



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:51 PM UTC

PDB ID : 2SBT / pdb_00002sbt
Title : A COMPARISON OF THE THREE-DIMENSIONAL STRUCTURES OF
SUBTILISIN BPN AND SUBTILISIN NOVO
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

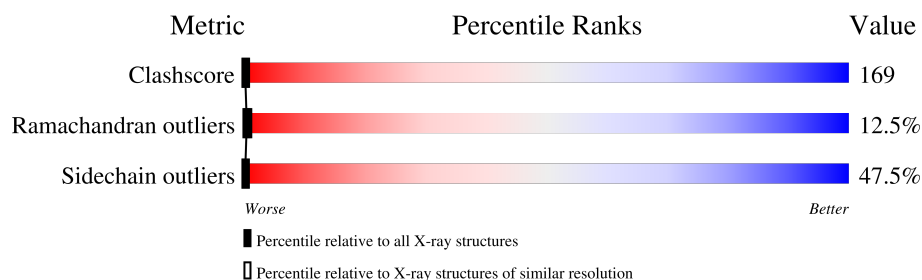
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

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.

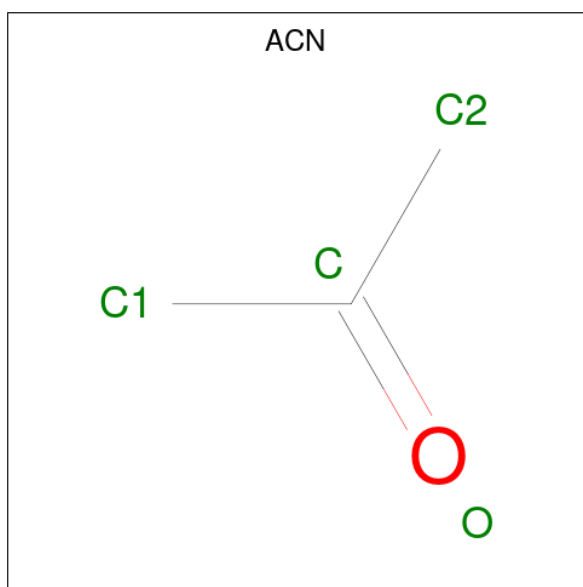
- Molecule 1 is a protein called SUBTILISIN NOVO.

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 (CCD ID: ACN) (formula: C₃H₆O).



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		

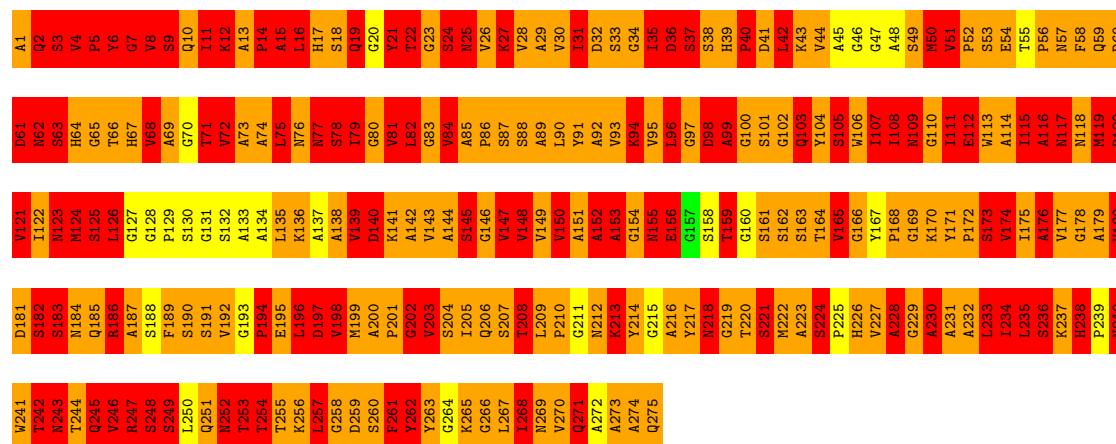
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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 is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.20Å 78.50Å 37.10Å 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 ²)	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	5.87	658/1971 (33.4%)	4.16	482/2688 (17.9%)

