OH-CZ-CE2	-6.02	103.86	120.10
1	A	209	LEU	CB-CA-C	-5.99	98.83	110.20
1	A	197	ASP	O-C-N	5.98	132.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	LYS	CB-CA-C	-5.97	98.47	110.40
1	A	52	PRO	N-CD-CG	5.96	112.14	103.20
1	A	149	VAL	O-C-N	5.95	132.22	122.70
1	A	228	ALA	N-CA-CB	-5.94	101.79	110.10
1	A	270	VAL	CB-CA-C	-5.93	100.13	111.40
1	A	154	GLY	N-CA-C	-5.92	98.29	113.10
1	A	36	ASP	OD1-CG-OD2	-5.92	112.06	123.30
1	A	165	VAL	CA-C-N	-5.92	104.37	116.20
1	A	267	LEU	CA-C-N	-5.92	104.19	117.20
1	A	17	HIS	CG-ND1-CE1	5.91	116.48	108.20
1	A	30	VAL	O-C-N	5.90	132.14	122.70
1	A	247	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	A	71	THR	CA-CB-CG2	-5.90	104.14	112.40
1	A	107	ILE	CA-CB-CG2	-5.87	99.17	110.90
1	A	241	TRP	NE1-CE2-CZ2	5.86	136.85	130.40
1	A	15	ALA	N-CA-CB	5.86	118.30	110.10
1	A	227	VAL	CG1-CB-CG2	-5.84	101.55	110.90
1	A	7	GLY	O-C-N	5.84	132.04	122.70
1	A	15	ALA	CA-C-O	5.83	132.35	120.10
1	A	210	PRO	O-C-N	-5.83	113.29	123.20
1	A	270	VAL	CA-C-N	-5.82	104.41	117.20
1	A	114	ALA	CB-CA-C	5.76	118.73	110.10
1	A	175	ILE	CB-CG1-CD1	-5.75	97.79	113.90
1	A	164	THR	O-C-N	-5.75	113.50	122.70
1	A	118	ASN	CB-CG-ND2	-5.74	102.92	116.70
1	A	214	TYR	CA-CB-CG	-5.74	102.50	113.40
1	A	52	PRO	CA-C-N	-5.73	104.59	117.20
1	A	12	LYS	N-CA-C	-5.73	95.54	111.00
1	A	236	SER	O-C-N	-5.72	113.54	122.70
1	A	235	LEU	CA-C-O	-5.72	108.09	120.10
1	A	90	LEU	N-CA-CB	-5.70	99.00	110.40
1	A	117	ASN	CA-CB-CG	-5.68	100.89	113.40
1	A	229	GLY	O-C-N	5.68	131.80	122.70
1	A	58	PHE	CA-C-N	-5.68	104.70	117.20
1	A	212	ASN	CA-CB-CG	-5.68	100.91	113.40
1	A	137	ALA	N-CA-CB	-5.67	102.17	110.10
1	A	241	TRP	N-CA-C	-5.66	95.71	111.00
1	A	129	PRO	N-CD-CG	5.66	111.69	103.20
1	A	214	TYR	CE1-CZ-CE2	-5.65	110.76	119.80
1	A	183	SER	O-C-N	5.64	131.73	122.70
1	A	262	TYR	C-N-CA	5.63	135.76	121.70
1	A	138	ALA	O-C-N	-5.61	113.73	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	TYR	CD1-CE1-CZ	-5.60	114.76	119.80
1	A	260	SER	N-CA-CB	-5.59	102.11	110.50
1	A	166	GLY	O-C-N	5.57	131.61	122.70
1	A	268	ILE	CG1-CB-CG2	-5.57	99.15	111.40
1	A	57	ASN	N-CA-C	-5.56	95.98	111.00
1	A	263	TYR	CA-CB-CG	-5.55	102.85	113.40
1	A	89	ALA	CA-C-O	5.54	131.74	120.10
1	A	211	GLY	CA-C-O	-5.54	110.62	120.60
1	A	115	ILE	CB-CA-C	-5.52	100.57	111.60
1	A	171	TYR	CA-C-N	-5.51	101.66	117.10
1	A	217	TYR	CB-CA-C	5.50	121.41	110.40
1	A	3	SER	CA-C-N	-5.50	105.10	117.20
1	A	142	ALA	N-CA-C	-5.49	96.18	111.00
1	A	235	LEU	CB-CA-C	5.47	120.60	110.20
1	A	242	THR	CA-C-N	-5.47	105.17	117.20
1	A	259	ASP	N-CA-CB	-5.46	100.76	110.60
1	A	55	THR	CA-C-O	-5.46	108.64	120.10
1	A	68	VAL	N-CA-CB	-5.46	99.50	111.50
1	A	35	ILE	CA-C-N	-5.45	105.20	117.20
1	A	21	TYR	CZ-CE2-CD2	5.45	124.70	119.80
1	A	143	VAL	CG1-CB-CG2	-5.44	102.19	110.90
1	A	11	ILE	C-N-CA	5.44	135.30	121.70
1	A	171	TYR	CG-CD1-CE1	5.40	125.62	121.30
1	A	171	TYR	N-CA-C	-5.39	96.44	111.00
1	A	56	PRO	CA-C-O	5.39	133.13	120.20
1	A	192	VAL	C-N-CA	5.38	133.60	122.30
1	A	39	HIS	CA-CB-CG	-5.38	104.46	113.60
1	A	227	VAL	C-N-CA	-5.35	108.33	121.70
1	A	38	SER	CA-C-N	-5.34	105.44	117.20
1	A	186	ARG	NH1-CZ-NH2	-5.34	113.53	119.40
1	A	41	ASP	O-C-N	-5.32	114.18	122.70
1	A	95	VAL	CA-CB-CG1	5.31	118.86	110.90
1	A	150	VAL	CA-CB-CG2	5.31	118.86	110.90
1	A	206	GLN	CA-CB-CG	-5.31	101.72	113.40
1	A	112	GLU	C-N-CA	5.30	134.94	121.70
1	A	45	ALA	C-N-CA	5.28	133.40	122.30
1	A	156	GLU	CG-CD-OE1	5.28	128.87	118.30
1	A	16	LEU	CA-CB-CG	-5.27	103.18	115.30
1	A	148	VAL	CA-C-O	5.26	131.14	120.10
1	A	45	ALA	N-CA-CB	-5.26	102.74	110.10
1	A	250	LEU	N-CA-CB	-5.25	99.90	110.40
1	A	112	GLU	N-CA-C	-5.25	96.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	HIS	CG-CD2-NE2	5.23	119.14	109.20
1	A	111	ILE	C-N-CA	-5.22	108.65	121.70
1	A	123	ASN	OD1-CG-ND2	5.22	133.90	121.90
1	A	135	LEU	CB-CG-CD1	5.21	119.86	111.00
1	A	247	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	A	104	TYR	CZ-CE2-CD2	5.21	124.49	119.80
1	A	154	GLY	CA-C-N	-5.21	105.74	117.20
1	A	189	PHE	CD1-CG-CD2	5.21	125.07	118.30
1	A	83	GLY	C-N-CA	5.20	134.71	121.70
1	A	104	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	A	195	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	A	249	SER	O-C-N	5.13	130.91	122.70
1	A	2	GLN	O-C-N	5.11	130.88	122.70
1	A	134	ALA	O-C-N	-5.11	114.53	122.70
1	A	222	MET	CA-CB-CG	-5.10	104.64	113.30
1	A	256	LYS	CA-C-N	-5.10	105.98	117.20
1	A	171	TYR	CA-C-O	5.09	130.79	120.10
1	A	113	TRP	NE1-CE2-CZ2	5.07	135.98	130.40
1	A	111	ILE	CA-C-N	-5.06	106.07	117.20
1	A	201	PRO	C-N-CA	-5.06	111.68	122.30
1	A	252	ASN	CB-CA-C	5.03	120.47	110.40
1	A	218	ASN	N-CA-CB	5.01	119.61	110.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLY	Mainchain
1	A	116	ALA	Mainchain
1	A	117	ASN	Mainchain
1	A	123	ASN	Sidechain
1	A	125	SER	Mainchain
1	A	140	ASP	Sidechain
1	A	173	SER	Mainchain
1	A	176	ALA	Mainchain
1	A	208	THR	Mainchain
1	A	21	TYR	Sidechain
1	A	230	ALA	Mainchain
1	A	243	ASN	Sidechain
1	A	40	PRO	Mainchain
1	A	5	PRO	Mainchain
1	A	6	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	61	ASP	Mainchain
1	A	79	ILE	Mainchain
1	A	89	ALA	Mainchain
1	A	94	LYS	Mainchain
1	A	98	ASP	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1934	0	1853	626	141
2	A	4	0	6	7	0
3	A	10	0	0	8	0
All	All	1948	0	1859	626	141

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 165.

