



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:58 PM UTC

PDB ID : 6TAA / pdb_00006taa
Title : STRUCTURE AND MOLECULAR MODEL REFINEMENT OF AS-
PERGILLUS ORYZAE (TAKA) ALPHA-AMYLASE: AN APPLICATION
OF THE SIMULATED-ANNEALING METHOD
Authors : Swift, H.J.; Brady, L.; Derewenda, Z.S.; Dodson, E.J.; Turkenburg, J.P.;
Wilkinson, A.J.
Deposited on : 1992-08-21
Resolution : 2.10 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

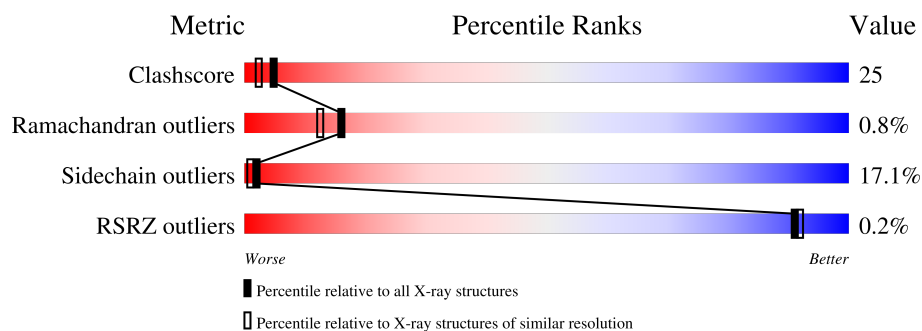
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3927 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 ALPHA-AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	31	0	0
			3686	2336	595	737	18			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

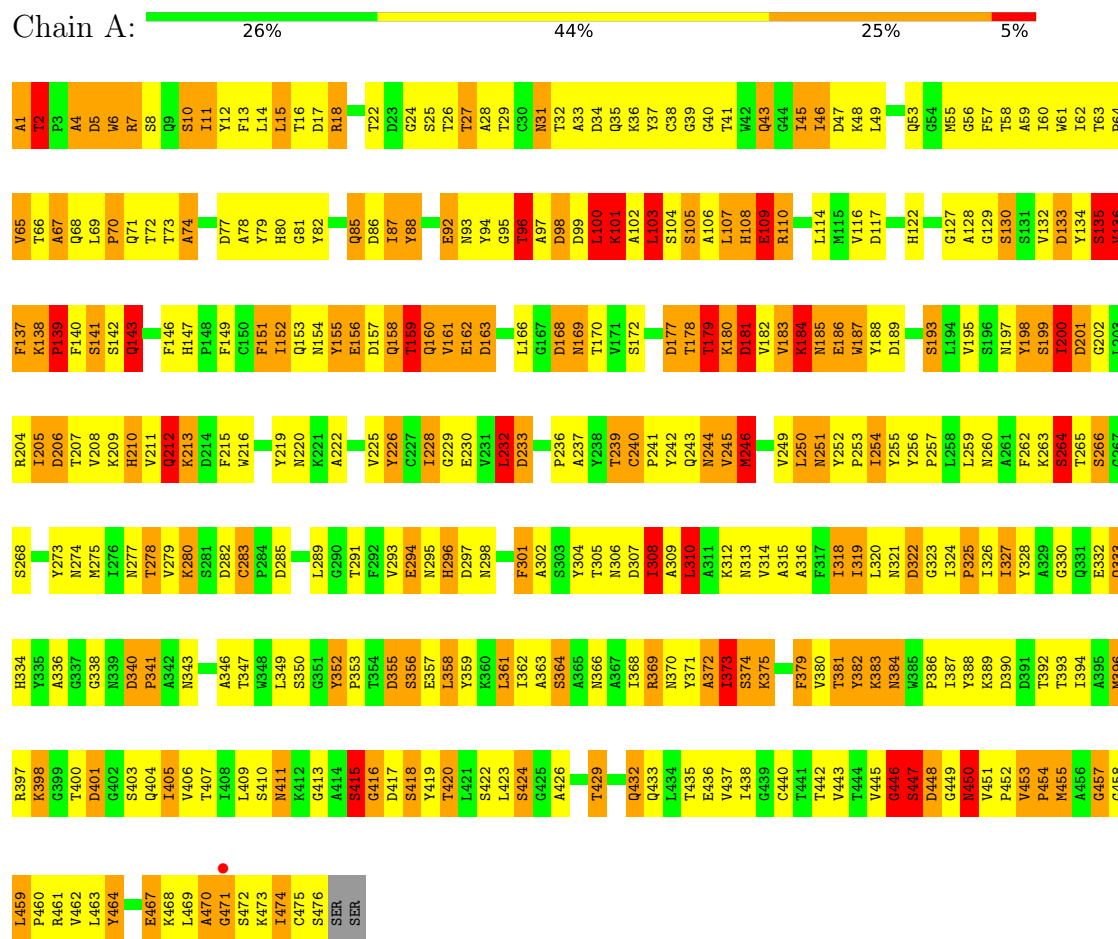
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	239	Total	O	0	0
			239	239		