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 (658) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	GLY	C-N	53.28	1.89	1.33
1	A	59	GLN	C-N	29.63	1.72	1.33
1	A	195	GLU	C-N	28.83	1.74	1.33
1	A	173	SER	C-N	-26.45	0.75	1.33
1	A	70	GLY	N-CA	-24.82	1.15	1.45
1	A	97	GLY	C-N	22.71	1.65	1.33
1	A	226	HIS	CE1-NE2	21.00	1.53	1.32
1	A	131	GLY	N-CA	19.84	1.66	1.45
1	A	123	ASN	C-N	19.73	1.58	1.33
1	A	113	TRP	NE1-CE2	19.39	1.58	1.37
1	A	100	GLY	C-O	19.20	1.36	1.23
1	A	111	ILE	C-O	-19.17	1.01	1.24
1	A	242	THR	N-CA	18.92	1.68	1.45
1	A	30	VAL	CA-C	17.97	1.75	1.52
1	A	59	GLN	N-CA	17.60	1.67	1.46
1	A	98	ASP	N-CA	-17.41	1.23	1.46
1	A	145	SER	N-CA	17.34	1.71	1.46
1	A	213	LYS	N-CA	-16.96	1.24	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	SER	C-N	-16.62	1.10	1.33
1	A	268	ILE	N-CA	16.61	1.66	1.46
1	A	54	GLU	CA-CB	16.59	1.74	1.52
1	A	231	ALA	CA-C	16.55	1.73	1.52
1	A	244	THR	N-CA	16.47	1.65	1.46
1	A	72	VAL	CA-C	16.30	1.71	1.52
1	A	71	THR	C-N	-16.26	1.14	1.33
1	A	114	ALA	C-N	-16.25	1.10	1.33
1	A	73	ALA	C-N	-16.09	1.12	1.33
1	A	235	LEU	N-CA	16.03	1.66	1.46
1	A	208	THR	CA-C	15.88	1.72	1.52
1	A	34	GLY	C-O	-15.86	1.01	1.23
1	A	259	ASP	N-CA	15.66	1.66	1.46
1	A	209	LEU	CA-C	15.54	1.68	1.52
1	A	52	PRO	C-N	-15.40	1.12	1.33
1	A	231	ALA	C-O	-15.39	1.06	1.24
1	A	4	VAL	CA-C	14.93	1.65	1.52
1	A	104	TYR	CA-C	14.84	1.72	1.52
1	A	128	GLY	C-N	-14.78	1.15	1.34
1	A	146	GLY	C-N	-14.77	1.16	1.33
1	A	146	GLY	CA-C	14.71	1.72	1.51
1	A	211	GLY	CA-C	14.52	1.72	1.51
1	A	94	LYS	C-N	-14.50	1.15	1.33
1	A	106	TRP	NE1-CE2	14.47	1.53	1.37
1	A	80	GLY	C-O	-14.43	1.04	1.23
1	A	96	LEU	N-CA	-14.30	1.27	1.45
1	A	114	ALA	C-O	14.27	1.42	1.24
1	A	111	ILE	CA-C	14.16	1.70	1.52
1	A	148	VAL	C-O	-14.08	1.08	1.24
1	A	42	LEU	C-O	-14.07	1.05	1.23
1	A	149	VAL	N-CA	-13.99	1.28	1.46
1	A	43	LYS	C-O	-13.95	1.07	1.23
1	A	108	ILE	C-N	-13.82	1.15	1.33
1	A	3	SER	N-CA	13.81	1.64	1.46
1	A	69	ALA	C-N	13.78	1.50	1.33
1	A	35	ILE	C-O	-13.77	1.07	1.23
1	A	211	GLY	C-N	-13.66	1.16	1.33
1	A	142	ALA	N-CA	13.66	1.63	1.46
1	A	136	LYS	CA-C	13.64	1.70	1.52
1	A	274	ALA	CA-CB	13.52	1.74	1.53
1	A	249	SER	C-N	-13.39	1.16	1.33
1	A	63	SER	N-CA	13.34	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	ILE	CA-CB	13.33	1.69	1.53
1	A	247	ARG	NE-CZ	13.33	1.47	1.33
1	A	52	PRO	N-CA	13.28	1.64	1.47
1	A	112	GLU	C-N	-13.16	1.15	1.33
1	A	121	VAL	C-N	-13.13	1.17	1.33
1	A	233	LEU	CA-CB	13.03	1.75	1.53
1	A	131	GLY	CA-C	13.01	1.64	1.52
1	A	238	HIS	CG-CD2	12.92	1.50	1.35
1	A	23	GLY	CA-C	12.79	1.70	1.51
1	A	33	SER	N-CA	-12.64	1.29	1.46
1	A	74	ALA	N-CA	12.61	1.61	1.46
1	A	67	HIS	ND1-CE1	12.60	1.45	1.32
1	A	15	ALA	CA-C	12.55	1.69	1.52
1	A	146	GLY	N-CA	-12.52	1.27	1.45
1	A	109	ASN	N-CA	12.52	1.61	1.46
1	A	234	ILE	CA-C	12.44	1.72	1.52
1	A	227	VAL	CA-C	12.43	1.68	1.52
1	A	147	VAL	C-N	12.36	1.48	1.33
1	A	208	THR	C-N	12.35	1.48	1.32
1	A	125	SER	N-CA	12.28	1.62	1.46
1	A	144	ALA	C-O	-12.28	1.06	1.24
1	A	140	ASP	CA-C	12.24	1.69	1.52
1	A	7	GLY	C-N	-12.22	1.17	1.33
1	A	238	HIS	CE1-NE2	12.16	1.44	1.32
1	A	251	GLN	CA-C	12.13	1.68	1.52
1	A	241	TRP	C-N	-12.07	1.14	1.33
1	A	39	HIS	CG-CD2	-12.05	1.22	1.35
1	A	213	LYS	CA-C	-12.05	1.36	1.52
1	A	94	LYS	C-O	12.04	1.38	1.24
1	A	174	VAL	CA-C	11.98	1.66	1.52
1	A	250	LEU	N-CA	11.97	1.60	1.46
1	A	112	GLU	C-O	11.94	1.38	1.24
1	A	89	ALA	CA-CB	11.93	1.67	1.52
1	A	38	SER	N-CA	-11.93	1.30	1.46
1	A	123	ASN	N-CA	11.90	1.60	1.46
1	A	229	GLY	C-O	-11.84	1.07	1.23
1	A	166	GLY	CA-C	11.83	1.72	1.52
1	A	252	ASN	N-CA	11.81	1.60	1.46
1	A	174	VAL	C-N	-11.80	1.18	1.33
1	A	59	GLN	C-O	-11.72	1.10	1.24
1	A	19	GLN	C-O	-11.71	1.09	1.24
1	A	210	PRO	CA-CB	11.57	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLN	CD-OE1	-11.54	1.01	1.23
1	A	113	TRP	CA-C	11.52	1.68	1.52
1	A	64	HIS	CA-CB	11.47	1.72	1.53
1	A	129	PRO	N-CD	11.40	1.63	1.47
1	A	113	TRP	C-O	-11.39	1.10	1.24
1	A	76	ASN	CA-C	11.34	1.67	1.52
1	A	134	ALA	C-O	-11.28	1.11	1.24
1	A	167	TYR	CA-C	11.27	1.64	1.52
1	A	148	VAL	N-CA	-11.26	1.30	1.46
1	A	228	ALA	CA-C	11.25	1.67	1.52
1	A	209	LEU	C-O	11.22	1.35	1.24
1	A	17	HIS	C-N	-11.22	1.18	1.33
1	A	174	VAL	C-O	11.17	1.39	1.24
1	A	87	SER	CA-C	-11.14	1.38	1.53
1	A	128	GLY	N-CA	11.12	1.59	1.44
1	A	144	ALA	CA-C	11.02	1.71	1.52
1	A	206	GLN	C-O	11.01	1.37	1.23
1	A	5	PRO	C-N	11.00	1.48	1.33
1	A	107	ILE	N-CA	-10.97	1.33	1.46
1	A	58	PHE	N-CA	10.96	1.60	1.46
1	A	117	ASN	N-CA	10.95	1.58	1.46
1	A	113	TRP	CG-CD2	-10.89	1.24	1.43
1	A	114	ALA	CA-C	10.88	1.67	1.52
1	A	183	SER	N-CA	10.84	1.60	1.46
1	A	186	ARG	CZ-NH2	10.83	1.47	1.33
1	A	61	ASP	C-N	10.81	1.48	1.33
1	A	141	LYS	CA-C	10.80	1.67	1.52
1	A	217	TYR	C-N	-10.77	1.19	1.33
1	A	243	ASN	CG-OD1	10.75	1.44	1.23
1	A	159	THR	N-CA	10.73	1.55	1.46
1	A	100	GLY	CA-C	-10.71	1.40	1.52
1	A	9	SER	CA-C	10.66	1.67	1.52
1	A	71	THR	CA-CB	10.63	1.71	1.53
1	A	99	ALA	C-O	-10.63	1.10	1.24
1	A	183	SER	CA-C	10.57	1.68	1.52
1	A	143	VAL	CA-C	10.56	1.66	1.52
1	A	253	THR	C-N	10.55	1.50	1.33
1	A	172	PRO	N-CA	10.53	1.61	1.47
1	A	255	THR	C-O	10.52	1.36	1.23
1	A	230	ALA	N-CA	10.51	1.59	1.46
1	A	116	ALA	CA-CB	10.51	1.69	1.53
1	A	83	GLY	C-O	10.48	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	LYS	CA-CB	10.47	1.72	1.53
1	A	22	THR	CA-C	-10.47	1.35	1.52
1	A	48	ALA	C-O	10.46	1.37	1.24
1	A	214	TYR	CE2-CZ	10.44	1.63	1.38
1	A	267	LEU	C-O	-10.39	1.10	1.23
1	A	103	GLN	CA-C	-10.38	1.39	1.52
1	A	237	LYS	CA-C	10.36	1.67	1.52
1	A	79	ILE	C-N	-10.35	1.18	1.33
1	A	36	ASP	N-CA	10.35	1.58	1.46
1	A	62	ASN	C-N	-10.34	1.19	1.33
1	A	182	SER	N-CA	10.32	1.59	1.46
1	A	139	VAL	N-CA	-10.29	1.34	1.46
1	A	251	GLN	C-N	-10.27	1.20	1.33
1	A	247	ARG	CA-C	10.24	1.67	1.52
1	A	1	ALA	C-N	-10.17	1.19	1.33
1	A	185	GLN	C-O	-10.15	1.11	1.24
1	A	264	GLY	N-CA	10.14	1.60	1.45
1	A	139	VAL	C-O	10.12	1.36	1.24
1	A	57	ASN	CA-C	10.09	1.65	1.52
1	A	17	HIS	CE1-NE2	10.02	1.42	1.32
1	A	74	ALA	CA-CB	10.01	1.68	1.53
1	A	236	SER	CA-C	-10.01	1.41	1.52
1	A	92	ALA	CA-CB	9.98	1.66	1.53
1	A	92	ALA	CA-C	9.95	1.65	1.52
1	A	99	ALA	C-N	9.91	1.46	1.32
1	A	120	ASP	N-CA	9.90	1.58	1.46
1	A	192	VAL	CA-C	9.90	1.65	1.52
1	A	133	ALA	C-N	9.88	1.47	1.33
1	A	218	ASN	C-N	9.85	1.43	1.33
1	A	46	GLY	CA-C	-9.85	1.39	1.51
1	A	60	ASP	CG-OD1	-9.83	1.06	1.25
1	A	258	GLY	C-O	-9.81	1.10	1.23
1	A	109	ASN	C-O	-9.78	1.12	1.24
1	A	151	ALA	C-N	-9.77	1.20	1.33
1	A	178	GLY	CA-C	9.75	1.62	1.51
1	A	126	LEU	C-O	-9.72	1.11	1.24
1	A	268	ILE	C-N	-9.68	1.20	1.33
1	A	21	TYR	CG-CD2	9.63	1.59	1.39
1	A	175	ILE	C-N	-9.60	1.19	1.33
1	A	74	ALA	C-O	-9.59	1.13	1.24
1	A	132	SER	N-CA	9.59	1.59	1.45
1	A	102	GLY	CA-C	9.58	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	GLN	C-N	-9.58	1.20	1.33
1	A	202	GLY	N-CA	9.57	1.59	1.45
1	A	220	THR	C-O	-9.54	1.11	1.24
1	A	197	ASP	CA-CB	9.53	1.67	1.53
1	A	87	SER	CA-CB	9.51	1.66	1.53
1	A	260	SER	CA-CB	9.50	1.64	1.52
1	A	99	ALA	N-CA	-9.48	1.33	1.46
1	A	139	VAL	C-N	-9.48	1.20	1.33
1	A	262	TYR	C-N	-9.43	1.21	1.33
1	A	35	ILE	C-N	9.38	1.46	1.33
1	A	190	SER	CB-OG	9.34	1.60	1.42
1	A	56	PRO	N-CA	-9.32	1.33	1.47
1	A	149	VAL	CA-C	9.30	1.64	1.52
1	A	113	TRP	N-CA	-9.30	1.34	1.46
1	A	186	ARG	N-CA	9.29	1.58	1.46
1	A	67	HIS	CD2-NE2	-9.29	1.27	1.37
1	A	101	SER	CB-OG	9.28	1.60	1.42
1	A	44	VAL	C-O	-9.27	1.14	1.24
1	A	76	ASN	N-CA	-9.27	1.34	1.46
1	A	14	PRO	N-CD	-9.26	1.34	1.47
1	A	221	SER	C-N	-9.26	1.19	1.33
1	A	235	LEU	C-N	-9.25	1.21	1.33
1	A	61	ASP	N-CA	9.23	1.59	1.46
1	A	141	LYS	C-O	-9.21	1.12	1.24
1	A	242	THR	C-N	9.18	1.45	1.33
1	A	175	ILE	CB-CG1	9.13	1.71	1.53
1	A	49	SER	CB-OG	9.12	1.60	1.42
1	A	43	LYS	CA-C	9.10	1.62	1.52
1	A	57	ASN	C-O	-9.09	1.06	1.24
1	A	25	ASN	CA-CB	-9.09	1.38	1.53
1	A	98	ASP	C-N	-9.06	1.21	1.33
1	A	47	GLY	N-CA	9.05	1.53	1.45
1	A	144	ALA	N-CA	9.04	1.59	1.46
1	A	238	HIS	CD2-NE2	9.04	1.47	1.37
1	A	256	LYS	C-N	9.04	1.46	1.33
1	A	99	ALA	CA-CB	9.02	1.68	1.53
1	A	246	VAL	CA-C	9.02	1.64	1.52
1	A	53	SER	N-CA	8.99	1.57	1.46
1	A	79	ILE	CA-CB	-8.99	1.42	1.54
1	A	163	SER	CB-OG	8.98	1.60	1.42
1	A	106	TRP	N-CA	8.98	1.57	1.46
1	A	118	ASN	C-O	8.97	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	TYR	CE2-CZ	8.96	1.59	1.38
1	A	151	ALA	CA-C	8.90	1.63	1.52
1	A	273	ALA	C-N	-8.88	1.22	1.33
1	A	202	GLY	C-N	-8.88	1.21	1.33
1	A	138	ALA	CA-C	8.87	1.65	1.52
1	A	201	PRO	C-O	-8.83	1.12	1.24
1	A	208	THR	C-O	-8.80	1.13	1.23
1	A	177	VAL	N-CA	-8.79	1.35	1.46
1	A	108	ILE	CA-C	8.76	1.64	1.52
1	A	161	SER	C-N	8.75	1.46	1.33
1	A	265	LYS	N-CA	-8.75	1.33	1.46
1	A	139	VAL	CA-C	8.75	1.63	1.52
1	A	149	VAL	CA-CB	8.72	1.65	1.54
1	A	3	SER	CA-C	-8.70	1.41	1.52
1	A	27	LYS	CA-C	8.68	1.63	1.52
1	A	106	TRP	C-N	8.67	1.44	1.33
1	A	81	VAL	C-N	-8.64	1.23	1.33
1	A	77	ASN	C-O	-8.63	1.13	1.24
1	A	248	SER	CA-CB	8.62	1.67	1.53
1	A	156	GLU	CD-OE1	-8.61	1.08	1.25
1	A	232	ALA	C-O	-8.58	1.14	1.24
1	A	17	HIS	CG-ND1	-8.56	1.28	1.38
1	A	35	ILE	CA-CB	-8.54	1.45	1.55
1	A	254	THR	N-CA	8.51	1.57	1.45
1	A	130	SER	C-N	8.50	1.44	1.33
1	A	136	LYS	N-CA	-8.49	1.34	1.46
1	A	126	LEU	C-N	-8.49	1.21	1.33
1	A	67	HIS	CE1-NE2	8.47	1.41	1.32
1	A	30	VAL	CA-CB	-8.45	1.43	1.54
1	A	209	LEU	N-CA	8.44	1.52	1.45
1	A	226	HIS	C-N	-8.42	1.22	1.33
1	A	164	THR	C-O	8.40	1.37	1.23
1	A	147	VAL	CA-CB	8.39	1.62	1.54
1	A	109	ASN	CA-C	8.38	1.63	1.52
1	A	64	HIS	ND1-CE1	8.38	1.41	1.32
1	A	231	ALA	C-N	8.37	1.44	1.33
1	A	190	SER	C-O	8.33	1.33	1.24
1	A	82	LEU	CA-CB	8.31	1.68	1.53
1	A	123	ASN	C-O	-8.31	1.14	1.24
1	A	233	LEU	CA-C	8.30	1.64	1.52
1	A	103	GLN	N-CA	8.30	1.56	1.46
1	A	12	LYS	CA-C	8.27	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	THR	C-N	-8.27	1.22	1.33
1	A	115	ILE	C-O	8.27	1.34	1.24
1	A	202	GLY	CA-C	8.24	1.63	1.51
1	A	132	SER	C-O	8.23	1.36	1.24
1	A	28	VAL	CA-C	8.23	1.62	1.52
1	A	16	LEU	C-O	-8.22	1.13	1.24
1	A	239	PRO	CA-C	8.21	1.64	1.52
1	A	268	ILE	CA-CB	8.21	1.63	1.54
1	A	154	GLY	C-O	-8.20	1.12	1.23
1	A	155	ASN	C-N	8.20	1.45	1.33
1	A	258	GLY	CA-C	8.17	1.63	1.51
1	A	103	GLN	C-O	-8.16	1.14	1.23
1	A	184	ASN	N-CA	-8.16	1.34	1.46
1	A	212	ASN	CA-CB	8.13	1.65	1.52
1	A	171	TYR	CA-CB	-8.13	1.42	1.53
1	A	179	ALA	C-O	8.13	1.33	1.24
1	A	249	SER	CA-CB	8.12	1.67	1.53
1	A	245	GLN	C-N	8.11	1.44	1.34
1	A	60	ASP	CA-CB	8.10	1.65	1.53
1	A	206	GLN	C-N	8.10	1.45	1.33
1	A	94	LYS	CA-CB	8.08	1.64	1.53
1	A	176	ALA	C-O	8.05	1.33	1.24
1	A	64	HIS	C-N	-8.03	1.21	1.33
1	A	239	PRO	C-O	8.03	1.34	1.24
1	A	58	PHE	C-N	-8.02	1.22	1.33
1	A	105	SER	C-N	-8.02	1.22	1.33
1	A	95	VAL	C-O	7.99	1.37	1.23
1	A	2	GLN	C-O	7.99	1.34	1.24
1	A	149	VAL	C-O	-7.99	1.14	1.24
1	A	197	ASP	CA-C	7.99	1.62	1.52
1	A	119	MET	C-O	7.98	1.33	1.23
1	A	140	ASP	N-CA	7.98	1.56	1.46
1	A	247	ARG	CZ-NH2	-7.96	1.23	1.33
1	A	221	SER	C-O	7.95	1.34	1.24
1	A	40	PRO	C-N	7.90	1.44	1.33
1	A	255	THR	CA-CB	7.89	1.66	1.53
1	A	175	ILE	N-CA	-7.88	1.36	1.46
1	A	212	ASN	C-O	7.88	1.31	1.23
1	A	177	VAL	CA-CB	7.82	1.65	1.54
1	A	224	SER	CA-C	7.81	1.62	1.52
1	A	266	GLY	C-N	-7.80	1.22	1.33
1	A	16	LEU	CA-C	7.80	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	ALA	CA-C	7.80	1.63	1.52
1	A	66	THR	C-N	7.79	1.43	1.33
1	A	10	GLN	N-CA	7.78	1.56	1.46
1	A	182	SER	CA-C	-7.78	1.42	1.52
1	A	53	SER	CA-C	7.76	1.63	1.52
1	A	10	GLN	C-N	-7.75	1.24	1.34
1	A	30	VAL	C-N	-7.71	1.24	1.33
1	A	40	PRO	N-CA	7.71	1.57	1.47
1	A	19	GLN	CD-OE1	7.69	1.38	1.23
1	A	22	THR	CB-CG2	7.68	1.77	1.52
1	A	146	GLY	C-O	7.68	1.34	1.23
1	A	96	LEU	C-O	-7.67	1.14	1.23
1	A	71	THR	CA-C	7.66	1.63	1.52
1	A	212	ASN	CB-CG	7.65	1.71	1.52