All (626) 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:175:ILE:CG1	1:A:175:ILE:CD1	1.76	1.62
1:A:22:THR:CG2	1:A:22:THR:CB	1.77	1.62
1:A:233:LEU:CA	1:A:233:LEU:CB	1.75	1.55
1:A:196:LEU:CG	1:A:196:LEU:CD2	1.77	1.55
1:A:242:THR:CA	1:A:242:THR:N	1.68	1.54
1:A:145:SER:N	1:A:145:SER:CA	1.71	1.54
1:A:257:LEU:HB3	1:A:263:TYR:CD1	1.44	1.53
1:A:30:VAL:CA	1:A:30:VAL:C	1.75	1.53
1:A:59:GLN:N	1:A:59:GLN:CA	1.67	1.53
1:A:59:GLN:C	1:A:60:ASP:N	1.72	1.42
1:A:195:GLU:C	1:A:196:LEU:N	1.74	1.41
1:A:234:ILE:HG12	1:A:274:ALA:CB	1.50	1.40
1:A:8:VAL:O	1:A:10:GLN:N	1.58	1.35
1:A:202:GLY:O	1:A:203:VAL:HG23	1.18	1.35
1:A:113:TRP:O	1:A:117:ASN:HB2	1.28	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD12	1:A:19:GLN:OE1	1.17	1.34
1:A:208:THR:HG22	1:A:214:TYR:CE1	1.62	1.32
1:A:56:PRO:O	1:A:57:ASN:ND2	1.67	1.27
1:A:173:SER:C	1:A:174:VAL:CA	2.03	1.25
1:A:249:SER:O	1:A:273:ALA:HB1	1.32	1.25
1:A:34:GLY:C	1:A:35:ILE:N	1.89	1.24
1:A:39:HIS:CE1	1:A:208:THR:HB	1.69	1.24
1:A:73:ALA:O	2:A:276:ACN:H21	1.36	1.23
1:A:173:SER:O	1:A:174:VAL:N	1.66	1.23
1:A:257:LEU:CB	1:A:263:TYR:CD1	2.20	1.23
1:A:12:LYS:O	1:A:270:VAL:HB	1.07	1.23
1:A:173:SER:CA	1:A:174:VAL:N	2.01	1.22
1:A:104:TYR:O	1:A:108:ILE:HG23	1.36	1.21
1:A:104:TYR:O	1:A:108:ILE:CG2	1.89	1.20
1:A:31:ILE:N	3:A:280:HOH:O	1.74	1.19
1:A:72:VAL:HG11	1:A:90:LEU:HD21	1.23	1.19
1:A:41:ASP:O	1:A:42:LEU:HD23	1.43	1.18
1:A:202:GLY:O	1:A:203:VAL:CG2	1.92	1.16
1:A:234:ILE:CG1	1:A:274:ALA:HB2	1.72	1.16
1:A:192:VAL:HG11	1:A:262:TYR:CD1	1.80	1.16
1:A:234:ILE:HG12	1:A:274:ALA:HB2	1.23	1.16
1:A:253:THR:OG1	1:A:273:ALA:HB2	1.44	1.15
1:A:16:LEU:CD2	1:A:270:VAL:HG12	1.77	1.15
1:A:125:SER:C	1:A:126:LEU:HG	1.53	1.13
1:A:216:ALA:O	1:A:217:TYR:HD1	1.32	1.13
1:A:26:VAL:HG13	1:A:120:ASP:HB2	1.12	1.12
1:A:124:MET:CE	1:A:168:PRO:HG2	1.79	1.12
1:A:39:HIS:HD2	1:A:40:PRO:HD2	0.95	1.12
1:A:24:SER:O	1:A:25:ASN:HB2	1.48	1.12
1:A:242:THR:O	1:A:246:VAL:HG23	1.50	1.11
1:A:254:THR:HG22	1:A:267:LEU:O	1.50	1.11
1:A:39:HIS:CD2	1:A:40:PRO:HD2	1.87	1.10
1:A:125:SER:O	1:A:126:LEU:HG	1.49	1.09
1:A:31:ILE:CA	3:A:280:HOH:O	1.99	1.09
1:A:234:ILE:HG12	1:A:274:ALA:HB1	1.23	1.09
1:A:11:ILE:HD12	1:A:268:ILE:HG21	1.34	1.08
1:A:5:PRO:HD3	1:A:81:VAL:HA	1.30	1.08
1:A:192:VAL:HG11	1:A:262:TYR:HD1	1.14	1.08
1:A:16:LEU:HD22	1:A:270:VAL:HG12	1.32	1.07
1:A:257:LEU:HB3	1:A:263:TYR:CE1	1.89	1.07
1:A:208:THR:O	1:A:209:LEU:HD12	1.51	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:HG11	1:A:121:VAL:CG2	1.84	1.06
1:A:26:VAL:CG1	1:A:120:ASP:HB2	1.85	1.06
1:A:29:ALA:O	1:A:123:ASN:N	1.87	1.06
1:A:30:VAL:C	3:A:280:HOH:O	1.88	1.06
1:A:248:SER:O	1:A:252:ASN:HB2	1.54	1.06
1:A:16:LEU:CD1	1:A:19:GLN:OE1	2.03	1.06
1:A:91:TYR:HB3	1:A:119:MET:HE1	1.32	1.05
1:A:67:HIS:CE1	1:A:207:SER:HB3	1.89	1.05
1:A:12:LYS:O	1:A:270:VAL:CB	2.03	1.05
1:A:258:GLY:H	1:A:263:TYR:CB	1.71	1.04
1:A:113:TRP:HZ3	1:A:119:MET:CE	1.69	1.04
1:A:124:MET:CE	1:A:168:PRO:CG	2.35	1.03
1:A:175:ILE:HG22	1:A:247:ARG:NH1	1.74	1.03
1:A:253:THR:HG23	1:A:273:ALA:CB	1.90	1.02
1:A:26:VAL:HG13	1:A:120:ASP:CB	1.90	1.01
1:A:11:ILE:HB	1:A:268:ILE:HB	1.42	1.01
1:A:253:THR:CG2	1:A:273:ALA:CB	2.38	1.01
1:A:189:PHE:O	1:A:189:PHE:CD1	2.13	1.00
1:A:114:ALA:O	1:A:119:MET:CB	2.10	0.99
1:A:73:ALA:O	2:A:276:ACN:C2	2.11	0.99
1:A:91:TYR:HB3	1:A:119:MET:CE	1.93	0.98
1:A:62:ASN:O	1:A:63:SER:HB3	1.62	0.98
1:A:122:ILE:CG2	1:A:149:VAL:HG13	1.94	0.98
1:A:192:VAL:CG1	1:A:262:TYR:HD1	1.76	0.98
1:A:111:ILE:CG1	1:A:111:ILE:O	2.10	0.98
1:A:11:ILE:HD12	1:A:268:ILE:CG2	1.94	0.98
1:A:107:ILE:O	1:A:111:ILE:CG2	2.11	0.97
1:A:39:HIS:HE1	1:A:208:THR:HB	1.16	0.97
1:A:114:ALA:O	1:A:119:MET:HB2	1.65	0.97
1:A:192:VAL:CG1	1:A:262:TYR:CD1	2.47	0.97
1:A:234:ILE:CG1	1:A:274:ALA:CB	2.34	0.97
1:A:59:GLN:C	1:A:60:ASP:CA	2.32	0.96
1:A:216:ALA:O	1:A:217:TYR:CD1	2.18	0.96
1:A:257:LEU:HD23	1:A:263:TYR:HE1	1.26	0.96
1:A:253:THR:CG2	1:A:273:ALA:HB2	1.95	0.96
1:A:26:VAL:CG1	1:A:121:VAL:HG23	1.95	0.96
1:A:208:THR:CG2	1:A:214:TYR:CE1	2.50	0.95
1:A:257:LEU:CB	1:A:263:TYR:HD1	1.69	0.95
1:A:253:THR:CB	1:A:273:ALA:HB2	1.98	0.94
1:A:146:GLY:O	1:A:243:ASN:OD1	1.86	0.94
1:A:121:VAL:HG11	1:A:228:ALA:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLY:C	1:A:243:ASN:HD21	1.72	0.93
1:A:5:PRO:CG	1:A:81:VAL:HG13	1.98	0.93
1:A:177:VAL:HG12	1:A:178:GLY:H	1.34	0.92
1:A:5:PRO:CD	1:A:81:VAL:HA	2.00	0.92
1:A:144:ALA:C	1:A:145:SER:CA	2.37	0.92
1:A:253:THR:HG21	1:A:273:ALA:HA	1.52	0.92
1:A:186:ARG:HD2	1:A:262:TYR:HB3	1.51	0.91
1:A:255:THR:O	1:A:266:GLY:HA3	1.69	0.91
1:A:58:PHE:C	1:A:59:GLN:CA	2.39	0.90
1:A:202:GLY:C	1:A:203:VAL:HG23	1.92	0.90
1:A:3:SER:O	1:A:81:VAL:N	2.05	0.89
1:A:73:ALA:HB2	1:A:85:ALA:O	1.71	0.89
1:A:113:TRP:O	1:A:117:ASN:CB	2.20	0.89
1:A:122:ILE:HG21	1:A:149:VAL:HG13	1.53	0.89
1:A:26:VAL:CG1	1:A:121:VAL:CG2	2.51	0.88
1:A:159:THR:CG2	1:A:159:THR:O	2.21	0.87
1:A:43:LYS:CB	2:A:276:ACN:O	2.23	0.87
1:A:82:LEU:HG	1:A:83:GLY:N	1.77	0.87
1:A:5:PRO:HD3	1:A:81:VAL:CA	2.05	0.86
1:A:8:VAL:CG2	1:A:9:SER:N	2.37	0.86
1:A:207:SER:C	1:A:214:TYR:HD1	1.78	0.86
1:A:166:GLY:O	1:A:169:GLY:HA3	1.76	0.86
1:A:72:VAL:CG1	1:A:90:LEU:HD21	2.04	0.86