1	A	270	VAL	CA-C	7.65	1.62	1.52
1	A	21	TYR	N-CA	7.64	1.56	1.46
1	A	72	VAL	C-N	-7.63	1.23	1.33
1	A	23	GLY	C-O	-7.62	1.13	1.23
1	A	120	ASP	CA-CB	7.61	1.65	1.53
1	A	263	TYR	C-O	7.60	1.34	1.23
1	A	60	ASP	CA-C	7.60	1.61	1.52
1	A	55	THR	N-CA	7.59	1.60	1.46
1	A	68	VAL	C-O	-7.59	1.15	1.24
1	A	196	LEU	CG-CD2	7.58	1.77	1.52
1	A	239	PRO	C-N	-7.56	1.23	1.33
1	A	113	TRP	CG-CD1	7.55	1.55	1.36
1	A	53	SER	C-N	-7.55	1.23	1.33
1	A	241	TRP	NE1-CE2	7.53	1.45	1.37
1	A	219	GLY	C-O	7.50	1.33	1.23
1	A	227	VAL	CA-CB	-7.50	1.44	1.54
1	A	236	SER	CB-OG	7.50	1.57	1.42
1	A	241	TRP	CG-CD2	-7.49	1.30	1.43
1	A	171	TYR	C-O	-7.46	1.16	1.24
1	A	134	ALA	C-N	-7.45	1.24	1.33
1	A	195	GLU	CD-OE1	7.42	1.39	1.25
1	A	56	PRO	CA-C	7.41	1.68	1.52
1	A	66	THR	CB-OG1	-7.41	1.31	1.43
1	A	31	ILE	N-CA	7.40	1.54	1.46
1	A	84	VAL	CA-C	7.39	1.62	1.52
1	A	132	SER	C-N	-7.38	1.22	1.33
1	A	196	LEU	N-CA	7.38	1.55	1.46
1	A	69	ALA	C-O	-7.37	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	VAL	C-O	-7.36	1.15	1.24
1	A	119	MET	N-CA	7.36	1.55	1.46
1	A	200	ALA	N-CA	7.36	1.56	1.46
1	A	224	SER	C-O	7.35	1.33	1.24
1	A	247	ARG	N-CA	7.35	1.55	1.46
1	A	131	GLY	C-O	7.34	1.33	1.23
1	A	208	THR	N-CA	-7.34	1.37	1.45
1	A	180	VAL	C-O	7.33	1.31	1.23
1	A	92	ALA	N-CA	-7.31	1.37	1.46
1	A	142	ALA	CA-C	7.31	1.62	1.52
1	A	86	PRO	N-CD	7.31	1.57	1.47
1	A	111	ILE	CA-CB	-7.30	1.44	1.54
1	A	27	LYS	C-N	-7.29	1.24	1.33
1	A	113	TRP	CD2-CE2	7.28	1.53	1.41
1	A	11	ILE	C-N	-7.28	1.23	1.33
1	A	19	GLN	CA-CB	7.27	1.65	1.53
1	A	217	TYR	CA-C	7.27	1.61	1.52
1	A	72	VAL	C-O	-7.27	1.16	1.24
1	A	5	PRO	CA-CB	-7.25	1.44	1.53
1	A	69	ALA	N-CA	7.23	1.55	1.46
1	A	140	ASP	C-N	7.23	1.44	1.33
1	A	270	VAL	C-O	-7.22	1.16	1.24
1	A	118	ASN	N-CA	7.22	1.57	1.46
1	A	91	TYR	CG-CD2	-7.20	1.24	1.39
1	A	274	ALA	C-N	-7.17	1.23	1.33
1	A	217	TYR	CG-CD2	-7.17	1.24	1.39
1	A	268	ILE	CB-CG1	7.12	1.67	1.53
1	A	232	ALA	CA-C	7.11	1.62	1.52
1	A	31	ILE	C-N	-7.11	1.23	1.33
1	A	263	TYR	C-N	-7.08	1.23	1.33
1	A	241	TRP	N-CA	7.05	1.54	1.45
1	A	184	ASN	CG-OD1	7.02	1.36	1.23
1	A	10	GLN	CA-C	-7.00	1.43	1.52
1	A	79	ILE	N-CA	6.99	1.55	1.46
1	A	220	THR	C-N	6.99	1.44	1.33
1	A	120	ASP	CA-C	-6.99	1.43	1.52
1	A	262	TYR	CB-CG	6.99	1.67	1.51
1	A	28	VAL	C-O	-6.98	1.16	1.24
1	A	94	LYS	CA-C	6.96	1.61	1.52
1	A	186	ARG	CD-NE	-6.96	1.36	1.46
1	A	60	ASP	C-N	-6.95	1.24	1.33
1	A	272	ALA	C-N	6.95	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	VAL	C-N	-6.93	1.24	1.33
1	A	196	LEU	CA-CB	6.93	1.65	1.53
1	A	98	ASP	CG-OD2	6.93	1.38	1.25
1	A	81	VAL	C-O	6.93	1.32	1.24
1	A	64	HIS	CA-C	-6.92	1.43	1.52
1	A	67	HIS	CB-CG	-6.91	1.40	1.50
1	A	6	TYR	CZ-OH	6.91	1.52	1.38
1	A	34	GLY	CA-C	6.90	1.60	1.52
1	A	204	SER	C-N	6.89	1.42	1.33
1	A	249	SER	CA-C	6.89	1.62	1.52
1	A	135	LEU	C-N	6.89	1.43	1.33
1	A	115	ILE	CA-CB	6.88	1.65	1.55
1	A	50	MET	C-O	6.88	1.32	1.24
1	A	60	ASP	C-O	-6.87	1.15	1.24
1	A	45	ALA	CA-C	6.87	1.61	1.52
1	A	240	ASN	CG-ND2	-6.86	1.18	1.33
1	A	217	TYR	CB-CG	6.86	1.66	1.51
1	A	196	LEU	C-N	-6.86	1.24	1.33
1	A	248	SER	CA-C	6.85	1.61	1.52
1	A	240	ASN	N-CA	-6.85	1.37	1.46
1	A	183	SER	CB-OG	6.82	1.55	1.42
1	A	238	HIS	CG-ND1	6.80	1.45	1.38
1	A	200	ALA	CA-C	6.79	1.61	1.52
1	A	2	GLN	CA-C	6.79	1.61	1.52
1	A	252	ASN	CG-OD1	6.76	1.36	1.23
1	A	183	SER	CA-CB	-6.76	1.41	1.53
1	A	252	ASN	CA-C	-6.75	1.43	1.52
1	A	209	LEU	C-N	-6.73	1.18	1.33
1	A	2	GLN	C-N	-6.72	1.24	1.33
1	A	96	LEU	CA-C	6.71	1.60	1.52
1	A	143	VAL	C-O	6.71	1.31	1.23
1	A	65	GLY	CA-C	6.70	1.61	1.51
1	A	142	ALA	C-O	6.68	1.32	1.24
1	A	91	TYR	C-N	-6.68	1.22	1.33
1	A	241	TRP	CA-C	6.66	1.61	1.52
1	A	87	SER	C-O	-6.64	1.14	1.23
1	A	264	GLY	C-N	6.64	1.43	1.33
1	A	112	GLU	N-CA	6.59	1.55	1.45
1	A	118	ASN	CA-CB	6.59	1.63	1.53
1	A	133	ALA	C-O	-6.58	1.15	1.24
1	A	272	ALA	CA-C	-6.57	1.44	1.52
1	A	114	ALA	N-CA	6.57	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	PRO	C-O	6.56	1.32	1.24
1	A	245	GLN	CA-C	-6.56	1.44	1.52
1	A	68	VAL	CA-CB	6.56	1.61	1.54
1	A	119	MET	CA-C	6.54	1.61	1.52
1	A	111	ILE	CB-CG1	6.53	1.66	1.53
1	A	60	ASP	CG-OD2	6.50	1.37	1.25
1	A	86	PRO	CA-C	6.50	1.62	1.52
1	A	25	ASN	C-O	6.50	1.32	1.24
1	A	180	VAL	CA-CB	-6.49	1.44	1.54
1	A	220	THR	N-CA	-6.48	1.37	1.45
1	A	236	SER	C-O	6.47	1.32	1.23
1	A	253	THR	C-O	-6.47	1.16	1.23
1	A	150	VAL	C-O	-6.47	1.17	1.24
1	A	213	LYS	CA-CB	6.46	1.64	1.53
1	A	112	GLU	CA-C	6.45	1.61	1.52
1	A	238	HIS	C-N	6.45	1.49	1.33
1	A	4	VAL	C-N	-6.44	1.26	1.33
1	A	112	GLU	CD-OE2	6.44	1.37	1.25
1	A	257	LEU	CA-C	6.43	1.61	1.52
1	A	129	PRO	N-CA	6.42	1.55	1.47
1	A	187	ALA	CA-C	6.41	1.60	1.52
1	A	41	ASP	C-N	-6.41	1.25	1.33
1	A	59	GLN	CD-NE2	-6.40	1.19	1.33
1	A	192	VAL	N-CA	-6.40	1.38	1.46
1	A	172	PRO	C-N	-6.39	1.24	1.33
1	A	181	ASP	C-O	-6.37	1.16	1.24
1	A	210	PRO	N-CD	6.37	1.56	1.47
1	A	40	PRO	N-CD	6.37	1.56	1.47
1	A	257	LEU	C-N	6.36	1.42	1.33
1	A	126	LEU	N-CA	6.34	1.54	1.46
1	A	229	GLY	CA-C	6.34	1.60	1.51
1	A	91	TYR	CE2-CZ	6.34	1.53	1.38
1	A	76	ASN	C-O	-6.34	1.16	1.24
1	A	136	LYS	CA-CB	6.33	1.63	1.53
1	A	174	VAL	CB-CG2	6.33	1.73	1.52
1	A	113	TRP	CD1-NE1	6.33	1.51	1.37
1	A	136	LYS	CG-CD	6.32	1.71	1.52
1	A	148	VAL	C-N	6.31	1.45	1.33
1	A	171	TYR	CA-C	6.30	1.61	1.52
1	A	86	PRO	C-O	-6.30	1.16	1.24
1	A	95	VAL	N-CA	6.28	1.54	1.46
1	A	158	SER	C-O	-6.28	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	TRP	CG-CD1	6.28	1.52	1.36
1	A	152	ALA	CA-C	6.26	1.61	1.52
1	A	26	VAL	CA-C	6.25	1.59	1.52
1	A	23	GLY	N-CA	6.25	1.54	1.45
1	A	145	SER	CB-OG	6.24	1.54	1.42
1	A	39	HIS	N-CA	6.24	1.53	1.45
1	A	175	ILE	CG1-CD1	6.23	1.76	1.51
1	A	128	GLY	CA-C	6.23	1.60	1.51
1	A	176	ALA	CA-CB	6.23	1.62	1.53
1	A	194	PRO	CG-CD	6.23	1.72	1.50
1	A	210	PRO	N-CA	6.22	1.55	1.47
1	A	163	SER	CA-CB	6.21	1.63	1.53
1	A	123	ASN	CB-CG	6.21	1.67	1.52
1	A	198	VAL	CA-CB	6.21	1.63	1.55
1	A	250	LEU	CA-C	-6.19	1.45	1.52
1	A	194	PRO	N-CA	-6.19	1.39	1.47
1	A	68	VAL	CA-C	-6.18	1.45	1.52
1	A	26	VAL	CB-CG1	6.17	1.73	1.52
1	A	17	HIS	N-CA	6.17	1.54	1.46
1	A	223	ALA	C-N	-6.16	1.20	1.33
1	A	240	ASN	CG-OD1	-6.16	1.11	1.23
1	A	58	PHE	CG-CD2	6.15	1.51	1.38
1	A	78	SER	C-O	-6.14	1.17	1.23
1	A	61	ASP	CG-OD1	-6.13	1.13	1.25
1	A	210	PRO	C-N	6.12	1.42	1.33
1	A	39	HIS	C-O	6.11	1.32	1.24
1	A	107	ILE	CA-CB	6.11	1.61	1.54
1	A	8	VAL	CA-CB	6.11	1.62	1.54
1	A	156	GLU	N-CA	-6.06	1.38	1.46
1	A	212	ASN	CA-C	-6.06	1.48	1.53
1	A	248	SER	C-N	6.06	1.42	1.33
1	A	245	GLN	N-CA	6.05	1.54	1.46
1	A	18	SER	N-CA	6.05	1.53	1.46
1	A	257	LEU	N-CA	6.04	1.53	1.46
1	A	18	SER	C-O	-6.03	1.16	1.24
1	A	5	PRO	CA-C	-6.02	1.46	1.52
1	A	68	VAL	C-N	-6.02	1.25	1.33
1	A	221	SER	CA-C	6.01	1.61	1.52
1	A	116	ALA	C-N	-6.01	1.24	1.34
1	A	194	PRO	CA-C	6.00	1.60	1.52
1	A	87	SER	C-N	6.00	1.41	1.33
1	A	56	PRO	C-O	-6.00	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	MET	N-CA	-5.99	1.38	1.46
1	A	237	LYS	CE-NZ	5.98	1.67	1.49
1	A	226	HIS	C-O	5.97	1.31	1.24
1	A	181	ASP	CA-C	5.96	1.60	1.52
1	A	18	SER	CA-C	5.95	1.60	1.52
1	A	53	SER	CA-CB	5.95	1.63	1.53
1	A	43	LYS	CD-CE	5.94	1.70	1.52
1	A	273	ALA	N-CA	5.91	1.53	1.46
1	A	275	GLN	C-O	-5.89	1.11	1.23
1	A	106	TRP	CD2-CE2	-5.88	1.31	1.41
1	A	164	THR	CB-OG1	5.87	1.53	1.43
1	A	246	VAL	N-CA	-5.87	1.39	1.46
1	A	148	VAL	CB-CG1	5.87	1.72	1.52
1	A	49	SER	CA-CB	-5.86	1.43	1.53
1	A	185	GLN	CA-C	-5.85	1.45	1.52
1	A	266	GLY	CA-C	5.83	1.60	1.51
1	A	219	GLY	CA-C	-5.83	1.45	1.51
1	A	235	LEU	CG-CD2	-5.83	1.33	1.52
1	A	91	TYR	CE1-CZ	-5.81	1.24	1.38
1	A	189	PHE	C-O	-5.80	1.17	1.23
1	A	181	ASP	C-N	-5.80	1.25	1.33
1	A	36	ASP	C-O	-5.79	1.17	1.24
1	A	190	SER	N-CA	-5.79	1.39	1.46
1	A	84	VAL	C-N	-5.78	1.26	1.33
1	A	130	SER	CA-C	-5.78	1.45	1.52
1	A	119	MET	CG-SD	5.77	1.95	1.80
1	A	135	LEU	CG-CD2	5.76	1.71	1.52
1	A	125	SER	CA-C	5.76	1.60	1.52
1	A	228	ALA	CA-CB	5.73	1.63	1.53
1	A	96	LEU	CG-CD2	5.70	1.71	1.52
1	A	227	VAL	C-N	5.69	1.41	1.33
1	A	243	ASN	CA-CB	5.69	1.62	1.53
1	A	207	SER	C-N	-5.69	1.25	1.33
1	A	214	TYR	C-O	-5.67	1.15	1.24
1	A	75	LEU	N-CA	5.65	1.53	1.46
1	A	36	ASP	CG-OD2	5.63	1.36	1.25
1	A	240	ASN	CB-CG	5.62	1.66	1.52
1	A	188	SER	N-CA	5.60	1.53	1.46
1	A	41	ASP	CG-OD2	5.59	1.35	1.25
1	A	5	PRO	CG-CD	5.59	1.69	1.50
1	A	47	GLY	C-N	-5.58	1.25	1.33
1	A	214	TYR	CG-CD2	5.58	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	LEU	C-O	-5.57	1.17	1.24
1	A	145	SER	C-O	5.57	1.31	1.23
1	A	188	SER	C-O	5.57	1.30	1.24
1	A	248	SER	C-O	-5.56	1.17	1.24
1	A	265	LYS	C-N	5.56	1.43	1.33
1	A	206	GLN	CB-CG	5.54	1.69	1.52
1	A	212	ASN	C-N	5.53	1.41	1.33
1	A	118	ASN	CG-OD1	-5.53	1.13	1.23
1	A	40	PRO	CA-C	-5.53	1.44	1.52
1	A	262	TYR	N-CA	5.52	1.53	1.46
1	A	155	ASN	C-O	-5.52	1.17	1.24
1	A	178	GLY	C-N	5.49	1.40	1.33
1	A	270	VAL	CA-CB	5.49	1.60	1.54
1	A	8	VAL	CA-C	-5.48	1.45	1.52
1	A	256	LYS	CA-C	5.47	1.60	1.52
1	A	170	LYS	CA-CB	5.47	1.61	1.53
1	A	115	ILE	CB-CG1	5.46	1.64	1.53
1	A	131	GLY	C-N	-5.46	1.23	1.33
1	A	123	ASN	CA-CB	5.45	1.61	1.53
1	A	253	THR	CA-C	5.45	1.61	1.52
1	A	32	ASP	C-N	-5.44	1.26	1.33
1	A	135	LEU	CA-C	-5.44	1.44	1.52
1	A	116	ALA	CA-C	5.43	1.61	1.52
1	A	33	SER	CA-C	5.42	1.60	1.52
1	A	241	TRP	CD1-NE1	-5.42	1.26	1.37
1	A	68	VAL	N-CA	-5.42	1.40	1.46
1	A	214	TYR	CD2-CE2	-5.42	1.22	1.38
1	A	261	PHE	C-O	5.41	1.30	1.24
1	A	24	SER	CA-CB	5.40	1.61	1.53
1	A	71	THR	CB-OG1	-5.39	1.35	1.43
1	A	86	PRO	CG-CD	5.38	1.69	1.50
1	A	93	VAL	C-O	5.38	1.30	1.24
1	A	262	TYR	CD1-CE1	5.37	1.54	1.38
1	A	134	ALA	CA-C	5.37	1.59	1.52
1	A	17	HIS	CA-CB	5.36	1.62	1.53
1	A	261	PHE	CB-CG	5.34	1.62	1.50
1	A	125	SER	C-N	5.34	1.41	1.33
1	A	197	ASP	CG-OD2	-5.34	1.15	1.25
1	A	204	SER	C-O	5.33	1.31	1.23
1	A	121	VAL	CA-C	5.33	1.59	1.52
1	A	214	TYR	N-CA	-5.32	1.38	1.45
1	A	185	GLN	CD-NE2	5.31	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	SER	CA-C	-5.31	1.45	1.52
1	A	171	TYR	CG-CD2	5.31	1.50	1.39
1	A	142	ALA	C-N	-5.31	1.26	1.33
1	A	17	HIS	CA-C	5.31	1.60	1.52
1	A	17	HIS	ND1-CE1	5.30	1.37	1.32
1	A	257	LEU	CA-CB	5.30	1.62	1.53
1	A	270	VAL	CB-CG2	5.29	1.70	1.52
1	A	115	ILE	CA-C	5.28	1.58	1.52
1	A	54	GLU	CD-OE2	-5.28	1.15	1.25
1	A	89	ALA	C-O	-5.28	1.17	1.23
1	A	243	ASN	C-O	-5.28	1.18	1.24
1	A	107	ILE	CG1-CD1	5.28	1.72	1.51
1	A	62	ASN	CA-C	5.27	1.59	1.52
1	A	70	GLY	C-O	5.26	1.30	1.23
1	A	77	ASN	CG-ND2	-5.26	1.22	1.33
1	A	243	ASN	CG-ND2	5.25	1.44	1.33
1	A	134	ALA	CA-CB	-5.25	1.45	1.53
1	A	244	THR	C-O	5.25	1.30	1.24
1	A	12	LYS	C-N	-5.24	1.22	1.33
1	A	124	MET	CG-SD	5.23	1.93	1.80
1	A	127	GLY	N-CA	5.21	1.52	1.45
1	A	160	GLY	N-CA	5.21	1.52	1.45
1	A	197	ASP	N-CA	-5.21	1.39	1.46
1	A	71	THR	C-O	5.20	1.30	1.24
1	A	263	TYR	CD2-CE2	5.18	1.54	1.38
1	A	35	ILE	N-CA	5.18	1.53	1.46
1	A	107	ILE	CB-CG1	-5.17	1.43	1.53
1	A	255	THR	CB-OG1	-5.16	1.35	1.43
1	A	72	VAL	CA-CB	5.16	1.59	1.54
1	A	18	SER	C-N	5.16	1.41	1.33
1	A	153	ALA	CA-C	5.15	1.59	1.52
1	A	151	ALA	N-CA	-5.14	1.39	1.45
1	A	213	LYS	C-N	5.14	1.42	1.33
1	A	136	LYS	C-N	-5.13	1.26	1.33
1	A	226	HIS	CA-CB	5.12	1.61	1.53
1	A	252	ASN	C-N	-5.11	1.26	1.33
1	A	150	VAL	CB-CG1	5.08	1.69	1.52
1	A	199	MET	C-O	-5.07	1.17	1.23
1	A	141	LYS	CA-CB	5.07	1.61	1.53
1	A	108	ILE	N-CA	5.06	1.52	1.46
1	A	13	ALA	C-O	-5.05	1.17	1.24
1	A	28	VAL	N-CA	5.05	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	LEU	CB-CG	5.05	1.63	1.53
1	A	41	ASP	CB-CG	5.04	1.64	1.52
1	A	54	GLU	CG-CD	-5.04	1.39	1.52
1	A	195	GLU	C-O	-5.03	1.18	1.24
1	A	113	TRP	CE3-CZ3	5.03	1.53	1.38
1	A	234	ILE	C-O	-5.03	1.17	1.24
1	A	110	GLY	CA-C	5.02	1.58	1.51
1	A	187	ALA	C-O	-5.01	1.18	1.23
1	A	197	ASP	CB-CG	5.01	1.64	1.52
1	A	273	ALA	CA-C	-5.00	1.45	1.52

All (482) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ILE	CA-C-O	22.48	142.09	120.96
1	A	59	GLN	CA-C-N	-21.90	92.78	123.00
1	A	59	GLN	C-N-CA	-21.90	92.78	123.00
1	A	34	GLY	CA-C-O	20.97	145.58	121.47
1	A	59	GLN	CA-C-O	20.21	141.62	120.40
1	A	69	ALA	CA-C-N	19.39	141.46	119.94
1	A	69	ALA	C-N-CA	19.39	141.46	119.94
1	A	52	PRO	O-C-N	19.07	148.39	122.64
1	A	101	SER	O-C-N	-17.24	99.66	122.59
1	A	123	ASN	CA-C-O	16.30	137.74	120.30
1	A	118	ASN	OD1-CG-ND2	16.27	138.87	122.60
1	A	5	PRO	N-CA-CB	15.89	117.31	103.17
1	A	275	GLN	OE1-CD-NE2	-15.86	106.74	122.60
1	A	34	GLY	O-C-N	-15.62	102.12	123.67
1	A	66	THR	CA-C-O	15.45	136.79	120.42
1	A	232	ALA	O-C-N	15.31	138.01	122.09
1	A	111	ILE	O-C-N	15.02	141.35	122.57
1	A	190	SER	CA-C-N	14.77	143.32	121.31
1	A	190	SER	C-N-CA	14.77	143.32	121.31
1	A	56	PRO	N-CA-CB	14.37	118.81	103.00
1	A	97	GLY	O-C-N	-14.14	104.31	122.70
1	A	270	VAL	CA-C-O	14.05	137.09	120.65
1	A	60	ASP	N-CA-CB	-13.84	88.85	110.57
1	A	69	ALA	O-C-N	-13.66	104.63	122.39
1	A	89	ALA	O-C-N	-13.66	105.34	122.68
1	A	142	ALA	N-CA-C	-13.48	96.18	111.82
1	A	217	TYR	CA-C-N	13.11	141.25	122.77
1	A	217	TYR	C-N-CA	13.11	141.25	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	SER	CA-C-O	12.87	138.92	120.51
1	A	92	ALA	CB-CA-C	-12.85	90.23	110.78
1	A	39	HIS	ND1-CG-CD2	12.74	118.84	106.10
1	A	52	PRO	CA-C-N	-12.71	97.26	121.54
1	A	52	PRO	C-N-CA	-12.71	97.26	121.54
1	A	108	ILE	CA-C-O	-12.31	107.40	120.57
1	A	186	ARG	NE-CZ-NH1	12.18	133.68	121.50
1	A	108	ILE	O-C-N	12.17	134.16	121.87
1	A	144	ALA	O-C-N	12.17	141.88	122.41
1	A	112	GLU	N-CA-C	-12.10	96.84	114.39
1	A	49	SER	CB-CA-C	12.06	133.77	109.76
1	A	64	HIS	CG-CD2-NE2	11.94	119.14	107.20
1	A	99	ALA	CA-C-O	11.89	137.52	120.51
1	A	57	ASN	N-CA-C	-11.85	95.98	113.40
1	A	66	THR	O-C-N	-11.84	108.65	122.15
1	A	115	ILE	CB-CA-C	-11.78	100.57	111.05
1	A	117	ASN	CA-CB-CG	-11.71	100.89	112.60
1	A	5	PRO	O-C-N	-11.70	110.22	122.98
1	A	212	ASN	CA-CB-CG	-11.69	100.91	112.60
1	A	87	SER	CA-C-O	11.67	135.00	120.65
1	A	123	ASN	O-C-N	-11.54	109.88	123.27
1	A	144	ALA	CA-C-N	-11.43	101.53	123.13
1	A	144	ALA	C-N-CA	-11.43	101.53	123.13
1	A	195	GLU	N-CA-CB	-11.42	93.22	110.13
1	A	29	ALA	O-C-N	11.40	136.60	122.93
1	A	49	SER	N-CA-CB	-11.31	93.26	110.45
1	A	123	ASN	OD1-CG-ND2	11.30	133.90	122.60
1	A	58	PHE	O-C-N	11.14	136.26	122.34
1	A	148	VAL	CA-C-O	11.05	131.14	120.31
1	A	35	ILE	O-C-N	-10.96	112.67	123.19
1	A	241	TRP	CH2-CZ2-CE2	10.95	131.74	117.50
1	A	243	ASN	O-C-N	10.95	133.86	122.03
1	A	66	THR	N-CA-C	-10.91	99.46	111.36
1	A	214	TYR	CG-CD2-CE2	10.82	137.43	121.20
1	A	68	VAL	N-CA-CB	-10.59	99.50	110.62
1	A	45	ALA	CA-C-N	10.56	133.40	120.51
1	A	45	ALA	C-N-CA	10.56	133.40	120.51
1	A	148	VAL	O-C-N	-10.50	112.85	123.03
1	A	68	VAL	O-C-N	10.46	133.26	121.96
1	A	89	ALA	CA-C-O	10.40	131.74	120.92
1	A	247	ARG	NE-CZ-NH1	-10.30	111.20	121.50
1	A	274	ALA	N-CA-CB	10.09	126.37	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ASN	OD1-CG-ND2	-10.03	112.57	122.60
1	A	54	GLU	O-C-N	9.97	135.93	122.57
1	A	263	TYR	N-CA-CB	9.93	125.61	110.42
1	A	238	HIS	CB-CG-CD2	-9.82	118.44	131.20
1	A	138	ALA	CA-C-N	9.79	133.87	120.46
1	A	138	ALA	C-N-CA	9.79	133.87	120.46
1	A	190	SER	O-C-N	-9.73	110.49	123.14
1	A	247	ARG	CD-NE-CZ	-9.65	110.89	124.40
1	A	123	ASN	CA-CB-CG	-9.64	102.96	112.60
1	A	209	LEU	CA-C-N	9.62	131.87	119.84
1	A	209	LEU	C-N-CA	9.62	131.87	119.84
1	A	95	VAL	CG1-CB-CG2	-9.54	89.82	110.80
1	A	212	ASN	OD1-CG-ND2	9.42	132.02	122.60
1	A	212	ASN	CA-C-O	-9.37	110.79	120.63
1	A	39	HIS	CA-CB-CG	-9.34	104.46	113.80
1	A	95	VAL	CA-CB-CG2	9.32	126.24	110.40
1	A	36	ASP	CA-CB-CG	-9.31	103.28	112.60
1	A	192	VAL	O-C-N	-9.29	112.79	123.00
1	A	114	ALA	N-CA-C	-9.27	101.97	113.28
1	A	171	TYR	N-CA-C	-9.25	96.44	110.50
1	A	103	GLN	CB-CA-C	9.24	127.65	109.35
1	A	106	TRP	O-C-N	-9.19	108.77	122.28
1	A	257	LEU	N-CA-C	-9.19	91.22	110.80
1	A	241	TRP	N-CA-C	-9.19	95.71	110.32
1	A	226	HIS	CB-CG-CD2	-9.16	119.30	131.20
1	A	201	PRO	O-C-N	9.07	134.88	122.64
1	A	253	THR	CA-C-N	-9.06	106.50	123.27
1	A	253	THR	C-N-CA	-9.06	106.50	123.27
1	A	136	LYS	N-CA-C	-9.06	102.35	113.50
1	A	118	ASN	CB-CG-ND2	-8.99	102.92	116.40
1	A	216	ALA	O-C-N	-8.97	112.68	123.27
1	A	64	HIS	ND1-CG-CD2	-8.97	97.13	106.10
1	A	41	ASP	CA-CB-CG	-8.95	103.65	112.60
1	A	270	VAL	CB-CA-C	-8.95	100.13	110.96
1	A	171	TYR	CA-C-O	8.94	130.79	120.87
1	A	67	HIS	ND1-CE1-NE2	-8.89	99.51	108.40
1	A	179	ALA	CA-C-O	8.88	130.12	120.71
1	A	120	ASP	CA-C-O	8.87	130.04	120.55
1	A	227	VAL	O-C-N	8.82	133.59	122.57
1	A	259	ASP	CA-CB-CG	-8.82	103.78	112.60
1	A	109	ASN	CA-C-O	-8.80	111.56	120.80
1	A	149	VAL	O-C-N	8.76	132.22	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ALA	O-C-N	-8.72	110.99	122.59
1	A	111	ILE	CA-C-N	-8.71	108.65	121.98
1	A	111	ILE	C-N-CA	-8.71	108.65	121.98
1	A	226	HIS	ND1-CG-CD2	8.71	114.81	106.10
1	A	235	LEU	CA-C-O	-8.69	108.09	120.51
1	A	121	VAL	CA-C-O	-8.66	111.30	120.48
1	A	118	ASN	N-CA-CB	-8.65	99.16	112.30
1	A	4	VAL	O-C-N	8.64	129.19	121.41
1	A	67	HIS	CG-CD2-NE2	8.63	115.83	107.20
1	A	208	THR	CB-CA-C	-8.59	94.99	109.50
1	A	113	TRP	CE2-CD2-CE3	-8.55	110.25	118.80
1	A	69	ALA	CA-C-O	8.53	129.81	119.49
1	A	92	ALA	N-CA-CB	-8.51	96.33	110.37
1	A	79	ILE	O-C-N	-8.50	111.95	122.57
1	A	39	HIS	CA-C-N	8.44	130.39	119.84
1	A	39	HIS	C-N-CA	8.44	130.39	119.84
1	A	128	GLY	CA-C-N	8.44	128.14	119.19
1	A	128	GLY	C-N-CA	8.44	128.14	119.19
1	A	52	PRO	CA-C-O	-8.42	105.28	120.60
1	A	214	TYR	N-CA-CB	-8.42	95.66	110.14
1	A	112	GLU	CA-C-N	8.40	134.94	120.58
1	A	112	GLU	C-N-CA	8.40	134.94	120.58
1	A	115	ILE	CB-CG1-CD1	-8.36	96.25	113.80
1	A	91	TYR	CA-C-O	-8.34	111.87	120.54
1	A	58	PHE	CA-C-N	-8.30	110.95	123.07
1	A	58	PHE	C-N-CA	-8.30	110.95	123.07
1	A	31	ILE	CB-CG1-CD1	-8.29	96.38	113.80
1	A	15	ALA	CA-C-O	8.28	132.35	120.51
1	A	67	HIS	CA-CB-CG	-8.24	105.56	113.80
1	A	238	HIS	ND1-CE1-NE2	8.18	116.58	108.40
1	A	274	ALA	N-CA-C	-8.17	102.34	112.88
1	A	106	TRP	CA-C-N	8.14	130.65	120.72
1	A	106	TRP	C-N-CA	8.14	130.65	120.72
1	A	149	VAL	N-CA-C	8.13	120.82	108.71
1	A	265	LYS	CA-C-O	8.12	128.59	118.43
1	A	212	ASN	CA-C-N	8.03	136.88	121.54
1	A	212	ASN	C-N-CA	8.03	136.88	121.54
1	A	58	PHE	N-CA-C	-7.96	103.14	113.17
1	A	235	LEU	N-CA-CB	-7.92	97.11	110.49
1	A	195	GLU	O-C-N	-7.86	112.66	122.17
1	A	79	ILE	CA-C-O	-7.83	110.99	120.78
1	A	19	GLN	CG-CD-NE2	7.82	128.12	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	THR	O-C-N	7.80	133.22	122.46
1	A	226	HIS	CA-CB-CG	-7.77	106.03	113.80
1	A	72	VAL	O-C-N	7.76	130.34	121.96
1	A	224	SER	CA-C-N	7.75	129.53	119.84
1	A	224	SER	C-N-CA	7.75	129.53	119.84
1	A	140	ASP	CA-CB-CG	-7.75	104.85	112.60
1	A	241	TRP	CZ3-CH2-CZ2	-7.68	111.52	121.50
1	A	30	VAL	O-C-N	7.66	132.14	122.57
1	A	262	TYR	N-CA-C	-7.66	104.84	114.56
1	A	82	LEU	CA-C-N	-7.63	106.46	121.41
1	A	82	LEU	C-N-CA	-7.63	106.46	121.41
1	A	175	ILE	CB-CG1-CD1	-7.62	97.79	113.80
1	A	35	ILE	N-CA-C	-7.62	98.31	108.06
1	A	113	TRP	CE2-CD2-CG	7.58	116.30	107.20
1	A	175	ILE	CA-C-O	-7.57	111.96	120.97
1	A	130	SER	CA-C-N	-7.55	113.57	121.35
1	A	130	SER	C-N-CA	-7.55	113.57	121.35
1	A	208	THR	CA-C-N	-7.53	109.49	123.65
1	A	208	THR	C-N-CA	-7.53	109.49	123.65
1	A	186	ARG	NE-CZ-NH2	-7.49	112.46	119.20
1	A	167	TYR	O-C-N	7.49	128.05	121.39
1	A	129	PRO	CA-N-CD	-7.47	101.53	112.00
1	A	192	VAL	CA-C-N	7.47	133.60	121.87
1	A	192	VAL	C-N-CA	7.47	133.60	121.87
1	A	174	VAL	CA-C-O	-7.47	112.43	121.54
1	A	208	THR	CA-C-O	-7.46	112.48	121.28
1	A	256	LYS	N-CA-C	-7.45	99.45	110.48
1	A	106	TRP	CA-CB-CG	-7.45	99.44	113.60
1	A	143	VAL	CB-CA-C	-7.45	102.56	111.94
1	A	36	ASP	N-CA-CB	-7.44	98.42	109.95
1	A	240	ASN	N-CA-C	7.41	123.39	112.94
1	A	89	ALA	CA-C-N	-7.40	110.59	121.24
1	A	89	ALA	C-N-CA	-7.40	110.59	121.24
1	A	197	ASP	O-C-N	7.39	132.26	122.36
1	A	17	HIS	CA-C-O	-7.38	111.93	120.20
1	A	164	THR	O-C-N	-7.38	113.50	122.65
1	A	46	GLY	CA-C-N	7.36	131.82	121.22
1	A	46	GLY	C-N-CA	7.36	131.82	121.22
1	A	78	SER	CA-C-O	-7.36	113.44	122.64
1	A	9	SER	N-CA-CB	7.32	122.86	110.49
1	A	175	ILE	CA-CB-CG1	-7.28	98.03	110.40
1	A	100	GLY	O-C-N	-7.28	115.34	124.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	SER	O-C-N	-7.27	112.46	122.20
1	A	172	PRO	N-CD-CG	7.24	114.06	103.20
1	A	79	ILE	CA-C-N	7.24	135.60	121.41
1	A	79	ILE	C-N-CA	7.24	135.60	121.41
1	A	183	SER	O-C-N	7.23	131.73	122.33
1	A	131	GLY	CA-C-O	-7.22	113.90	121.63
1	A	220	THR	CA-C-O	7.21	126.98	119.05
1	A	11	ILE	CA-C-N	7.20	135.30	121.54
1	A	11	ILE	C-N-CA	7.20	135.30	121.54
1	A	123	ASN	CB-CG-ND2	-7.20	105.61	116.40
1	A	97	GLY	CA-C-O	7.20	133.09	120.57
1	A	7	GLY	O-C-N	7.19	132.04	122.70
1	A	265	LYS	CB-CA-C	-7.17	98.47	109.29
1	A	12	LYS	N-CA-C	-7.17	95.54	110.80
1	A	210	PRO	N-CA-CB	7.16	110.77	103.25
1	A	55	THR	CA-C-O	-7.15	108.64	120.80
1	A	147	VAL	N-CA-C	7.15	119.74	109.51
1	A	246	VAL	N-CA-C	-7.15	102.47	110.62
1	A	208	THR	O-C-N	-7.14	114.89	123.10
1	A	148	VAL	CA-C-N	7.10	133.07	122.91
1	A	148	VAL	C-N-CA	7.10	133.07	122.91
1	A	83	GLY	CA-C-N	7.08	134.71	121.97
1	A	83	GLY	C-N-CA	7.08	134.71	121.97
1	A	166	GLY	O-C-N	7.07	131.61	122.71
1	A	171	TYR	O-C-N	7.05	127.55	121.20
1	A	119	MET	N-CA-C	-7.04	99.40	109.96
1	A	142	ALA	CA-C-O	-7.03	111.88	119.97
1	A	17	HIS	ND1-CE1-NE2	-7.01	101.39	108.40
1	A	183	SER	CA-C-O	-7.00	111.35	119.61
1	A	134	ALA	O-C-N	-7.00	114.53	122.09
1	A	229	GLY	O-C-N	7.00	131.80	122.70
1	A	19	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	A	250	LEU	N-CA-CB	-6.97	99.90	110.01
1	A	106	TRP	CG-CD2-CE3	-6.97	126.93	133.90
1	A	243	ASN	CA-C-N	-6.97	110.11	121.19
1	A	243	ASN	C-N-CA	-6.97	110.11	121.19
1	A	145	SER	N-CA-CB	-6.97	101.20	111.51
1	A	275	GLN	CG-CD-OE1	6.96	134.73	120.80
1	A	90	LEU	N-CA-CB	-6.95	99.00	109.71
1	A	195	GLU	CB-CA-C	6.93	122.44	110.79
1	A	203	VAL	CA-C-O	6.93	129.44	120.78
1	A	210	PRO	O-C-N	-6.92	113.29	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	VAL	CA-C-N	-6.92	108.33	121.54
1	A	227	VAL	C-N-CA	-6.92	108.33	121.54