1:A:35:ILE:CG2	1:A:66:THR:HA	2.05	0.86
1:A:196:LEU:CD1	1:A:196:LEU:CD2	2.53	0.86
1:A:242:THR:O	1:A:246:VAL:CG2	2.23	0.86
1:A:107:ILE:O	1:A:111:ILE:HG21	1.73	0.85
1:A:253:THR:HG23	1:A:273:ALA:HB1	1.56	0.85
1:A:200:ALA:HB1	1:A:201:PRO:HD2	1.57	0.85
1:A:111:ILE:HG12	1:A:111:ILE:O	1.76	0.85
1:A:104:TYR:O	1:A:108:ILE:HG22	1.75	0.85
1:A:51:VAL:HG21	1:A:106:TRP:CZ3	2.11	0.85
1:A:26:VAL:HG12	1:A:121:VAL:HG23	1.57	0.85
1:A:16:LEU:CD2	1:A:270:VAL:CG1	2.55	0.85
1:A:124:MET:HE2	1:A:168:PRO:HG2	1.56	0.85
1:A:73:ALA:CB	1:A:85:ALA:O	2.25	0.84
1:A:155:ASN:ND2	1:A:155:ASN:O	2.10	0.84
1:A:257:LEU:HD23	1:A:263:TYR:CE1	2.11	0.84
1:A:113:TRP:CZ3	1:A:119:MET:CE	2.59	0.84
1:A:39:HIS:CE1	1:A:208:THR:CB	2.58	0.83
1:A:163:SER:HB2	1:A:193:GLY:CA	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:O	1:A:116:ALA:HB3	1.77	0.83
1:A:271:GLN:O	1:A:271:GLN:CG	2.25	0.83
1:A:62:ASN:HB2	1:A:98:ASP:HB3	1.59	0.83
1:A:200:ALA:HA	1:A:267:LEU:HD11	1.58	0.83
1:A:247:ARG:NE	1:A:251:GLN:OE1	2.12	0.82
1:A:255:THR:O	1:A:266:GLY:CA	2.28	0.82
1:A:29:ALA:HB3	1:A:122:ILE:HA	1.59	0.82
1:A:124:MET:HE1	1:A:168:PRO:HG2	1.60	0.81
1:A:43:LYS:HB3	2:A:276:ACN:O	1.79	0.81
1:A:199:MET:O	1:A:267:LEU:HD12	1.78	0.81
1:A:96:LEU:HD21	1:A:101:SER:HA	1.63	0.81
1:A:8:VAL:HG23	1:A:14:PRO:HD3	1.62	0.81
1:A:253:THR:O	1:A:253:THR:OG1	1.90	0.81
1:A:254:THR:CG2	1:A:267:LEU:O	2.28	0.81
1:A:257:LEU:HB2	1:A:263:TYR:HD1	1.45	0.81
1:A:8:VAL:HG23	1:A:9:SER:N	1.93	0.81
1:A:125:SER:O	1:A:126:LEU:CG	2.29	0.81
1:A:28:VAL:HG22	1:A:121:VAL:CG2	2.09	0.81
1:A:5:PRO:HG3	1:A:81:VAL:HG13	1.63	0.81
1:A:97:GLY:O	1:A:98:ASP:HB2	1.80	0.81
1:A:97:GLY:O	1:A:98:ASP:CB	2.29	0.81
1:A:270:VAL:O	1:A:271:GLN:HB3	1.80	0.80
1:A:59:GLN:O	1:A:60:ASP:HA	1.80	0.80
1:A:173:SER:C	1:A:174:VAL:N	0.75	0.80
1:A:107:ILE:O	1:A:111:ILE:HG22	1.81	0.80
1:A:104:TYR:C	1:A:108:ILE:CG2	2.50	0.80
1:A:39:HIS:HD2	1:A:40:PRO:CD	1.88	0.80
1:A:20:GLY:O	1:A:22:THR:HG23	1.82	0.80
1:A:234:ILE:CD1	1:A:274:ALA:HB2	2.12	0.79
1:A:258:GLY:N	1:A:263:TYR:CG	2.50	0.79
1:A:249:SER:O	1:A:253:THR:HG23	1.82	0.79
1:A:253:THR:OG1	1:A:273:ALA:CB	2.29	0.79
1:A:35:ILE:CG2	1:A:69:ALA:HB3	2.12	0.79
1:A:62:ASN:O	1:A:63:SER:CB	2.31	0.79
1:A:175:ILE:HG13	1:A:175:ILE:O	1.83	0.79
1:A:27:LYS:HB3	1:A:91:TYR:CE1	2.17	0.79
1:A:33:SER:O	1:A:94:LYS:HD3	1.83	0.79
1:A:175:ILE:CB	1:A:175:ILE:CD1	2.61	0.78
1:A:253:THR:HG21	1:A:273:ALA:CA	2.13	0.78
1:A:200:ALA:HA	1:A:267:LEU:CD1	2.14	0.78
1:A:35:ILE:HG22	1:A:66:THR:HA	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:C	1:A:155:ASN:ND2	2.35	0.78
1:A:16:LEU:HD23	1:A:270:VAL:CG1	2.14	0.78
1:A:26:VAL:HA	1:A:120:ASP:OD2	1.83	0.78
1:A:115:ILE:HG12	1:A:116:ALA:N	1.97	0.78
1:A:241:TRP:C	1:A:242:THR:CA	2.48	0.78
1:A:248:SER:O	1:A:252:ASN:N	2.17	0.78
1:A:121:VAL:HG21	1:A:232:ALA:HB2	1.67	0.77
1:A:186:ARG:HH22	1:A:192:VAL:CG1	1.95	0.77
1:A:196:LEU:CD2	1:A:196:LEU:CB	2.62	0.77
1:A:98:ASP:O	1:A:99:ALA:HB3	1.85	0.76
1:A:35:ILE:HG21	1:A:69:ALA:HB3	1.66	0.76
1:A:5:PRO:HD3	1:A:81:VAL:HG22	1.68	0.76
1:A:271:GLN:O	1:A:271:GLN:HG2	1.86	0.76
1:A:249:SER:C	1:A:273:ALA:HB1	2.05	0.76
1:A:122:ILE:HG22	1:A:149:VAL:HG13	1.66	0.76
1:A:2:GLN:O	3:A:277:HOH:O	2.01	0.76
1:A:39:HIS:HE1	1:A:208:THR:CB	1.95	0.76
1:A:59:GLN:N	1:A:59:GLN:CB	2.49	0.76
1:A:246:VAL:HA	1:A:249:SER:HB2	1.68	0.76
1:A:159:THR:O	1:A:159:THR:HG22	1.86	0.76
1:A:189:PHE:O	1:A:189:PHE:HD1	1.67	0.75
1:A:49:SER:O	1:A:50:MET:SD	2.44	0.75
1:A:26:VAL:HG11	1:A:121:VAL:HG22	1.68	0.75
1:A:249:SER:O	1:A:273:ALA:CB	2.26	0.75
1:A:54:GLU:OE2	1:A:97:GLY:O	2.04	0.75
1:A:259:ASP:OD1	1:A:261:PHE:HB2	1.87	0.75
1:A:68:VAL:HG12	1:A:69:ALA:N	2.00	0.75
1:A:22:THR:CG2	1:A:22:THR:CA	2.65	0.75
1:A:150:VAL:HG21	1:A:228:ALA:HB2	1.68	0.75
1:A:208:THR:C	1:A:209:LEU:HD12	2.06	0.74
1:A:230:ALA:O	1:A:234:ILE:N	2.20	0.74
1:A:56:PRO:HB2	1:A:58:PHE:H	1.49	0.74
1:A:11:ILE:HG13	1:A:270:VAL:HG23	1.69	0.74
1:A:35:ILE:HA	1:A:66:THR:HA	1.69	0.74
1:A:186:ARG:NH2	1:A:192:VAL:HG12	2.01	0.74
1:A:233:LEU:O	1:A:236:SER:HB2	1.87	0.74
1:A:247:ARG:O	1:A:251:GLN:HG3	1.88	0.74
1:A:145:SER:CB	1:A:145:SER:N	2.51	0.74
1:A:124:MET:HE3	1:A:168:PRO:CG	2.18	0.73
1:A:17:HIS:NE2	1:A:84:VAL:O	2.20	0.73
1:A:207:SER:O	1:A:214:TYR:CA	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:CD2	1:A:101:SER:HA	2.18	0.73
1:A:106:TRP:N	1:A:106:TRP:CD1	2.54	0.73
1:A:207:SER:C	1:A:214:TYR:CD1	2.60	0.73
1:A:30:VAL:CA	1:A:31:ILE:N	2.50	0.73
1:A:155:ASN:O	1:A:156:GLU:HB2	1.88	0.73
1:A:91:TYR:CB	1:A:119:MET:CE	2.66	0.73
1:A:17:HIS:HE1	1:A:83:GLY:O	1.70	0.73
1:A:234:ILE:HG21	1:A:246:VAL:HG13	1.71	0.73
1:A:186:ARG:NH2	1:A:192:VAL:CG1	2.52	0.72
1:A:27:LYS:HD2	1:A:118:ASN:O	1.89	0.72
1:A:13:ALA:H	1:A:14:PRO:HD2	1.54	0.72
1:A:258:GLY:H	1:A:263:TYR:HB3	1.55	0.72
1:A:8:VAL:CG2	1:A:14:PRO:HD3	2.19	0.72
1:A:59:GLN:CA	1:A:60:ASP:N	2.52	0.72
1:A:39:HIS:ND1	1:A:208:THR:HB	2.03	0.72
1:A:59:GLN:O	1:A:60:ASP:CA	2.38	0.72
1:A:35:ILE:HG21	1:A:69:ALA:CB	2.19	0.72
1:A:111:ILE:HG13	1:A:111:ILE:O	1.90	0.71
1:A:258:GLY:N	1:A:263:TYR:CB	2.51	0.71
1:A:248:SER:O	1:A:252:ASN:CB	2.37	0.71
1:A:207:SER:O	1:A:214:TYR:CB	2.38	0.71