1	A	213	LYS	CA-C-O	-6.92	110.62	120.51
1	A	172	PRO	CB-CA-C	-6.90	102.10	113.06
1	A	262	TYR	CA-C-N	6.89	135.76	122.53
1	A	262	TYR	C-N-CA	6.89	135.76	122.53
1	A	109	ASN	O-C-N	6.88	130.10	122.11
1	A	155	ASN	CA-CB-CG	-6.87	105.73	112.60
1	A	175	ILE	N-CA-C	6.85	117.30	106.88
1	A	209	LEU	CB-CA-C	-6.84	98.83	109.22
1	A	246	VAL	CA-C-O	-6.83	113.95	121.05
1	A	191	SER	CA-C-N	6.81	132.73	122.92
1	A	191	SER	C-N-CA	6.81	132.73	122.92
1	A	246	VAL	CB-CA-C	-6.81	103.12	112.04
1	A	10	GLN	CG-CD-NE2	-6.81	106.19	116.40
1	A	106	TRP	CE2-CD2-CG	6.79	115.35	107.20
1	A	143	VAL	CA-CB-CG2	-6.79	98.86	110.40
1	A	87	SER	N-CA-C	6.78	121.44	111.87
1	A	134	ALA	CA-C-O	6.77	127.68	120.70
1	A	234	ILE	N-CA-C	-6.77	102.37	111.44
1	A	71	THR	N-CA-C	-6.76	104.51	112.89
1	A	125	SER	N-CA-CB	-6.75	100.30	110.35
1	A	210	PRO	CA-N-CD	-6.72	102.59	112.00
1	A	6	TYR	N-CA-CB	-6.72	98.09	110.32
1	A	238	HIS	ND1-CG-CD2	6.70	112.80	106.10
1	A	77	ASN	CA-C-N	-6.69	111.93	122.23
1	A	77	ASN	C-N-CA	-6.69	111.93	122.23
1	A	121	VAL	O-C-N	6.69	130.20	123.18
1	A	148	VAL	CA-CB-CG1	6.68	121.75	110.40
1	A	107	ILE	CA-CB-CG2	-6.67	99.17	110.50
1	A	167	TYR	CA-C-O	-6.66	112.89	119.69
1	A	90	LEU	CA-C-N	6.64	131.47	122.84
1	A	90	LEU	C-N-CA	6.64	131.47	122.84
1	A	111	ILE	CA-C-O	-6.63	112.49	120.78
1	A	236	SER	O-C-N	-6.60	113.54	122.19
1	A	150	VAL	O-C-N	-6.60	116.07	123.20
1	A	268	ILE	O-C-N	6.60	129.80	122.61
1	A	94	LYS	N-CA-CB	-6.59	99.53	110.47
1	A	242	THR	CA-C-O	6.55	129.69	121.50
1	A	116	ALA	N-CA-CB	-6.53	101.55	110.56
1	A	47	GLY	N-CA-C	6.52	120.53	110.88
1	A	183	SER	N-CA-C	-6.51	103.87	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ALA	CA-C-O	-6.51	111.43	119.18
1	A	158	SER	CA-C-O	6.50	129.42	121.56
1	A	113	TRP	CA-C-O	6.47	127.43	120.24
1	A	219	GLY	O-C-N	-6.47	116.18	123.62
1	A	215	GLY	O-C-N	-6.46	115.87	123.55
1	A	163	SER	CA-C-O	6.43	128.86	121.47
1	A	219	GLY	CA-C-O	-6.42	114.64	121.38
1	A	6	TYR	N-CA-C	-6.41	105.17	112.87
1	A	270	VAL	CA-CB-CG2	-6.41	99.50	110.40
1	A	245	GLN	OE1-CD-NE2	6.38	128.99	122.60
1	A	214	TYR	CA-CB-CG	-6.33	102.50	113.90
1	A	267	LEU	CA-C-N	-6.33	112.11	120.91
1	A	267	LEU	C-N-CA	-6.33	112.11	120.91
1	A	260	SER	CB-CA-C	-6.33	102.29	111.91
1	A	41	ASP	O-C-N	-6.32	114.18	122.59
1	A	165	VAL	O-C-N	6.32	130.06	123.05
1	A	240	ASN	CB-CG-ND2	-6.31	106.93	116.40
1	A	113	TRP	NE1-CE2-CD2	-6.31	99.20	107.40
1	A	217	TYR	CB-CA-C	6.30	121.41	109.37
1	A	154	GLY	N-CA-C	-6.28	98.29	113.18
1	A	197	ASP	CA-CB-CG	-6.26	106.33	112.60
1	A	214	TYR	CD1-CG-CD2	-6.26	108.71	118.10
1	A	249	SER	O-C-N	6.26	130.91	122.59
1	A	2	GLN	O-C-N	6.24	130.88	122.59
1	A	184	ASN	CB-CG-ND2	6.23	125.75	116.40
1	A	89	ALA	N-CA-CB	-6.23	101.07	110.35
1	A	67	HIS	CA-C-O	-6.21	114.48	121.00
1	A	41	ASP	CA-C-O	6.20	129.37	120.51
1	A	17	HIS	CA-CB-CG	-6.19	107.61	113.80
1	A	66	THR	CA-C-N	6.19	128.82	120.65
1	A	66	THR	C-N-CA	6.19	128.82	120.65
1	A	206	GLN	CA-CB-CG	-6.19	101.72	114.10
1	A	17	HIS	N-CA-C	-6.17	103.86	111.75
1	A	67	HIS	N-CA-C	-6.15	104.27	110.97
1	A	263	TYR	CA-CB-CG	-6.14	102.85	113.90
1	A	82	LEU	CA-CB-CG	-6.14	94.82	116.30
1	A	198	VAL	O-C-N	-6.13	115.23	122.58
1	A	123	ASN	N-CA-C	-6.12	98.44	108.41
1	A	82	LEU	O-C-N	6.11	129.51	123.46
1	A	34	GLY	CA-C-N	6.11	131.30	121.95
1	A	34	GLY	C-N-CA	6.11	131.30	121.95
1	A	243	ASN	OD1-CG-ND2	-6.10	116.50	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ALA	O-C-N	-6.08	113.73	122.36
1	A	191	SER	O-C-N	-6.07	115.83	123.12
1	A	218	ASN	O-C-N	-6.06	116.18	123.27
1	A	92	ALA	N-CA-C	6.06	118.56	108.20
1	A	84	VAL	N-CA-CB	-6.05	101.25	111.23
1	A	39	HIS	CG-CD2-NE2	-6.04	101.16	107.20
1	A	94	LYS	CA-C-O	-6.03	114.01	120.46
1	A	202	GLY	O-C-N	6.03	130.53	122.70
1	A	131	GLY	O-C-N	6.01	129.16	123.57
1	A	241	TRP	CD2-CE2-CZ2	-6.01	116.39	122.40
1	A	13	ALA	CA-C-O	6.00	128.38	120.16
1	A	68	VAL	CA-CB-CG1	-6.00	100.21	110.40
1	A	75	LEU	CA-C-O	5.98	129.07	120.51
1	A	101	SER	CA-C-N	5.98	130.62	121.12
1	A	101	SER	C-N-CA	5.98	130.62	121.12
1	A	104	TYR	CE1-CZ-CE2	-5.97	108.36	120.30
1	A	107	ILE	CB-CA-C	5.97	119.57	111.87
1	A	139	VAL	CB-CA-C	-5.96	104.09	112.14
1	A	1	ALA	CA-C-N	5.96	132.93	121.54
1	A	1	ALA	C-N-CA	5.96	132.93	121.54
1	A	258	GLY	O-C-N	5.96	130.45	122.70
1	A	52	PRO	N-CD-CG	5.96	112.14	103.20
1	A	217	TYR	CB-CG-CD1	-5.94	111.89	120.80
1	A	109	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	24	SER	N-CA-C	5.92	119.18	109.76
1	A	269	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	192	VAL	CA-C-O	-5.91	115.64	121.67
1	A	46	GLY	N-CA-C	5.91	120.65	111.08
1	A	60	ASP	N-CA-C	5.91	118.58	109.07
1	A	253	THR	N-CA-C	5.91	117.53	110.44
1	A	60	ASP	CB-CG-OD1	5.89	131.94	118.40
1	A	38	SER	CA-CB-OG	5.88	122.86	111.10
1	A	252	ASN	CB-CA-C	5.86	120.47	110.74
1	A	28	VAL	O-C-N	5.85	129.58	123.26
1	A	173	SER	O-C-N	-5.84	114.82	122.59
1	A	103	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	39	HIS	CG-ND1-CE1	-5.83	99.39	109.30
1	A	249	SER	CA-C-O	-5.83	112.18	120.51
1	A	243	ASN	CA-C-O	5.82	126.89	120.90
1	A	120	ASP	O-C-N	-5.78	115.18	122.17
1	A	252	ASN	CA-C-O	-5.78	114.45	120.92
1	A	195	GLU	CA-CB-CG	-5.76	102.58	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	N-CA-CB	-5.76	100.76	110.49
1	A	152	ALA	CA-C-O	5.75	128.73	120.51
1	A	113	TRP	CG-CD1-NE1	-5.74	102.74	110.20
1	A	51	VAL	CA-C-O	5.74	127.64	119.95
1	A	114	ALA	O-C-N	5.73	130.54	122.41
1	A	90	LEU	O-C-N	-5.72	115.75	122.96
1	A	211	GLY	CA-C-O	-5.72	110.62	120.57
1	A	103	GLN	N-CA-C	-5.71	99.70	109.24
1	A	230	ALA	CB-CA-C	5.71	121.19	110.63
1	A	267	LEU	CA-C-O	5.70	128.62	121.66
1	A	138	ALA	CA-C-O	5.70	126.27	119.60
1	A	229	GLY	CA-C-N	-5.69	112.08	120.28
1	A	229	GLY	C-N-CA	-5.69	112.08	120.28
1	A	109	ASN	N-CA-CB	-5.69	101.71	110.07
1	A	3	SER	O-C-N	5.67	130.14	122.59
1	A	256	LYS	CA-C-N	-5.67	110.71	121.54
1	A	256	LYS	C-N-CA	-5.67	110.71	121.54
1	A	108	ILE	CA-CB-CG1	5.67	120.04	110.40
1	A	120	ASP	OD1-CG-OD2	-5.67	109.30	122.90
1	A	129	PRO	N-CD-CG	5.66	111.69	103.20
1	A	104	TYR	CD1-CE1-CZ	5.66	129.78	119.60
1	A	237	LYS	O-C-N	5.66	130.26	122.46
1	A	239	PRO	CA-C-N	5.65	131.08	122.37
1	A	239	PRO	C-N-CA	5.65	131.08	122.37
1	A	221	SER	N-CA-C	-5.65	105.88	112.89
1	A	194	PRO	N-CA-CB	5.64	109.17	103.25
1	A	167	TYR	CZ-CE2-CD2	5.64	129.75	119.60
1	A	218	ASN	N-CA-CB	5.63	119.61	110.77
1	A	45	ALA	N-CA-C	-5.63	104.77	111.69
1	A	252	ASN	CB-CG-ND2	5.61	124.81	116.40
1	A	43	LYS	CA-CB-CG	-5.60	102.90	114.10
1	A	137	ALA	CA-C-N	-5.60	111.22	121.52
1	A	137	ALA	C-N-CA	-5.60	111.22	121.52
1	A	78	SER	O-C-N	5.59	129.89	122.56
1	A	175	ILE	CA-C-N	5.57	130.04	122.19
1	A	175	ILE	C-N-CA	5.57	130.04	122.19
1	A	85	ALA	O-C-N	5.56	126.49	121.04
1	A	189	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	253	THR	O-C-N	5.55	129.21	121.83
1	A	106	TRP	N-CA-C	-5.55	104.74	112.45
1	A	11	ILE	O-C-N	-5.55	116.65	122.20
1	A	217	TYR	CA-C-O	-5.52	114.74	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ILE	O-C-N	5.52	129.38	121.82
1	A	4	VAL	CA-C-N	5.51	126.37	119.98
1	A	4	VAL	C-N-CA	5.51	126.37	119.98
1	A	256	LYS	CA-CB-CG	-5.50	103.10	114.10
1	A	91	TYR	CB-CA-C	5.50	119.58	110.78
1	A	176	ALA	CA-C-O	-5.50	114.33	120.54
1	A	216	ALA	CA-C-O	5.49	126.36	120.32
1	A	155	ASN	N-CA-C	-5.47	99.14	110.80
1	A	106	TRP	CG-CD1-NE1	5.47	117.31	110.20
1	A	21	TYR	CD1-CG-CD2	-5.47	109.90	118.10
1	A	84	VAL	CA-C-N	-5.47	115.43	123.30
1	A	84	VAL	C-N-CA	-5.47	115.43	123.30
1	A	154	GLY	O-C-N	5.47	129.81	122.70
1	A	144	ALA	N-CA-C	5.44	119.67	113.19
1	A	5	PRO	CA-C-O	5.43	126.97	121.27
1	A	255	THR	O-C-N	-5.43	116.86	123.10
1	A	196	LEU	CD1-CG-CD2	-5.42	98.88	110.80
1	A	141	LYS	CB-CG-CD	-5.42	98.84	111.30
1	A	113	TRP	O-C-N	5.41	129.27	122.23
1	A	76	ASN	O-C-N	5.39	129.46	123.05
1	A	94	LYS	CA-CB-CG	-5.37	103.36	114.10
1	A	133	ALA	CA-C-O	5.36	125.96	119.31
1	A	120	ASP	N-CA-C	5.36	117.94	111.40
1	A	168	PRO	N-CD-CG	5.36	110.23	103.80
1	A	6	TYR	OH-CZ-CE2	-5.35	103.86	119.90
1	A	90	LEU	N-CA-C	5.33	117.43	109.59
1	A	201	PRO	N-CA-CB	5.33	108.85	103.25
1	A	218	ASN	CA-CB-CG	-5.33	107.27	112.60
1	A	214	TYR	CD1-CE1-CZ	5.33	129.19	119.60
1	A	143	VAL	N-CA-C	-5.32	105.94	111.58
1	A	117	ASN	N-CA-C	-5.31	105.08	112.30
1	A	260	SER	N-CA-CB	-5.30	102.11	110.49
1	A	39	HIS	CB-CG-ND1	-5.29	114.76	122.70
1	A	137	ALA	N-CA-CB	-5.28	102.17	110.30
1	A	214	TYR	CB-CG-CD1	5.28	128.72	120.80
1	A	220	THR	N-CA-CB	-5.28	102.89	110.65
1	A	2	GLN	OE1-CD-NE2	5.25	127.85	122.60
1	A	60	ASP	OD1-CG-OD2	-5.24	110.33	122.90
1	A	53	SER	N-CA-C	-5.23	99.66	110.80
1	A	60	ASP	CA-CB-CG	-5.23	107.37	112.60
1	A	37	SER	N-CA-C	-5.23	104.51	112.04
1	A	196	LEU	CA-CB-CG	-5.22	98.02	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	HIS	CA-C-N	5.22	126.36	119.84
1	A	238	HIS	C-N-CA	5.22	126.36	119.84
1	A	184	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	194	PRO	O-C-N	5.21	129.67	122.64
1	A	150	VAL	N-CA-C	5.20	115.61	108.12
1	A	274	ALA	O-C-N	5.20	128.44	122.25
1	A	34	GLY	N-CA-C	-5.19	103.01	110.38
1	A	129	PRO	N-CA-CB	5.18	109.01	103.52
1	A	28	VAL	CB-CA-C	5.17	118.28	110.63
1	A	10	GLN	CB-CG-CD	-5.16	103.83	112.60
1	A	228	ALA	N-CA-CB	-5.15	101.79	110.49
1	A	107	ILE	N-CA-CB	-5.14	104.84	110.65
1	A	168	PRO	N-CA-CB	5.14	108.25	102.60
1	A	103	GLN	CG-CD-OE1	5.14	131.07	120.80
1	A	235	LEU	CB-CA-C	5.11	120.60	110.42
1	A	110	GLY	O-C-N	5.11	128.16	122.54
1	A	235	LEU	CA-C-N	5.11	132.20	122.60
1	A	235	LEU	C-N-CA	5.11	132.20	122.60
1	A	262	TYR	CB-CG-CD1	-5.09	113.17	120.80
1	A	50	MET	N-CA-CB	-5.09	104.27	110.98
1	A	54	GLU	N-CA-CB	-5.09	102.87	110.24
1	A	37	SER	O-C-N	-5.08	115.45	122.30
1	A	247	ARG	NH1-CZ-NH2	5.07	125.89	119.30
1	A	210	PRO	CA-C-O	5.07	129.83	120.60
1	A	160	GLY	CA-C-N	5.05	130.14	122.56
1	A	160	GLY	C-N-CA	5.05	130.14	122.56
1	A	113	TRP	CE3-CZ3-CH2	-5.05	114.54	121.10
1	A	231	ALA	O-C-N	5.04	127.27	122.03
1	A	32	ASP	CA-C-N	5.04	128.66	120.60
1	A	32	ASP	C-N-CA	5.04	128.66	120.60
1	A	138	ALA	CB-CA-C	-5.03	99.56	109.67
1	A	21	TYR	CB-CG-CD1	5.01	128.32	120.80
1	A	45	ALA	N-CA-CB	-5.01	102.74	110.20
1	A	94	LYS	N-CA-C	5.01	116.85	107.99