1:A:77:ASN:OD1	1:A:79:ILE:HG12	1.91	0.71
1:A:24:SER:O	1:A:25:ASN:CB	2.32	0.71
1:A:30:VAL:C	1:A:30:VAL:CB	2.56	0.71
1:A:163:SER:HB2	1:A:193:GLY:HA2	1.73	0.71
1:A:180:VAL:O	1:A:201:PRO:HA	1.89	0.71
1:A:12:LYS:HB3	1:A:270:VAL:O	1.90	0.70
1:A:30:VAL:HA	1:A:123:ASN:HB3	1.72	0.70
1:A:164:THR:O	1:A:191:SER:OG	2.07	0.70
1:A:13:ALA:HB3	1:A:14:PRO:HD3	1.73	0.70
1:A:71:THR:HB	1:A:225:PRO:HB2	1.72	0.70
1:A:33:SER:O	1:A:98:ASP:OD2	2.09	0.70
1:A:113:TRP:HZ3	1:A:119:MET:HE2	1.56	0.69
1:A:253:THR:HG23	1:A:273:ALA:HB2	1.65	0.69
1:A:11:ILE:CG1	1:A:270:VAL:HG23	2.21	0.69
1:A:12:LYS:C	1:A:270:VAL:HB	2.08	0.69
1:A:11:ILE:CD1	1:A:268:ILE:HG21	2.20	0.69
1:A:1:ALA:O	1:A:2:GLN:HG3	1.92	0.69
1:A:233:LEU:CA	1:A:233:LEU:CG	2.70	0.69
1:A:23:GLY:HA3	1:A:85:ALA:HB1	1.74	0.69
1:A:56:PRO:O	1:A:57:ASN:CG	2.30	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HG13	1:A:199:MET:N	2.07	0.69
1:A:156:GLU:HB3	1:A:164:THR:HB	1.74	0.69
1:A:124:MET:CE	1:A:168:PRO:HG3	2.23	0.69
1:A:104:TYR:C	1:A:108:ILE:HG23	2.10	0.68
1:A:13:ALA:N	1:A:14:PRO:HD2	2.07	0.68
1:A:208:THR:HG22	1:A:214:TYR:CZ	2.27	0.68
1:A:186:ARG:HG2	1:A:187:ALA:H	1.58	0.68
1:A:185:GLN:HG2	1:A:186:ARG:N	2.08	0.68
1:A:125:SER:C	1:A:126:LEU:CG	2.47	0.68
1:A:258:GLY:C	1:A:263:TYR:HB2	2.14	0.68
1:A:113:TRP:HZ3	1:A:119:MET:SD	2.16	0.68
1:A:114:ALA:O	1:A:119:MET:HB3	1.93	0.68
1:A:115:ILE:HD12	1:A:142:ALA:HA	1.75	0.68
1:A:8:VAL:O	1:A:9:SER:C	2.27	0.67
1:A:163:SER:CB	1:A:193:GLY:HA2	2.23	0.67
1:A:124:MET:HE3	1:A:168:PRO:HG3	1.76	0.67
1:A:1:ALA:O	1:A:2:GLN:CB	2.42	0.67
1:A:117:ASN:O	1:A:118:ASN:HB2	1.94	0.67
1:A:6:TYR:HA	1:A:9:SER:HB2	1.76	0.67
1:A:159:THR:O	1:A:159:THR:HG23	1.95	0.67
1:A:197:ASP:N	1:A:197:ASP:OD1	2.28	0.67
1:A:177:VAL:HG12	1:A:178:GLY:N	2.09	0.67
1:A:146:GLY:C	1:A:243:ASN:ND2	2.48	0.66
1:A:59:GLN:C	1:A:59:GLN:N	2.48	0.66
1:A:171:TYR:HB3	1:A:172:PRO:HD2	1.77	0.66
1:A:150:VAL:CG2	1:A:228:ALA:HB2	2.25	0.66
1:A:186:ARG:HD2	1:A:262:TYR:CB	2.25	0.66
1:A:165:VAL:HG22	1:A:192:VAL:O	1.95	0.66
1:A:173:SER:O	1:A:174:VAL:CA	2.29	0.66
1:A:27:LYS:HG3	1:A:120:ASP:OD2	1.96	0.66
1:A:14:PRO:O	1:A:17:HIS:HB2	1.95	0.66
1:A:1:ALA:O	1:A:2:GLN:HB2	1.96	0.66
1:A:112:GLU:HA	1:A:115:ILE:CG2	2.26	0.65
1:A:28:VAL:HG13	1:A:121:VAL:HB	1.79	0.65
1:A:152:ALA:O	1:A:153:ALA:CB	2.44	0.65
1:A:36:ASP:H	1:A:66:THR:HG23	1.62	0.65
1:A:207:SER:O	1:A:214:TYR:HA	1.96	0.65
1:A:221:SER:OG	1:A:222:MET:HE1	1.97	0.64
1:A:208:THR:HG22	1:A:214:TYR:CD1	2.30	0.64
1:A:81:VAL:CG1	1:A:82:LEU:N	2.60	0.64
1:A:257:LEU:CD2	1:A:263:TYR:CE1	2.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:CG2	1:A:13:ALA:HB3	2.27	0.64
1:A:104:TYR:H	1:A:104:TYR:HD1	1.44	0.64
1:A:113:TRP:CZ3	1:A:119:MET:HE1	2.33	0.64
1:A:34:GLY:CA	1:A:60:ASP:OD1	2.46	0.64
1:A:56:PRO:HB2	1:A:58:PHE:HB2	1.78	0.64
1:A:30:VAL:HG11	1:A:69:ALA:HB2	1.79	0.64
1:A:223:ALA:O	1:A:226:HIS:HB2	1.98	0.64
1:A:235:LEU:HD11	1:A:246:VAL:HG21	1.80	0.63
1:A:237:LYS:HB3	1:A:238:HIS:NE2	2.13	0.63
1:A:159:THR:HG21	1:A:162:SER:CB	2.27	0.63
1:A:98:ASP:O	1:A:99:ALA:CB	2.47	0.63
1:A:233:LEU:N	1:A:233:LEU:CB	2.59	0.63
1:A:77:ASN:OD1	1:A:79:ILE:CG1	2.47	0.62
1:A:22:THR:CG2	1:A:22:THR:N	2.61	0.62
1:A:57:ASN:HB2	1:A:94:LYS:HB3	1.81	0.62
1:A:186:ARG:HH21	1:A:262:TYR:HB3	1.64	0.62
1:A:186:ARG:HH22	1:A:192:VAL:HG12	1.62	0.62
1:A:155:ASN:C	1:A:155:ASN:HD22	2.01	0.62
1:A:242:THR:N	1:A:242:THR:CB	2.60	0.62
1:A:27:LYS:HB3	1:A:91:TYR:CD1	2.35	0.62
1:A:17:HIS:CE1	1:A:83:GLY:O	2.52	0.62
1:A:81:VAL:HG12	1:A:82:LEU:N	2.13	0.62
1:A:112:GLU:CA	1:A:115:ILE:HG23	2.29	0.62
1:A:113:TRP:HZ3	1:A:119:MET:HE1	1.60	0.62
1:A:237:LYS:HB3	1:A:238:HIS:CE1	2.35	0.61
1:A:4:VAL:HG22	1:A:82:LEU:HB3	1.81	0.61
1:A:27:LYS:N	1:A:120:ASP:OD2	2.27	0.61
1:A:216:ALA:C	1:A:217:TYR:CD1	2.73	0.61
1:A:32:ASP:OD1	1:A:64:HIS:ND1	2.29	0.61
1:A:112:GLU:HA	1:A:115:ILE:HG23	1.81	0.61
1:A:150:VAL:HG13	1:A:175:ILE:CD1	2.30	0.61
1:A:216:ALA:C	1:A:217:TYR:HD1	2.03	0.61
1:A:31:ILE:HG23	1:A:93:VAL:CG1	2.30	0.61
1:A:163:SER:HB2	1:A:193:GLY:HA3	1.81	0.61
1:A:31:ILE:CG1	3:A:280:HOH:O	2.48	0.61
1:A:113:TRP:CZ3	1:A:119:MET:HE2	2.34	0.61
1:A:175:ILE:HG22	1:A:247:ARG:HH11	1.62	0.61
1:A:51:VAL:HB	1:A:106:TRP:CD2	2.36	0.61
1:A:1:ALA:O	1:A:2:GLN:CG	2.49	0.61
1:A:163:SER:CB	1:A:193:GLY:CA	2.78	0.60
1:A:35:ILE:HG23	1:A:66:THR:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:VAL:CA	1:A:249:SER:HB2	2.31	0.60
1:A:234:ILE:HD11	1:A:274:ALA:HB2	1.84	0.60
1:A:221:SER:H	1:A:222:MET:HE2	1.67	0.60
1:A:18:SER:O	1:A:20:GLY:N	2.34	0.60
1:A:180:VAL:O	1:A:202:GLY:N	2.35	0.60
1:A:248:SER:C	1:A:252:ASN:HB2	2.22	0.60
1:A:146:GLY:O	1:A:243:ASN:CG	2.39	0.59
1:A:23:GLY:HA3	1:A:85:ALA:CB	2.31	0.59
1:A:257:LEU:HB2	1:A:263:TYR:CD1	2.22	0.59
1:A:111:ILE:O	1:A:115:ILE:CG2	2.51	0.59
1:A:200:ALA:HB1	1:A:201:PRO:CD	2.32	0.59
1:A:142:ALA:O	1:A:147:VAL:HG23	2.03	0.58
1:A:84:VAL:O	1:A:86:PRO:HD3	2.03	0.58
1:A:136:LYS:O	1:A:140:ASP:HB2	2.02	0.58
1:A:187:ALA:HB3	1:A:190:SER:HB2	1.84	0.58
1:A:106:TRP:HD1	1:A:106:TRP:N	2.02	0.58
1:A:141:LYS:O	1:A:145:SER:OG	2.22	0.57
1:A:51:VAL:HG21	1:A:106:TRP:CH2	2.39	0.57
1:A:36:ASP:HB2	1:A:66:THR:CG2	2.34	0.57
1:A:224:SER:N	1:A:225:PRO:HD2	2.20	0.57