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

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Mol	Chain	Res	Type	Group
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
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	1878	647	141
2	A	4	0	6	7	0
3	A	10	0	0	8	0
All	All	1948	0	1884	647	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 169.

All (647) 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:CD1	1:A:175:ILE:CG1	1.76	1.62
1:A:22:THR:CB	1:A:22:THR:CG2	1.77	1.62
1:A:30:VAL:C	1:A:30:VAL:CA	1.75	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:CD2	1:A:196:LEU:CG	1.77	1.55
1:A:233:LEU:CA	1:A:233:LEU:CB	1.75	1.55
1:A:145:SER:CA	1:A:145:SER:N	1.71	1.54
1:A:242:THR:N	1:A:242:THR:CA	1.68	1.54
1:A:257:LEU:HB3	1:A:263:TYR:CD1	1.44	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	1.47
1:A:195:GLU:C	1:A:196:LEU:N	1.74	1.46
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
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:34:GLY:C	1:A:35:ILE:N	1.89	1.31
1:A:173:SER:C	1:A:174:VAL:CA	2.03	1.29
1:A:56:PRO:O	1:A:57:ASN:ND2	1.67	1.27
1:A:249:SER:O	1:A:273:ALA:HB1	1.32	1.25
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:125:SER:C	1:A:126:LEU:HG	1.53	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:30:VAL:C	3:A:280:HOH:O	1.88	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:39:HIS:HD2	1:A:40:PRO:HD2	0.95	1.12
1:A:124:MET:CE	1:A:168:PRO:HG2	1.79	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:5:PRO:HD3	1:A:81:VAL:HA	1.30	1.08
1:A:11:ILE:HD12	1:A:268:ILE:HG21	1.34	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
1:A:26:VAL:CG1	1:A:120:ASP:HB2	1.85	1.06
1:A:26:VAL:HG11	1:A:121:VAL:CG2	1.84	1.06
1:A:29:ALA:O	1:A:123:ASN:N	1.87	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:12:LYS:O	1:A:270:VAL:CB	2.03	1.05
1:A:67:HIS:CE1	1:A:207:SER:HB3	1.89	1.05
1:A:113:TRP:HZ3	1:A:119:MET:HE1	1.17	1.04
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:113:TRP:CZ3	1:A:119:MET:HE1	1.90	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:59:GLN:C	1:A:60:ASP:CA	2.32	1.01
1:A:11:ILE:HB	1:A:268:ILE:HB	1.42	1.01
1:A:124:MET:HE2	1:A:168:PRO:HG2	1.40	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:11:ILE:HD12	1:A:268:ILE:CG2	1.94	0.98
1:A:111:ILE:CG1	1:A:111:ILE:O	2.10	0.98