1:A:113:TRP:CE3	1:A:113:TRP:C	2.78	0.57
1:A:207:SER:O	1:A:214:TYR:HB3	2.04	0.57
1:A:271:GLN:O	1:A:271:GLN:HG3	2.04	0.57
1:A:253:THR:CG2	1:A:273:ALA:CA	2.78	0.57
1:A:16:LEU:HD22	1:A:270:VAL:CG1	2.20	0.57
1:A:82:LEU:CG	1:A:83:GLY:N	2.61	0.57
1:A:113:TRP:CZ3	1:A:119:MET:SD	2.98	0.57
1:A:5:PRO:HG3	1:A:81:VAL:CG1	2.32	0.57
1:A:221:SER:OG	1:A:222:MET:CE	2.52	0.57
1:A:186:ARG:NH2	1:A:262:TYR:HB3	2.20	0.56
1:A:69:ALA:HA	1:A:72:VAL:HB	1.87	0.56
1:A:31:ILE:HA	1:A:93:VAL:HB	1.86	0.56
1:A:35:ILE:HD11	1:A:92:ALA:HA	1.87	0.56
1:A:207:SER:O	1:A:214:TYR:CD1	2.59	0.56
1:A:60:ASP:O	1:A:210:PRO:HG3	2.05	0.56
1:A:30:VAL:N	1:A:30:VAL:C	2.54	0.56
1:A:49:SER:HB2	1:A:57:ASN:HB3	1.88	0.56
1:A:91:TYR:CB	1:A:119:MET:HE1	2.22	0.56
1:A:122:ILE:HD12	1:A:149:VAL:HG22	1.87	0.56
1:A:224:SER:CB	1:A:225:PRO:HD3	2.35	0.56
1:A:62:ASN:ND2	1:A:64:HIS:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG21	1:A:229:GLY:HA3	1.87	0.56
1:A:246:VAL:O	1:A:249:SER:HB2	2.06	0.56
1:A:8:VAL:C	1:A:10:GLN:N	2.41	0.55
1:A:68:VAL:CG1	1:A:69:ALA:N	2.69	0.55
1:A:69:ALA:O	1:A:72:VAL:HG12	2.06	0.55
1:A:8:VAL:HG22	1:A:9:SER:N	2.21	0.55
1:A:192:VAL:HG11	1:A:262:TYR:CE1	2.40	0.55
1:A:78:SER:O	1:A:79:ILE:HD13	2.07	0.55
1:A:270:VAL:O	1:A:271:GLN:CB	2.52	0.55
1:A:148:VAL:HG22	1:A:148:VAL:O	2.05	0.55
1:A:28:VAL:HG22	1:A:121:VAL:HG21	1.85	0.55
1:A:258:GLY:O	1:A:263:TYR:HB2	2.06	0.55
1:A:242:THR:N	1:A:242:THR:C	2.56	0.55
1:A:268:ILE:N	1:A:268:ILE:HD13	2.22	0.55
1:A:56:PRO:HB2	1:A:58:PHE:N	2.21	0.55
1:A:72:VAL:HG12	1:A:73:ALA:N	2.21	0.55
1:A:123:ASN:C	1:A:123:ASN:HD22	2.08	0.55
1:A:146:GLY:O	1:A:243:ASN:ND2	2.39	0.55
1:A:11:ILE:CD1	1:A:268:ILE:CG2	2.76	0.55
1:A:5:PRO:HD3	1:A:81:VAL:CG2	2.34	0.55
1:A:219:GLY:HA3	1:A:222:MET:HE3	1.89	0.55
1:A:154:GLY:O	1:A:220:THR:HG21	2.06	0.55
1:A:150:VAL:HG13	1:A:175:ILE:CG1	2.36	0.54
1:A:175:ILE:CG1	1:A:175:ILE:O	2.54	0.54
1:A:14:PRO:HA	1:A:17:HIS:ND1	2.22	0.54
1:A:72:VAL:CG1	1:A:73:ALA:N	2.71	0.54
1:A:255:THR:O	1:A:266:GLY:HA2	2.06	0.54
1:A:209:LEU:N	1:A:209:LEU:HD12	2.20	0.54
1:A:175:ILE:CG2	1:A:247:ARG:NH1	2.61	0.54
1:A:26:VAL:HG21	1:A:232:ALA:O	2.06	0.54
1:A:34:GLY:O	1:A:35:ILE:N	2.32	0.54
1:A:150:VAL:HG13	1:A:175:ILE:HG13	1.90	0.54
1:A:27:LYS:HB3	1:A:91:TYR:HE1	1.70	0.54
1:A:28:VAL:HG22	1:A:121:VAL:HB	1.89	0.54
1:A:198:VAL:CG1	1:A:199:MET:N	2.66	0.53
1:A:104:TYR:O	1:A:108:ILE:N	2.33	0.53
1:A:39:HIS:CE1	1:A:208:THR:CG2	2.91	0.53
1:A:115:ILE:HD12	1:A:142:ALA:CA	2.39	0.53
1:A:8:VAL:O	1:A:11:ILE:N	2.39	0.53
1:A:6:TYR:O	1:A:7:GLY:C	2.45	0.53
1:A:124:MET:HE2	1:A:168:PRO:CG	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:HA3	1:A:60:ASP:OD1	2.08	0.53
1:A:155:ASN:O	1:A:156:GLU:CB	2.54	0.53
1:A:63:SER:OG	1:A:217:TYR:HE2	1.91	0.53
1:A:93:VAL:HB	3:A:280:HOH:O	2.08	0.53
1:A:13:ALA:N	1:A:14:PRO:CD	2.72	0.52
1:A:228:ALA:HA	1:A:231:ALA:HB3	1.91	0.52
1:A:73:ALA:HB1	1:A:85:ALA:O	2.10	0.52
1:A:30:VAL:CG2	1:A:72:VAL:HG21	2.38	0.52
1:A:27:LYS:HB2	1:A:119:MET:HG3	1.92	0.52
1:A:112:GLU:O	1:A:116:ALA:CB	2.52	0.52
1:A:238:HIS:HB2	1:A:241:TRP:CG	2.44	0.52
1:A:11:ILE:O	1:A:12:LYS:HB2	2.08	0.52
1:A:11:ILE:O	1:A:269:ASN:HA	2.09	0.52
1:A:104:TYR:HA	1:A:107:ILE:HG13	1.92	0.52
1:A:175:ILE:HG22	1:A:247:ARG:CZ	2.38	0.51
1:A:113:TRP:HE3	1:A:114:ALA:N	2.09	0.51
1:A:8:VAL:HG21	1:A:13:ALA:HB3	1.93	0.51
1:A:43:LYS:HB2	2:A:276:ACN:O	2.07	0.51
1:A:80:GLY:O	1:A:81:VAL:O	2.29	0.51
1:A:234:ILE:CG2	1:A:246:VAL:HG13	2.37	0.51
1:A:29:ALA:HB3	1:A:122:ILE:HG12	1.91	0.51
1:A:150:VAL:CG1	1:A:175:ILE:HG13	2.41	0.51
1:A:203:VAL:H	1:A:205:ILE:CD1	2.24	0.51
1:A:152:ALA:O	1:A:153:ALA:HB3	2.10	0.51
1:A:81:VAL:CG1	1:A:82:LEU:H	2.24	0.51
1:A:159:THR:HG21	1:A:162:SER:HB2	1.92	0.51
1:A:13:ALA:O	1:A:15:ALA:N	2.44	0.50
1:A:224:SER:HB3	1:A:225:PRO:HD3	1.94	0.50
1:A:31:ILE:HG22	1:A:95:VAL:HG22	1.92	0.50
1:A:233:LEU:C	1:A:233:LEU:CB	2.74	0.50
1:A:255:THR:HG22	1:A:267:LEU:H	1.76	0.50
1:A:36:ASP:HB2	1:A:66:THR:HG21	1.92	0.50
1:A:54:GLU:CD	1:A:97:GLY:O	2.49	0.50
1:A:179:ALA:HB1	1:A:202:GLY:O	2.12	0.50
1:A:154:GLY:O	1:A:155:ASN:HB3	2.11	0.50
1:A:105:SER:O	1:A:109:ASN:HB2	2.11	0.50
1:A:208:THR:N	1:A:214:TYR:CD1	2.80	0.50
1:A:31:ILE:HG23	1:A:93:VAL:HG11	1.93	0.50
1:A:34:GLY:C	1:A:60:ASP:OD1	2.50	0.50
1:A:20:GLY:O	1:A:22:THR:CG2	2.55	0.50
1:A:65:GLY:HA2	1:A:68:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ILE:O	1:A:115:ILE:HG21	2.12	0.49
1:A:224:SER:CB	1:A:225:PRO:CD	2.90	0.49
1:A:64:HIS:O	1:A:68:VAL:HB	2.12	0.49
1:A:180:VAL:HG22	1:A:185:GLN:O	2.11	0.49
1:A:257:LEU:CD2	1:A:263:TYR:HE1	2.08	0.49
1:A:214:TYR:CD2	1:A:214:TYR:N	2.79	0.49
1:A:43:LYS:O	1:A:90:LEU:HB2	2.11	0.49
1:A:56:PRO:CB	1:A:58:PHE:HB2	2.41	0.49
1:A:13:ALA:C	1:A:15:ALA:H	2.16	0.49
1:A:4:VAL:HG22	1:A:82:LEU:HD23	1.94	0.49
1:A:32:ASP:O	1:A:94:LYS:HA	2.12	0.49
1:A:159:THR:HB	1:A:162:SER:O	2.13	0.49
1:A:11:ILE:HD12	1:A:268:ILE:CB	2.43	0.49
1:A:16:LEU:HA	1:A:19:GLN:OE1	2.13	0.48
1:A:186:ARG:HH22	1:A:192:VAL:HG13	1.78	0.48
1:A:5:PRO:CD	1:A:81:VAL:HG22	2.38	0.48
1:A:51:VAL:HG23	1:A:52:PRO:HD2	1.95	0.48
1:A:22:THR:CG2	1:A:22:THR:OG1	2.55	0.48
1:A:136:LYS:NZ	1:A:140:ASP:OD2	2.38	0.48
1:A:13:ALA:HB3	1:A:14:PRO:CD	2.41	0.48
1:A:5:PRO:HD3	1:A:81:VAL:CB	2.44	0.48
1:A:199:MET:HB3	1:A:266:GLY:O	2.13	0.48
1:A:186:ARG:CD	1:A:262:TYR:HB3	2.33	0.48
1:A:123:ASN:ND2	1:A:224:SER:OG	2.47	0.48
1:A:122:ILE:CD1	1:A:149:VAL:HG22	2.43	0.48
1:A:192:VAL:HB	1:A:261:PHE:O	2.14	0.48
1:A:150:VAL:HG13	1:A:175:ILE:HD11	1.96	0.48
1:A:200:ALA:HA	1:A:267:LEU:HD12	1.96	0.48
1:A:63:SER:OG	1:A:217:TYR:CE2	2.67	0.47
1:A:88:SER:O	2:A:276:ACN:C1	2.62	0.47
1:A:164:THR:O	1:A:191:SER:CB	2.62	0.47
1:A:112:GLU:HA	1:A:115:ILE:HG21	1.95	0.47
1:A:10:GLN:HE22	1:A:182:SER:HA	1.79	0.47
1:A:23:GLY:H	1:A:233:LEU:HD12	1.80	0.47
1:A:227:VAL:C	1:A:229:GLY:N	2.67	0.47
1:A:35:ILE:HD11	1:A:92:ALA:CA	2.45	0.47
1:A:244:THR:O	1:A:247:ARG:HB2	2.15	0.47
1:A:208:THR:N	1:A:214:TYR:HD1	2.11	0.47
1:A:28:VAL:HG22	1:A:121:VAL:CB	2.44	0.47
1:A:112:GLU:CA	1:A:115:ILE:CG2	2.92	0.47
1:A:199:MET:O	1:A:267:LEU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD22	1:A:42:LEU:HA	1.76	0.47
1:A:151:ALA:O	1:A:176:ALA:HA	2.15	0.47
1:A:124:MET:HG2	1:A:126:LEU:HD12	1.96	0.47
1:A:180:VAL:N	1:A:200:ALA:O	2.48	0.47
1:A:207:SER:O	1:A:214:TYR:CG	2.68	0.47
1:A:31:ILE:HG21	1:A:31:ILE:HD13	1.49	0.47
1:A:208:THR:CG2	1:A:214:TYR:HE1	2.21	0.47
1:A:75:LEU:HA	1:A:75:LEU:HD12	1.37	0.47
1:A:228:ALA:HA	1:A:231:ALA:CB	2.45	0.46
1:A:31:ILE:HG12	3:A:280:HOH:O	2.11	0.46
1:A:5:PRO:CD	1:A:81:VAL:CA	2.76	0.46
1:A:163:SER:HB3	1:A:193:GLY:HA2	1.97	0.46
1:A:142:ALA:O	1:A:147:VAL:CG2	2.63	0.46
1:A:140:ASP:O	1:A:144:ALA:HB2	2.15	0.46
1:A:202:GLY:O	1:A:203:VAL:HG22	2.05	0.46
1:A:138:ALA:O	1:A:142:ALA:N	2.39	0.46
1:A:37:SER:O	1:A:38:SER:C	2.54	0.46
1:A:138:ALA:O	1:A:142:ALA:CB	2.64	0.46
1:A:227:VAL:C	1:A:229:GLY:H	2.18	0.46
1:A:108:ILE:C	1:A:111:ILE:HG23	2.37	0.46
1:A:56:PRO:O	1:A:57:ASN:CB	2.63	0.46
1:A:29:ALA:HB3	1:A:122:ILE:CG1	2.45	0.46
1:A:212:ASN:O	1:A:213:LYS:HB3	2.16	0.46
1:A:142:ALA:O	1:A:147:VAL:HB	2.16	0.45
1:A:104:TYR:CA	1:A:107:ILE:HG13	2.46	0.45
1:A:110:GLY:O	1:A:113:TRP:HB3	2.16	0.45
1:A:36:ASP:HB2	1:A:66:THR:HG23	1.98	0.45
1:A:25:ASN:HA	1:A:25:ASN:HD22	1.59	0.45
1:A:95:VAL:O	1:A:106:TRP:HB3	2.16	0.45
1:A:72:VAL:HG12	1:A:73:ALA:H	1.81	0.45
1:A:203:VAL:H	1:A:205:ILE:HD12	1.81	0.45
1:A:149:VAL:O	1:A:175:ILE:HG12	2.16	0.45
1:A:88:SER:O	2:A:276:ACN:H12	2.17	0.45
1:A:170:LYS:HA	1:A:195:GLU:CG	2.47	0.45
1:A:29:ALA:N	1:A:121:VAL:O	2.43	0.45
1:A:63:SER:O	1:A:67:HIS:HB2	2.16	0.45
1:A:8:VAL:HA	1:A:11:ILE:CG2	2.47	0.45
1:A:237:LYS:C	1:A:238:HIS:CG	2.88	0.45
1:A:245:GLN:O	1:A:246:VAL:C	2.55	0.45
1:A:154:GLY:O	1:A:220:THR:CG2	2.65	0.45
1:A:237:LYS:CB	1:A:238:HIS:CE1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PRO:CD	1:A:81:VAL:HG13	2.46	0.44
1:A:82:LEU:CD1	1:A:86:PRO:HG3	2.47	0.44
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.64	0.44
1:A:192:VAL:HA	1:A:196:LEU:HD12	2.00	0.44
1:A:84:VAL:HG11	1:A:230:ALA:N	2.32	0.44
1:A:16:LEU:HA	1:A:16:LEU:HD12	1.50	0.44
1:A:243:ASN:N	1:A:243:ASN:OD1	2.50	0.44
1:A:23:GLY:N	1:A:233:LEU:HD12	2.33	0.44
1:A:4:VAL:CG2	1:A:82:LEU:HD23	2.48	0.44
1:A:155:ASN:CG	1:A:155:ASN:O	2.55	0.44
1:A:12:LYS:O	1:A:270:VAL:CG1	2.60	0.43
1:A:35:ILE:HA	1:A:66:THR:CA	2.44	0.43
1:A:173:SER:CB	1:A:174:VAL:N	2.76	0.43
1:A:170:LYS:HA	1:A:195:GLU:HG2	1.99	0.43
1:A:29:ALA:HB2	1:A:114:ALA:HB1	2.00	0.43
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.78	0.43
1:A:224:SER:N	1:A:225:PRO:CD	2.81	0.43
1:A:145:SER:OG	1:A:145:SER:N	2.52	0.43
1:A:11:ILE:O	1:A:11:ILE:HG13	2.19	0.43
1:A:60:ASP:CG	1:A:66:THR:OG1	2.56	0.43
1:A:180:VAL:HG13	1:A:181:ASP:N	2.33	0.43
1:A:102:GLY:HA2	1:A:106:TRP:CZ3	2.53	0.43
1:A:195:GLU:O	1:A:197:ASP:OD1	2.36	0.43
1:A:189:PHE:CE1	1:A:219:GLY:HA2	2.53	0.43
1:A:122:ILE:HG21	1:A:149:VAL:CG1	2.35	0.43
1:A:30:VAL:CA	1:A:30:VAL:O	2.47	0.43
1:A:39:HIS:CD2	1:A:40:PRO:CD	2.79	0.43
1:A:16:LEU:N	1:A:16:LEU:HD13	2.32	0.42
1:A:208:THR:HA	1:A:214:TYR:HA	2.01	0.42
1:A:138:ALA:O	1:A:142:ALA:HB2	2.18	0.42
1:A:139:VAL:HG12	1:A:140:ASP:N	2.32	0.42
1:A:153:ALA:C	1:A:220:THR:HG21	2.40	0.42
1:A:234:ILE:CD1	1:A:249:SER:HB3	2.50	0.42
1:A:159:THR:HG21	1:A:162:SER:HB3	1.98	0.42
1:A:104:TYR:HA	1:A:107:ILE:HB	2.01	0.42
1:A:108:ILE:HG13	1:A:108:ILE:O	2.20	0.42
1:A:13:ALA:C	1:A:15:ALA:N	2.72	0.42
1:A:175:ILE:CG2	1:A:247:ARG:CZ	2.97	0.42
1:A:19:GLN:HB2	1:A:21:TYR:HD2	1.85	0.42
1:A:247:ARG:O	1:A:251:GLN:CG	2.63	0.42
1:A:94:LYS:HD2	1:A:96:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HG21	1:A:149:VAL:HG22	2.01	0.42
1:A:31:ILE:HA	3:A:280:HOH:O	1.86	0.42
1:A:28:VAL:HG22	1:A:121:VAL:HG23	1.93	0.42
1:A:68:VAL:HG21	1:A:125:SER:OG	2.20	0.42
1:A:91:TYR:CB	1:A:119:MET:HE3	2.49	0.41
1:A:11:ILE:CB	1:A:268:ILE:HB	2.30	0.41
1:A:209:LEU:CD1	1:A:209:LEU:N	2.84	0.41
1:A:147:VAL:O	1:A:243:ASN:ND2	2.53	0.41
1:A:244:THR:O	1:A:245:GLN:C	2.59	0.41
1:A:35:ILE:CG2	1:A:69:ALA:CB	2.85	0.41
1:A:195:GLU:C	1:A:196:LEU:CA	2.82	0.41
1:A:204:SER:H	1:A:218:ASN:HB3	1.85	0.41
1:A:255:THR:CG2	1:A:267:LEU:H	2.34	0.41
1:A:8:VAL:O	1:A:10:GLN:CA	2.61	0.41
1:A:28:VAL:CG1	1:A:121:VAL:HB	2.47	0.41
1:A:207:SER:CA	1:A:214:TYR:HD1	2.33	0.41
1:A:274:ALA:O	1:A:275:GLN:HB3	2.21	0.41