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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	0.97
1:A:91:TYR:HB3	1:A:119:MET:HE3	1.44	0.97
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:144:ALA:C	1:A:145:SER:CA	2.37	0.97
1:A:234:ILE:CG1	1:A:274:ALA:CB	2.34	0.97
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:58:PHE:C	1:A:59:GLN:CA	2.39	0.95
1:A:202:GLY:C	1:A:203:VAL:HG23	1.92	0.94
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
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:8:VAL:CG2	1:A:9:SER:H	1.82	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:207:SER:C	1:A:214:TYR:HD1	1.78	0.91
1:A:255:THR:O	1:A:266:GLY:HA3	1.69	0.91
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:91:TYR:CB	1:A:119:MET:HE3	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLY:HA3	1:A:222:MET:HE3	1.57	0.86
1:A:196:LEU:CD2	1:A:196:LEU:CD1	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:200:ALA:HB1	1:A:201:PRO:HD2	1.57	0.85
1:A:253:THR:HG23	1:A:273:ALA:HB1	1.56	0.85
1:A:111:ILE:O	1:A:111:ILE:HG12	1.76	0.85
1:A:26:VAL:HG12	1:A:121:VAL:HG23	1.57	0.85
1:A:51:VAL:HG21	1:A:106:TRP:CZ3	2.11	0.85
1:A:104:TYR:O	1:A:108:ILE:HG22	1.75	0.85
1:A:16:LEU:CD2	1:A:270:VAL:CG1	2.55	0.85
1:A:173:SER:C	1:A:174:VAL:N	0.75	0.85
1:A:73:ALA:CB	1:A:85:ALA:O	2.25	0.84
1:A:104:TYR:C	1:A:108:ILE:CG2	2.50	0.84
1:A:155:ASN:O	1:A:155:ASN:ND2	2.10	0.84
1:A:257:LEU:HD23	1:A:263:TYR:CE1	2.11	0.84
1:A:221:SER:OG	1:A:222:MET:HE2	1.77	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
1:A:112:GLU:O	1:A:116:ALA:HB3	1.77	0.83
1:A:271:GLN:CG	1:A:271:GLN:O	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:241:TRP:C	1:A:242:THR:CA	2.48	0.82
1:A:247:ARG:NE	1:A:251:GLN:OE1	2.12	0.82
1:A:8:VAL:HG22	1:A:9:SER:H	1.43	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: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:8:VAL:HG23	1:A:14:PRO:HD3	1.62	0.81
1:A:96:LEU:HD21	1:A:101:SER:HA	1.63	0.81
1:A:253:THR:OG1	1:A:253:THR:O	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:155:ASN:ND2	1:A:155:ASN:C	2.35	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:249:SER:C	1:A:273:ALA:HB1	2.05	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:107:ILE:O	1:A:111:ILE:HG22	1.81	0.80
1:A:20:GLY:O	1:A:22:THR:HG23	1.82	0.80
1:A:39:HIS:HD2	1:A:40:PRO:CD	1.88	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:208:THR:C	1:A:209:LEU:HD12	2.06	0.79
1:A:207:SER:C	1:A:214:TYR:CD1	2.60	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:CD1	1:A:175:ILE:CB	2.61	0.78
1:A:200:ALA:HA	1:A:267:LEU:CD1	2.14	0.78
1:A:253:THR:HG21	1:A:273:ALA:CA	2.13	0.78
1:A:35:ILE:HG22	1:A:66:THR:HA	1.66	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: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:8:VAL:O	1:A:9:SER:C	2.27	0.77
1:A:248:SER:O	1:A:252:ASN:N	2.17	0.77
1:A:12:LYS:C	1:A:270:VAL:HB	2.08	0.76
1:A:98:ASP:O	1:A:99:ALA:HB3	1.85	0.76
1:A:5:PRO:HD3	1:A:81:VAL:HG22	1.68	0.76
1:A:35:ILE:HG21	1:A:69:ALA:HB3	1.66	0.76
1:A:271:GLN:O	1:A:271:GLN:HG2	1.86	0.76
1:A:104:TYR:C	1:A:108:ILE:HG23	2.10	0.76
1:A:2:GLN:O	3:A:277:HOH:O	2.01	0.76
1:A:122:ILE:HG22	1:A:149:VAL:HG13	1.66	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:159:THR:O	1:A:159:THR:HG22	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:VAL:HA	1:A:249:SER:HB2	1.68	0.76
1:A:189:PHE:O	1:A:189:PHE:HD1	1.67	0.75
1:A:30:VAL:C	1:A:30:VAL:CB	2.56	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: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:56:PRO:O	1:A:57:ASN:CG	2.30	0.74
1:A:145:SER:N	1:A:145:SER:CB	2.51	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:17:HIS:NE2	1:A:84:VAL:O	2.20	0.73
1:A:113:TRP:CZ3	1:A:119:MET:CE	2.59	0.73
1:A:207:SER:O	1:A:214:TYR:CA	2.36	0.73
1:A:96:LEU:CD2	1:A:101:SER:HA	2.18	0.73
1:A:124:MET:HE3	1:A:168:PRO:CG	2.19	0.73
1:A:106:TRP:CD1	1:A:106:TRP:N	2.54	0.73
1:A:155:ASN:O	1:A:156:GLU:HB2	1.88	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:164:THR:O	1:A:191:SER:OG	2.07	0.72
1:A:186:ARG:NH2	1:A:192:VAL:CG1	2.52	0.72
1:A:258:GLY:C	1:A:263:TYR:HB2	2.14	0.72
1:A:13:ALA:H	1:A:14:PRO:HD2	1.54	0.72
1:A:27:LYS:HD2	1:A:118:ASN:O	1.89	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:35:ILE:HG21	1:A:69:ALA:CB	2.19	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:111:ILE:O	1:A:111:ILE:HG13	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:GLN:N	1:A:59:GLN:C	2.48	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:146:GLY:C	1:A:243:ASN:ND2	2.48	0.71
1:A:24:SER:O	1:A:25:ASN:CB	2.32	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:91:TYR:CB	1:A:119:MET:CE	2.66	0.70
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: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: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:1:ALA:O	1:A:2:GLN:HG3	1.92	0.69
1:A:11:ILE:CD1	1:A:268:ILE:HG21	2.20	0.69
1:A:233:LEU:CA	1:A:233:LEU:CG	2.70	0.69
1:A:155:ASN:C	1:A:155:ASN:HD22	2.01	0.69
1:A:23:GLY:HA3	1:A:85:ALA:HB1	1.74	0.69
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:13:ALA:N	1:A:14:PRO:HD2	2.07	0.68
1:A:124:MET:HE1	1:A:168:PRO:HG3	1.74	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: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:125:SER:C	1:A:126:LEU:CG	2.47	0.67
1:A:163:SER:CB	1:A:193:GLY:HA2	2.23	0.67
1:A:1:ALA:O	1:A:2:GLN:CB	2.42	0.67
1:A:6:TYR:HA	1:A:9:SER:HB2	1.76	0.67
1:A:117:ASN:O	1:A:118:ASN:HB2	1.94	0.67
1:A:159:THR:O	1:A:159:THR:HG23	1.95	0.67
1:A:177:VAL:HG12	1:A:178:GLY:N	2.09	0.67
1:A:197:ASP:OD1	1:A:197:ASP:N	2.28	0.67
1:A:171:TYR:HB3	1:A:172:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:CG2	1:A:228:ALA:HB2	2.25	0.66
1:A:216:ALA:C	1:A:217:TYR:CD1	2.73	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:216:ALA:C	1:A:217:TYR:HD1	2.03	0.66
1:A:30:VAL:CA	1:A:31:ILE:N	2.50	0.66
1:A:1:ALA:O	1:A:2:GLN:HB2	1.96	0.66
1:A:14:PRO:O	1:A:17:HIS:HB2	1.95	0.66
1:A:27:LYS:HG3	1:A:120:ASP:OD2	1.96	0.66
1:A:112:GLU:HA	1:A:115:ILE:CG2	2.26	0.65
1:A:185:GLN:HG2	1:A:186:ARG:N	2.08	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:248:SER:C	1:A:252:ASN:HB2	2.22	0.65
1:A:207:SER:O	1:A:214:TYR:HA	1.96	0.65
1:A:81:VAL:CG1	1:A:82:LEU:N	2.60	0.64
1:A:124:MET:HE1	1:A:168:PRO:CG	2.22	0.64
1:A:146:GLY:O	1:A:243:ASN:CG	2.39	0.64
1:A:208:THR:HG22	1:A:214:TYR:CD1	2.30	0.64
1:A:257:LEU:CD2	1:A:263:TYR:CE1	2.79	0.64
1:A:8:VAL:CG2	1:A:13:ALA:HB3	2.27	0.64
1:A:104:TYR:HD1	1:A:104:TYR:H	1.44	0.64
1:A:34:GLY:CA	1:A:60:ASP:OD1	2.46	0.64
1:A:221:SER:H	1:A:222:MET:HE2	1.63	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:159:THR:HG21	1:A:162:SER:CB	2.27	0.63
1:A:237:LYS:HB3	1:A:238:HIS:NE2	2.13	0.63
1:A:98:ASP:O	1:A:99:ALA:CB	2.47	0.63
1:A:233:LEU:CB	1:A:233:LEU:N	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:HH22	1:A:192:VAL:HG12	1.62	0.62
1:A:186:ARG:HH21	1:A:262:TYR:HB3	1.64	0.62
1:A:27:LYS:HB3	1:A:91:TYR:CD1	2.35	0.62
1:A:242:THR:N	1:A:242:THR:CB	2.60	0.62
1:A:17:HIS:CE1	1:A:83:GLY:O	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE3	1:A:113:TRP:C	2.78	0.62
1:A:4:VAL:HG22	1:A:82:LEU:HB3	1.81	0.61
1:A:237:LYS:HB3	1:A:238:HIS:CE1	2.35	0.61
1:A:27:LYS:N	1:A:120:ASP:OD2	2.27	0.61
1:A:32:ASP:OD1	1:A:64:HIS:ND1	2.29	0.61
1:A:31:ILE:HG23	1:A:93:VAL:CG1	2.30	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: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:173:SER:O	1:A:174:VAL:CA	2.29	0.61
1:A:51:VAL:HB	1:A:106:TRP:CD2	2.36	0.61
1:A:175:ILE:HG22	1:A:247:ARG:HH11	1.62	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
1:A:30:VAL:C	1:A:30:VAL:N	2.54	0.60
1:A:246:VAL:CA	1:A:249:SER:HB2	2.31	0.60
1:A:8:VAL:C	1:A:10:GLN:N	2.41	0.60
1:A:234:ILE:HD11	1:A:274:ALA:HB2	1.84	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:242:THR:N	1:A:242:THR:C	2.56	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:123:ASN:C	1:A:123:ASN:HD22	2.08	0.59
1:A:84:VAL:O	1:A:86:PRO:HD3	2.03	0.58
1:A:142:ALA:O	1:A:147:VAL:HG23	2.03	0.58
1:A:91:TYR:HB3	1:A:119:MET:HE1	1.82	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:219:GLY:CA	1:A:222:MET:HE3	2.33	0.58
1:A:6:TYR:O	1:A:7:GLY:C	2.45	0.58
1:A:106:TRP:N	1:A:106:TRP:HD1	2.02	0.58
1:A:141:LYS:O	1:A:145:SER:OG	2.22	0.57
1:A:202:GLY:C	1:A:203:VAL:CG2	2.61	0.57
1:A:51:VAL:HG21	1:A:106:TRP:CH2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:207:SER:O	1:A:214:TYR:HB3	2.04	0.57
1:A:253:THR:CG2	1:A:273:ALA:CA	2.78	0.57
1:A:271:GLN:O	1:A:271:GLN:HG3	2.04	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:5:PRO:HG3	1:A:81:VAL:CG1	2.32	0.57
1:A:113:TRP:CZ3	1:A:119:MET:SD	2.98	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:60:ASP:O	1:A:210:PRO:HG3	2.05	0.56
1:A:207:SER:O	1:A:214:TYR:CD1	2.59	0.56
1:A:49:SER:HB2	1:A:57:ASN:HB3	1.88	0.56
1:A:62:ASN:ND2	1:A:64:HIS:HB2	2.20	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: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:69:ALA:O	1:A:72:VAL:HG12	2.06	0.55
1:A:78:SER:O	1:A:79:ILE:HD13	2.07	0.55
1:A:192:VAL:HG11	1:A:262:TYR:CE1	2.40	0.55
1:A:270:VAL:O	1:A:271:GLN:CB	2.52	0.55
1:A:28:VAL:HG22	1:A:121:VAL:HG21	1.85	0.55
1:A:233:LEU:CB	1:A:233:LEU:C	2.74	0.55
1:A:54:GLU:CD	1:A:97:GLY:O	2.49	0.55
1:A:148:VAL:O	1:A:148:VAL:HG22	2.05	0.55
1:A:56:PRO:HB2	1:A:58:PHE:N	2.21	0.55
1:A:268:ILE:N	1:A:268:ILE:HD13	2.22	0.55
1:A:5:PRO:HD3	1:A:81:VAL:CG2	2.34	0.55
1:A:11:ILE:CD1	1:A:268:ILE:CG2	2.76	0.55
1:A:146:GLY:O	1:A:243:ASN:ND2	2.39	0.55
1:A:154:GLY:O	1:A:220:THR:HG21	2.06	0.55
1:A:238:HIS:C	1:A:240:ASN:H	2.14	0.55
1:A:14:PRO:HA	1:A:17:HIS:ND1	2.22	0.54
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:72:VAL:CG1	1:A:73:ALA:N	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HG12	1:A:73:ALA:N	2.21	0.54
1:A:234:ILE:C	1:A:236:SER:H	2.15	0.54
1:A:255:THR:O	1:A:266:GLY:HA2	2.06	0.54
1:A:209:LEU:HD12	1:A:209:LEU:N	2.20	0.54
1:A:124:MET:HE3	1:A:168:PRO:CD	2.38	0.54
1:A:26:VAL:HG21	1:A:232:ALA:O	2.06	0.54
1:A:175:ILE:CG2	1:A:247:ARG:NH1	2.61	0.54
1:A:34:GLY:O	1:A:35:ILE:N	2.32	0.54
1:A:27:LYS:HB3	1:A:91:TYR:HE1	1.70	0.54
1:A:150:VAL:HG13	1:A:175:ILE:HG13	1.90	0.54
1:A:28:VAL:HG22	1:A:121:VAL:HB	1.89	0.54
1:A:34:GLY:C	1:A:60:ASP:OD1	2.50	0.54
1:A:258:GLY:O	1:A:263:TYR:HB2	2.06	0.54
1:A:13:ALA:C	1:A:15:ALA:H	2.16	0.53
1:A:39:HIS:CE1	1:A:208:THR:CG2	2.91	0.53
1:A:104:TYR:O	1:A:108:ILE:N	2.33	0.53
1:A:8:VAL:O	1:A:11:ILE:N	2.39	0.53
1:A:115:ILE:HD12	1:A:142:ALA:CA	2.39	0.53
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:91:TYR:HB2	1:A:119:MET:HE3	1.85	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:73:ALA:HB1	1:A:85:ALA:O	2.10	0.52
1:A:228:ALA:HA	1:A:231:ALA:HB3	1.91	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:C	1:A:108:ILE:HG22	2.29	0.52
1:A:104:TYR:HA	1:A:107:ILE:HG13	1.92	0.52
1:A:227:VAL:C	1:A:229:GLY:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:227:VAL:C	1:A:229:GLY:H	2.18	0.51
1:A:13:ALA:O	1:A:15:ALA:N	2.44	0.50
1:A:31:ILE:HG22	1:A:95:VAL:HG22	1.92	0.50
1:A:108:ILE:C	1:A:111:ILE:HG23	2.37	0.50
1:A:224:SER:HB3	1:A:225:PRO:HD3	1.94	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:105:SER:O	1:A:109:ASN:HB2	2.11	0.50
1:A:154:GLY:O	1:A:155:ASN:HB3	2.11	0.50
1:A:179:ALA:HB1	1:A:202:GLY:O	2.12	0.50
1:A:31:ILE:HG23	1:A:93:VAL:HG11	1.93	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
1:A:64:HIS:O	1:A:68:VAL:HB	2.12	0.49
1:A:111:ILE:O	1:A:115:ILE:HG21	2.12	0.49
1:A:180:VAL:HG22	1:A:185:GLN:O	2.11	0.49
1:A:224:SER:CB	1:A:225:PRO:CD	2.90	0.49
1:A:257:LEU:CD2	1:A:263:TYR:HE1	2.08	0.49
1:A:43:LYS:O	1:A:90:LEU:HB2	2.11	0.49
1:A:214:TYR:N	1:A:214:TYR:CD2	2.79	0.49
1:A:56:PRO:CB	1:A:58:PHE:HB2	2.41	0.49
1:A:245:GLN:O	1:A:246:VAL:C	2.55	0.49
1:A:4:VAL:HG22	1:A:82:LEU:HD23	1.94	0.49
1:A:208:THR:N	1:A:214:TYR:CD1	2.80	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:237:LYS:C	1:A:238:HIS:CG	2.88	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:155:ASN:O	1:A:155:ASN:CG	2.55	0.48
1:A:22:THR:CG2	1:A:22:THR:OG1	2.55	0.48
1:A:51:VAL:HG23	1:A:52:PRO:HD2	1.95	0.48
1:A:136:LYS:NZ	1:A:140:ASP:OD2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:186:ARG:CD	1:A:262:TYR:HB3	2.33	0.48
1:A:199:MET:HB3	1:A:266:GLY:O	2.13	0.48
1:A:123:ASN:ND2	1:A:224:SER:OG	2.47	0.48
1:A:60:ASP:CG	1:A:66:THR:OG1	2.56	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:145:SER:N	1:A:145:SER:C	2.64	0.47
1:A:164:THR:O	1:A:191:SER:CB	2.62	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:112:GLU:HA	1:A:115:ILE:HG21	1.95	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:28:VAL:HG22	1:A:121:VAL:CB	2.44	0.47
1:A:208:THR:N	1:A:214:TYR:HD1	2.11	0.47
1:A:37:SER:O	1:A:38:SER:C	2.54	0.47
1:A:42:LEU:HD22	1:A:42:LEU:HA	1.76	0.47
1:A:112:GLU:CA	1:A:115:ILE:CG2	2.92	0.47
1:A:151:ALA:O	1:A:176:ALA:HA	2.15	0.47
1:A:199:MET:O	1:A:267:LEU:HA	2.14	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:13:ALA:C	1:A:15:ALA:N	2.72	0.47
1:A:31:ILE:HG21	1:A:31:ILE:HD13	1.49	0.47
1:A:207:SER:O	1:A:214:TYR:CG	2.68	0.47
1:A:75:LEU:HA	1:A:75:LEU:HD12	1.37	0.47
1:A:208:THR:CG2	1:A:214:TYR:HE1	2.21	0.47
1:A:31:ILE:HG12	3:A:280:HOH:O	2.11	0.46
1:A:228:ALA:HA	1:A:231:ALA:CB	2.45	0.46
1:A:5:PRO:CD	1:A:81:VAL:CA	2.76	0.46
1:A:153:ALA:C	1:A:220:THR:HG21	2.40	0.46
1:A:163:SER:HB3	1:A:193:GLY:HA2	1.97	0.46
1:A:140:ASP:O	1:A:144:ALA:HB2	2.15	0.46
1:A:142:ALA:O	1:A:147:VAL:CG2	2.63	0.46
1:A:202:GLY:O	1:A:203:VAL:HG22	2.05	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:CB	1:A:119:MET:HE2	2.46	0.46
1:A:138:ALA:O	1:A:142:ALA:N	2.39	0.46
1:A:138:ALA:O	1:A:142:ALA:CB	2.64	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:18:SER:C	1:A:20:GLY:N	2.73	0.45
1:A:195:GLU:C	1:A:196:LEU:CA	2.82	0.45
1:A:142:ALA:O	1:A:147:VAL:HB	2.16	0.45
1:A:25:ASN:HD22	1:A:25:ASN:HA	1.59	0.45
1:A:36:ASP:HB2	1:A:66:THR:HG23	1.98	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:244:THR:O	1:A:245:GLN:C	2.59	0.45
1:A:72:VAL:HG12	1:A:73:ALA:H	1.81	0.45
1:A:95:VAL:O	1:A:106:TRP:HB3	2.16	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:49:SER:C	1:A:50:MET:SD	2.98	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
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:30:VAL:C	1:A:30:VAL:CG1	2.90	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:113:TRP:C	1:A:113:TRP:HE3	2.22	0.44
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.50	0.44
1:A:105:SER:C	1:A:106:TRP:HD1	2.25	0.44
1:A:4:VAL:CG2	1:A:82:LEU:HD23	2.48	0.44
1:A:23:GLY:N	1:A:233:LEU:HD12	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ALA:HB2	1:A:114:ALA:HB1	2.00	0.43
1:A:41:ASP:C	1:A:75:LEU:HB2	2.44	0.43
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.78	0.43
1:A:145:SER:N	1:A:145:SER:OG	2.52	0.43
1:A:224:SER:N	1:A:225:PRO:CD	2.81	0.43
1:A:243:ASN:OD1	1:A:243:ASN:N	2.50	0.43
1:A:74:ALA:O	1:A:75:LEU:C	2.60	0.43
1:A:11:ILE:HG13	1:A:11:ILE:O	2.19	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:189:PHE:CE1	1:A:219:GLY:HA2	2.53	0.43
1:A:195:GLU:O	1:A:197:ASP:OD1	2.36	0.43
1:A:122:ILE:HG21	1:A:149:VAL:CG1	2.35	0.43
1:A:209:LEU:HD13	1:A:214:TYR:C	2.43	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:195:GLU:O	1:A:196:LEU:C	2.62	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:159:THR:HG21	1:A:162:SER:HB3	1.98	0.42
1:A:182:SER:C	1:A:184:ASN:N	2.77	0.42
1:A:234:ILE:CD1	1:A:249:SER:HB3	2.50	0.42
1:A:104:TYR:HA	1:A:107:ILE:HB	2.01	0.42
1:A:19:GLN:HB2	1:A:21:TYR:HD2	1.85	0.42
1:A:94:LYS:HD2	1:A:96:LEU:O	2.20	0.42
1:A:97:GLY:O	1:A:98:ASP:CG	2.62	0.42
1:A:175:ILE:CG2	1:A:247:ARG:CZ	2.97	0.42
1:A:247:ARG:O	1:A:251:GLN:CG	2.63	0.42
1:A:31:ILE:HA	3:A:280:HOH:O	1.86	0.42
1:A:122:ILE:HG21	1:A:149:VAL:HG22	2.01	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:11:ILE:CB	1:A:268:ILE:HB	2.30	0.41
1:A:35:ILE:CG2	1:A:69:ALA:CB	2.85	0.41
1:A:147:VAL:O	1:A:243:ASN:ND2	2.53	0.41
1:A:204:SER:H	1:A:218:ASN:HB3	1.85	0.41
1:A:209:LEU:N	1:A:209:LEU:CD1	2.84	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:56:PRO:C	1:A:58:PHE:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLY:C	1:A:195:GLU:N	2.76	0.41
1:A:28:VAL:CG1	1:A:121:VAL:HB	2.47	0.41
1:A:51:VAL:HA	1:A:52:PRO:HD3	1.90	0.41
1:A:182:SER:C	1:A:184:ASN:H	2.27	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:4:VAL:HA	1:A:81:VAL:HA	2.02	0.41
1:A:18:SER:O	1:A:19:GLN:C	2.62	0.41
1:A:33:SER:HA	1:A:98:ASP:OD1	2.21	0.41
1:A:227:VAL:O	1:A:231:ALA:N	2.43	0.41
1:A:31:ILE:HD11	1:A:111:ILE:HB	2.02	0.41
1:A:258:GLY:HA3	1:A:263:TYR:CD2	2.55	0.41
1:A:69:ALA:O	1:A:72:VAL:CG1	2.69	0.41
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.65	0.41
1:A:122:ILE:HG21	1:A:122:ILE:HD13	1.81	0.41
1:A:237:LYS:C	1:A:238:HIS:CD2	2.99	0.41
1:A:60:ASP:CB	1:A:66:THR:OG1	2.69	0.41
1:A:121:VAL:HG21	1:A:232:ALA:CB	2.44	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:15:ALA:O	1:A:16:LEU:C	2.65	0.40
1:A:62:ASN:OD1	1:A:99:ALA:N	2.55	0.40
1:A:112:GLU:C	1:A:115:ILE:HG23	2.46	0.40
1:A:222:MET:H	1:A:222:MET:HG2	1.35	0.40
1:A:11:ILE:CG1	1:A:11:ILE:O	2.68	0.40
1:A:217:TYR:CD1	1:A:217:TYR:N	2.88	0.40
1:A:30:VAL:C	1:A:30:VAL:HG12	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:19:GLN:OE1	1:A:52:PRO:CA[2_656]	1.20	1.00
1:A:21:TYR:CE2	1:A:53:SER:CB[2_656]	1.20	1.00
1:A:21:TYR:N	1:A:106:TRP:CH2[2_656]	1.21	0.99
1:A:206:GLN:CD	1:A:242:THR:CB[1_556]	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:19:GLN:CG	1:A:51:VAL:C[2_656]	1.71	0.49
1:A:20:GLY:N	1:A:106:TRP:CZ3[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:20:GLY:N	1:A:106:TRP:CE3[2_656]	1.76	0.44
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:38:SER:N	1:A:260:SER:N[1_455]	1.77	0.43
1:A:16:LEU:O	1:A:52:PRO:CD[2_656]	1.78	0.42
1:A:18:SER:O	1:A:106:TRP:CG[2_656]	1.78	0.42
1:A:19:GLN:CA	1:A:51:VAL:CG2[2_656]	1.78	0.42
1:A:38:SER:CB	1:A:261:PHE:N[1_455]	1.78	0.42
1:A:19:GLN:N	1:A:51:VAL:CG1[2_656]	1.79	0.41
1:A:37:SER:N	1:A:260:SER:CB[1_455]	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:19:GLN:OE1	1:A:52:PRO:N[2_656]	1.82	0.38
1:A:36:ASP:CG	1:A:259:ASP:OD1[1_455]	1.82	0.38
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:16:LEU:C	1:A:52:PRO:CG[2_656]	1.88	0.32
1:A:39:HIS:N	1:A:260:SER:N[1_455]	1.88	0.32
1:A:115:ILE:O	1:A:213:LYS:NZ[1_554]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:20:GLY:C	1:A:106:TRP:CZ2[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:21:TYR:CG	1:A:53:SER:OG[2_656]	1.92	0.28
1:A:53:SER:O	1:A:237:LYS:NZ[2_646]	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:18:SER:O	1:A:51:VAL:CB[2_656]	1.97	0.23
1:A:38:SER:OG	1:A:261:PHE:CA[1_455]	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:19:GLN:CB	1:A:51:VAL:C[2_656]	1.99	0.21
1:A:20:GLY:N	1:A:51:VAL:CB[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: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:21:TYR:CZ	1:A:53:SER:CB[2_656]	2.09	0.11
1:A:21:TYR:N	1:A:106:TRP:CZ2[2_656]	2.09	0.11
1:A:36:ASP:OD2	1:A:259:ASP:CB[1_455]	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:37:SER:CA	1:A:260:SER:OG[1_455]	2.11	0.09
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:144:ALA:O	1:A:209:LEU:CD2[1_554]	2.14	0.06
1:A:18:SER:OG	1:A:50:MET:C[2_656]	2.15	0.05
1:A:19:GLN:CA	1:A:51:VAL:CA[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:19:GLN:NE2	1:A:51:VAL:O[2_656]	2.18	0.02
1:A:206:GLN:OE1	1:A:242:THR:CA[1_556]	2.18	0.02
1:A:19:GLN:OE1	1:A:51:VAL:C[2_656]	2.19	0.01
1:A:20:GLY:CA	1:A:106:TRP:CD2[2_656]	2.19	0.01
1:A:38:SER:C	1:A:260:SER:N[1_455]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	271/275 (98%)	186 (69%)	51 (19%)	34 (12%)	0 0

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
1	A	153	ALA
1	A	155	ASN
1	A	156	GLU
1	A	186	ARG
1	A	203	VAL

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Mol	Chain	Res	Type
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%)	107 (52%)	97 (48%)	0 0

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	3	SER
1	A	4	VAL

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Mol	Chain	Res	Type
1	A	8	VAL
1	A	9	SER
1	A	11	ILE
1	A	12	LYS
1	A	16	LEU
1	A	22	THR
1	A	24	SER
1	A	25	ASN
1	A	27	LYS
1	A	31	ILE
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	51	VAL
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	112	GLU
1	A	115	ILE
1	A	117	ASN
1	A	119	MET
1	A	120	ASP

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Mol	Chain	Res	Type
1	A	121	VAL
1	A	122	ILE
1	A	124	MET
1	A	125	SER
1	A	126	LEU
1	A	135	LEU
1	A	139	VAL
1	A	143	VAL
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	196	LEU
1	A	197	ASP
1	A	198	VAL
1	A	205	ILE
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	234	ILE
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	246	VAL
1	A	247	ARG
1	A	248	SER
1	A	249	SER

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Mol	Chain	Res	Type
1	A	252	ASN
1	A	253	THR
1	A	254	THR
1	A	256	LYS
1	A	257	LEU
1	A	261	PHE
1	A	262	TYR
1	A	265	LYS
1	A	268	ILE
1	A	271	GLN

Sometimes 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	118	ASN
1	A	123	ASN
1	A	155	ASN
1	A	238	HIS
1	A	243	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	2.52	2 (66%)	3,3,3	1.87	1 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	276	ACN	O-C	-3.11	1.02	1.22
2	A	276	ACN	C2-C	3.04	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	2.72	136.23	120.79

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	34

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	55:THR	C	56:PRO	N	4.26
1	A	34:GLY	C	35:ILE	N	1.89
1	A	195:GLU	C	196:LEU	N	1.74
1	A	59:GLN	C	60:ASP	N	1.72
1	A	97:GLY	C	98:ASP	N	1.65
1	A	139:VAL	C	140:ASP	N	1.20
1	A	151:ALA	C	152:ALA	N	1.20
1	A	185:GLN	C	186:ARG	N	1.20
1	A	268:ILE	C	269:ASN	N	1.20
1	A	1:ALA	C	2:GLN	N	1.19
1	A	62:ASN	C	63:SER	N	1.19
1	A	175:ILE	C	176:ALA	N	1.19
1	A	217:TYR	C	218:ASN	N	1.19
1	A	221:SER	C	222:MET	N	1.19
1	A	17:HIS	C	18:SER	N	1.18
1	A	79:ILE	C	80:GLY	N	1.18
1	A	174:VAL	C	175:ILE	N	1.18
1	A	209:LEU	C	210:PRO	N	1.18
1	A	7:GLY	C	8:VAL	N	1.17
1	A	121:VAL	C	122:ILE	N	1.17
1	A	146:GLY	C	147:VAL	N	1.16
1	A	211:GLY	C	212:ASN	N	1.16
1	A	249:SER	C	250:LEU	N	1.16
1	A	94:LYS	C	95:VAL	N	1.15
1	A	108:ILE	C	109:ASN	N	1.15
1	A	112:GLU	C	113:TRP	N	1.15
1	A	128:GLY	C	129:PRO	N	1.15
1	A	71:THR	C	72:VAL	N	1.14
1	A	241:TRP	C	242:THR	N	1.14
1	A	52:PRO	C	53:SER	N	1.12
1	A	73:ALA	C	74:ALA	N	1.12
1	A	114:ALA	C	115:ILE	N	1.10
1	A	190:SER	C	191:SER	N	1.10
1	A	173:SER	C	174:VAL	N	0.75

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.