1:A:51:VAL:HA	1:A:52:PRO:HD3	1.90	0.41
1:A:227:VAL:O	1:A:231:ALA:N	2.43	0.41
1:A:33:SER:HA	1:A:98:ASP:OD1	2.21	0.41
1:A:4:VAL:HA	1:A:81:VAL:HA	2.02	0.41
1:A:31:ILE:HD11	1:A:111:ILE:HB	2.02	0.41
1:A:18:SER:C	1:A:20:GLY:N	2.73	0.41
1:A:258:GLY:HA3	1:A:263:TYR:CD2	2.55	0.41
1:A:122:ILE:HG21	1:A:122:ILE:HD13	1.81	0.41
1:A:69:ALA:O	1:A:72:VAL:CG1	2.69	0.41
1:A:90:LEU:HA	1:A:90:LEU:HD23	1.65	0.41
1:A:104:TYR:C	1:A:108:ILE:HG22	2.29	0.41
1:A:121:VAL:HG21	1:A:232:ALA:CB	2.44	0.41
1:A:60:ASP:CB	1:A:66:THR:OG1	2.69	0.41
1:A:181:ASP:OD2	1:A:183:SER:OG	2.34	0.41
1:A:81:VAL:HG13	1:A:82:LEU:H	1.86	0.40
1:A:62:ASN:OD1	1:A:99:ALA:N	2.55	0.40
1:A:11:ILE:O	1:A:11:ILE:CG1	2.68	0.40
1:A:217:TYR:N	1:A:217:TYR:CD1	2.88	0.40
1:A:54:GLU:CB	1:A:94:LYS:NZ	2.85	0.40
1:A:153:ALA:O	1:A:220:THR:OG1	2.19	0.40

All (141) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:CB	1:A:50:MET:O[2_656]	0.34	1.86
1:A:206:GLN:OE1	1:A:242:THR:CG2[1_556]	0.36	1.84
1:A:20:GLY:CA	1:A:106:TRP:CZ3[2_656]	0.38	1.82
1:A:20:GLY:C	1:A:106:TRP:CH2[2_656]	0.56	1.64
1:A:38:SER:OG	1:A:261:PHE:N[1_455]	0.56	1.64
1:A:17:HIS:O	1:A:106:TRP:NE1[2_656]	0.57	1.63
1:A:16:LEU:CA	1:A:52:PRO:CG[2_656]	0.60	1.60
1:A:36:ASP:OD2	1:A:259:ASP:CG[1_455]	0.68	1.52
1:A:19:GLN:N	1:A:51:VAL:CB[2_656]	0.73	1.47
1:A:19:GLN:CG	1:A:51:VAL:O[2_656]	0.87	1.33
1:A:19:GLN:CA	1:A:51:VAL:CG1[2_656]	0.87	1.33
1:A:16:LEU:N	1:A:52:PRO:CG[2_656]	0.89	1.31
1:A:19:GLN:N	1:A:51:VAL:CA[2_656]	0.90	1.30
1:A:21:TYR:CD2	1:A:53:SER:OG[2_656]	0.96	1.24
1:A:38:SER:N	1:A:260:SER:CA[1_455]	0.97	1.23
1:A:18:SER:CB	1:A:50:MET:C[2_656]	1.01	1.19
1:A:37:SER:N	1:A:260:SER:OG[1_455]	1.02	1.18
1:A:21:TYR:CE2	1:A:53:SER:OG[2_656]	1.06	1.14
1:A:36:ASP:OD2	1:A:259:ASP:OD1[1_455]	1.06	1.14
1:A:20:GLY:CA	1:A:106:TRP:CE3[2_656]	1.07	1.13
1:A:19:GLN:OE1	1:A:53:SER:N[2_656]	1.10	1.10
1:A:38:SER:OG	1:A:260:SER:C[1_455]	1.11	1.09
1:A:18:SER:OG	1:A:50:MET:O[2_656]	1.14	1.06
1:A:206:GLN:CD	1:A:242:THR:CG2[1_556]	1.15	1.05
1:A:38:SER:N	1:A:260:SER:CB[1_455]	1.16	1.04
1:A:20:GLY:C	1:A:106:TRP:CZ3[2_656]	1.17	1.03
1:A:19:GLN:OE1	1:A:52:PRO:C[2_656]	1.19	1.01
1:A:36:ASP:CG	1:A:259:ASP:OD2[1_455]	1.19	1.01
1:A:21:TYR:CE2	1:A:53:SER:CB[2_656]	1.20	1.00
1:A:19:GLN:OE1	1:A:52:PRO:CA[2_656]	1.20	1.00
1:A:206:GLN:CD	1:A:242:THR:CB[1_556]	1.21	0.99
1:A:21:TYR:N	1:A:106:TRP:CH2[2_656]	1.21	0.99
1:A:38:SER:CA	1:A:260:SER:CA[1_455]	1.22	0.98
1:A:16:LEU:CD1	1:A:52:PRO:CB[2_656]	1.23	0.97
1:A:19:GLN:CA	1:A:51:VAL:CB[2_656]	1.26	0.94
1:A:16:LEU:CD1	1:A:52:PRO:O[2_656]	1.27	0.93
1:A:16:LEU:CD1	1:A:52:PRO:CA[2_656]	1.28	0.92
1:A:36:ASP:OD2	1:A:259:ASP:OD2[1_455]	1.32	0.88
1:A:16:LEU:CA	1:A:52:PRO:CD[2_656]	1.33	0.87
1:A:19:GLN:CD	1:A:51:VAL:O[2_656]	1.34	0.86
1:A:38:SER:CB	1:A:259:ASP:O[1_455]	1.37	0.83
1:A:37:SER:C	1:A:260:SER:CB[1_455]	1.38	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:C	1:A:52:PRO:CD[2_656]	1.40	0.80
1:A:22:THR:OG1	1:A:103:GLN:NE2[2_656]	1.40	0.80
1:A:18:SER:C	1:A:51:VAL:CB[2_656]	1.43	0.77
1:A:16:LEU:CD1	1:A:52:PRO:C[2_656]	1.46	0.74
1:A:206:GLN:OE1	1:A:242:THR:CB[1_556]	1.47	0.73
1:A:36:ASP:CB	1:A:259:ASP:OD2[1_455]	1.48	0.72
1:A:38:SER:CB	1:A:260:SER:CA[1_455]	1.49	0.71
1:A:18:SER:CA	1:A:50:MET:O[2_656]	1.51	0.69
1:A:38:SER:CB	1:A:259:ASP:C[1_455]	1.53	0.67
1:A:19:GLN:CD	1:A:53:SER:N[2_656]	1.54	0.66
1:A:20:GLY:O	1:A:106:TRP:CH2[2_656]	1.56	0.64
1:A:19:GLN:C	1:A:51:VAL:CG1[2_656]	1.57	0.63
1:A:20:GLY:CA	1:A:106:TRP:CH2[2_656]	1.60	0.60
1:A:20:GLY:N	1:A:51:VAL:CG2[2_656]	1.62	0.58
1:A:38:SER:CA	1:A:260:SER:N[1_455]	1.65	0.55
1:A:38:SER:CB	1:A:260:SER:N[1_455]	1.65	0.55
1:A:16:LEU:CA	1:A:52:PRO:CB[2_656]	1.66	0.54
1:A:17:HIS:O	1:A:106:TRP:CE2[2_656]	1.66	0.54
1:A:36:ASP:CG	1:A:259:ASP:CG[1_455]	1.66	0.54
1:A:37:SER:CA	1:A:260:SER:CB[1_455]	1.67	0.53
1:A:20:GLY:N	1:A:106:TRP:CZ3[2_656]	1.71	0.49
1:A:19:GLN:CG	1:A:51:VAL:C[2_656]	1.71	0.49
1:A:16:LEU:CG	1:A:52:PRO:O[2_656]	1.72	0.48
1:A:17:HIS:C	1:A:106:TRP:NE1[2_656]	1.73	0.47
1:A:16:LEU:N	1:A:52:PRO:CB[2_656]	1.74	0.46
1:A:16:LEU:CB	1:A:52:PRO:CG[2_656]	1.75	0.45
1:A:212:ASN:OD1	1:A:258:GLY:CA[1_455]	1.75	0.45
1:A:36:ASP:C	1:A:260:SER:OG[1_455]	1.76	0.44
1:A:145:SER:CA	1:A:209:LEU:CD2[1_554]	1.76	0.44
1:A:20:GLY:N	1:A:106:TRP:CE3[2_656]	1.76	0.44
1:A:38:SER:N	1:A:260:SER:N[1_455]	1.77	0.43
1:A:38:SER:CB	1:A:261:PHE:N[1_455]	1.78	0.42
1:A:19:GLN:CA	1:A:51:VAL:CG2[2_656]	1.78	0.42
1:A:18:SER:O	1:A:106:TRP:CG[2_656]	1.78	0.42
1:A:16:LEU:O	1:A:52:PRO:CD[2_656]	1.78	0.42
1:A:37:SER:N	1:A:260:SER:CB[1_455]	1.79	0.41
1:A:19:GLN:N	1:A:51:VAL:CG1[2_656]	1.79	0.41
1:A:17:HIS:O	1:A:106:TRP:CD1[2_656]	1.80	0.40
1:A:206:GLN:NE2	1:A:242:THR:CB[1_556]	1.80	0.40
1:A:36:ASP:CG	1:A:259:ASP:OD1[1_455]	1.82	0.38
1:A:19:GLN:OE1	1:A:52:PRO:N[2_656]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:N	1:A:51:VAL:N[2_656]	1.83	0.37
1:A:15:ALA:O	1:A:52:PRO:CD[2_656]	1.86	0.34
1:A:115:ILE:O	1:A:213:LYS:NZ[1_554]	1.88	0.32
1:A:39:HIS:N	1:A:260:SER:N[1_455]	1.88	0.32
1:A:16:LEU:C	1:A:52:PRO:CG[2_656]	1.88	0.32
1:A:16:LEU:N	1:A:52:PRO:CD[2_656]	1.89	0.31
1:A:18:SER:O	1:A:106:TRP:CD2[2_656]	1.90	0.30
1:A:38:SER:CB	1:A:260:SER:C[1_455]	1.90	0.30
1:A:38:SER:OG	1:A:260:SER:CA[1_455]	1.90	0.30
1:A:20:GLY:C	1:A:106:TRP:CZ2[2_656]	1.90	0.30
1:A:53:SER:O	1:A:237:LYS:NZ[2_646]	1.92	0.28
1:A:21:TYR:CG	1:A:53:SER:OG[2_656]	1.92	0.28
1:A:16:LEU:CG	1:A:52:PRO:CB[2_656]	1.93	0.27
1:A:19:GLN:C	1:A:51:VAL:CB[2_656]	1.93	0.27
1:A:19:GLN:C	1:A:51:VAL:CG2[2_656]	1.94	0.26
1:A:206:GLN:CG	1:A:242:THR:OG1[1_556]	1.94	0.26
1:A:36:ASP:OD1	1:A:259:ASP:OD1[1_455]	1.95	0.25
1:A:38:SER:OG	1:A:261:PHE:CA[1_455]	1.97	0.23
1:A:18:SER:O	1:A:51:VAL:CB[2_656]	1.97	0.23
1:A:19:GLN:N	1:A:51:VAL:CG2[2_656]	1.98	0.22
1:A:146:GLY:CA	1:A:214:TYR:O[1_554]	1.98	0.22
1:A:18:SER:C	1:A:51:VAL:CA[2_656]	1.99	0.21
1:A:20:GLY:N	1:A:51:VAL:CB[2_656]	1.99	0.21
1:A:19:GLN:CB	1:A:51:VAL:C[2_656]	1.99	0.21
1:A:206:GLN:CD	1:A:242:THR:OG1[1_556]	1.99	0.21
1:A:22:THR:CB	1:A:103:GLN:NE2[2_656]	2.00	0.20
1:A:18:SER:CB	1:A:51:VAL:N[2_656]	2.01	0.19
1:A:19:GLN:CB	1:A:51:VAL:O[2_656]	2.02	0.18
1:A:21:TYR:CZ	1:A:53:SER:OG[2_656]	2.04	0.16
1:A:15:ALA:C	1:A:52:PRO:CG[2_656]	2.05	0.15
1:A:146:GLY:N	1:A:214:TYR:O[1_554]	2.06	0.14
1:A:21:TYR:CZ	1:A:53:SER:CB[2_656]	2.09	0.11
1:A:36:ASP:OD2	1:A:259:ASP:CB[1_455]	2.09	0.11
1:A:21:TYR:N	1:A:106:TRP:CZ2[2_656]	2.09	0.11
1:A:19:GLN:CB	1:A:51:VAL:CG2[2_656]	2.09	0.11
1:A:20:GLY:O	1:A:106:TRP:CZ3[2_656]	2.09	0.11
1:A:19:GLN:CD	1:A:51:VAL:C[2_656]	2.10	0.10
1:A:21:TYR:CD2	1:A:53:SER:CB[2_656]	2.10	0.10
1:A:22:THR:CG2	1:A:103:GLN:NE2[2_656]	2.10	0.10
1:A:38:SER:O	1:A:258:GLY:O[1_455]	2.11	0.09
1:A:39:HIS:N	1:A:259:ASP:C[1_455]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:CA	1:A:260:SER:OG[1_455]	2.11	0.09
1:A:38:SER:CA	1:A:259:ASP:C[1_455]	2.12	0.08
1:A:206:GLN:NE2	1:A:242:THR:CG2[1_556]	2.12	0.08
1:A:21:TYR:N	1:A:106:TRP:CZ3[2_656]	2.13	0.07
1:A:56:PRO:CG	1:A:194:PRO:CB[1_455]	2.13	0.07
1:A:144:ALA:O	1:A:209:LEU:CD2[1_554]	2.14	0.06
1:A:15:ALA:C	1:A:52:PRO:CD[2_656]	2.14	0.06
1:A:38:SER:OG	1:A:260:SER:O[1_455]	2.14	0.06
1:A:19:GLN:CA	1:A:51:VAL:CA[2_656]	2.15	0.05
1:A:18:SER:OG	1:A:50:MET:C[2_656]	2.15	0.05
1:A:19:GLN:N	1:A:51:VAL:C[2_656]	2.16	0.04
1:A:36:ASP:CA	1:A:260:SER:OG[1_455]	2.17	0.03
1:A:206:GLN:OE1	1:A:242:THR:CA[1_556]	2.18	0.02
1:A:19:GLN:NE2	1:A:51:VAL:O[2_656]	2.18	0.02
1:A:19:GLN:OE1	1:A:51:VAL:C[2_656]	2.19	0.01
1:A:38:SER:C	1:A:260:SER:N[1_455]	2.19	0.01
1:A:20:GLY:CA	1:A:106:TRP:CD2[2_656]	2.19	0.01

## 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	271/275 (98%)	186 (69%)	51 (19%)	34 (12%)	<b>0</b> <b>1</b>

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	12	LYS
1	A	62	ASN
1	A	63	SER
1	A	81	VAL
1	A	152	ALA

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Mol	Chain	Res	Type
1	A	153	ALA
1	A	155	ASN
1	A	156	GLU
1	A	186	ARG
1	A	203	VAL
1	A	271	GLN
1	A	2	GLN
1	A	3	SER
1	A	19	GLN
1	A	25	ASN
1	A	182	SER
1	A	15	ALA
1	A	77	ASN
1	A	126	LEU
1	A	169	GLY
1	A	196	LEU
1	A	235	LEU
1	A	75	LEU
1	A	98	ASP
1	A	245	GLN
1	A	213	LYS
1	A	228	ALA
1	A	249	SER
1	A	99	ALA
1	A	7	GLY
1	A	14	PRO
1	A	202	GLY
1	A	194	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	A	204/205 (100%)	116 (57%)	88 (43%)	<b>0</b> <b>0</b>

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	6	TYR
1	A	8	VAL
1	A	9	SER
1	A	11	ILE
1	A	16	LEU
1	A	22	THR
1	A	24	SER
1	A	25	ASN
1	A	27	LYS
1	A	32	ASP
1	A	35	ILE
1	A	36	ASP
1	A	37	SER
1	A	42	LEU
1	A	44	VAL
1	A	50	MET
1	A	61	ASP
1	A	62	ASN
1	A	63	SER
1	A	68	VAL
1	A	71	THR
1	A	72	VAL
1	A	75	LEU
1	A	76	ASN
1	A	78	SER
1	A	82	LEU
1	A	84	VAL
1	A	87	SER
1	A	88	SER
1	A	96	LEU
1	A	103	GLN
1	A	105	SER
1	A	107	ILE
1	A	108	ILE
1	A	109	ASN
1	A	111	ILE
1	A	115	ILE
1	A	117	ASN
1	A	119	MET
1	A	120	ASP
1	A	121	VAL
1	A	122	ILE

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Mol	Chain	Res	Type
1	A	123	ASN
1	A	124	MET
1	A	125	SER
1	A	126	LEU
1	A	135	LEU
1	A	145	SER
1	A	147	VAL
1	A	148	VAL
1	A	150	VAL
1	A	155	ASN
1	A	156	GLU
1	A	159	THR
1	A	161	SER
1	A	162	SER
1	A	165	VAL
1	A	174	VAL
1	A	180	VAL
1	A	183	SER
1	A	191	SER
1	A	196	LEU
1	A	197	ASP
1	A	199	MET
1	A	213	LYS
1	A	218	ASN
1	A	221	SER
1	A	222	MET
1	A	224	SER
1	A	233	LEU
1	A	235	LEU
1	A	236	SER
1	A	238	HIS
1	A	240	ASN
1	A	242	THR
1	A	243	ASN
1	A	247	ARG
1	A	248	SER
1	A	249	SER
1	A	252	ASN
1	A	253	THR
1	A	254	THR
1	A	256	LYS
1	A	257	LEU

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Mol	Chain	Res	Type
1	A	261	PHE
1	A	262	TYR
1	A	271	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	25	ASN
1	A	39	HIS
1	A	67	HIS
1	A	76	ASN
1	A	103	GLN
1	A	109	ASN
1	A	117	ASN
1	A	123	ASN
1	A	155	ASN
1	A	238	HIS
1	A	243	ASN
1	A	275	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ACN	A	276	-	3,3,3	2.30	2 (66%)	3,3,3	1.70	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACN	A	276	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	276	ACN	O-C	-2.81	1.02	1.22
2	A	276	ACN	C2-C	2.78	1.66	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	276	ACN	O-C-C1	2.49	136.23	120.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	276	ACN	7	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.