3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ALPHA-AMYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.04Å 67.18Å 133.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.70 – 2.10 7.70 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.70-2.10) 85.2 (7.70-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.93 (at 2.10Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.198 , (Not available) 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3927	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.68	28/3781 (0.7%)	3.09	517/5164 (10.0%)

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	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	LYS	CE-NZ	-10.60	1.17	1.49
1	A	169	ASN	CG-OD1	10.34	1.43	1.23
1	A	92	GLU	CD-OE1	9.21	1.42	1.25
1	A	92	GLU	CD-OE2	-7.22	1.11	1.25
1	A	208	VAL	C-O	7.08	1.32	1.24
1	A	181	ASP	CB-CG	6.92	1.69	1.52
1	A	2	THR	CA-CB	6.58	1.63	1.53
1	A	246	MET	C-O	6.48	1.31	1.23
1	A	324	ILE	CA-CB	6.34	1.60	1.53
1	A	313	ASN	C-O	6.23	1.31	1.24
1	A	471	GLY	N-CA	6.16	1.54	1.45
1	A	183	VAL	N-CA	6.06	1.53	1.46
1	A	469	LEU	C-O	6.06	1.31	1.24
1	A	380	VAL	C-O	6.01	1.31	1.24
1	A	211	VAL	C-O	5.98	1.30	1.24
1	A	198	TYR	N-CA	5.90	1.54	1.45
1	A	310	LEU	N-CA	5.84	1.53	1.46
1	A	39	GLY	C-O	5.67	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	TYR	N-CA	5.67	1.53	1.46
1	A	210	HIS	C-N	-5.55	1.26	1.33
1	A	280	LYS	N-CA	5.54	1.53	1.46
1	A	127	GLY	N-CA	5.50	1.50	1.45
1	A	435	THR	CA-CB	5.40	1.61	1.53
1	A	326	ILE	C-N	-5.35	1.26	1.33
1	A	379	PHE	C-O	5.20	1.30	1.24
1	A	239	THR	CA-CB	5.09	1.61	1.53
1	A	327	ILE	C-O	5.07	1.29	1.24
1	A	46	ILE	C-N	-5.05	1.27	1.33

All (517) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ASN	OD1-CG-ND2	-18.17	104.43	122.60
1	A	451	VAL	CA-C-O	17.71	132.71	119.25
1	A	453	VAL	CA-C-O	15.46	129.24	119.19
1	A	163	ASP	CA-CB-CG	14.42	127.02	112.60
1	A	451	VAL	O-C-N	-13.13	113.10	121.37
1	A	197	ASN	CA-CB-CG	13.04	125.64	112.60
1	A	450	ASN	CA-CB-CG	-12.91	99.69	112.60
1	A	181	ASP	CA-CB-CG	-12.72	99.88	112.60
1	A	215	PHE	CA-CB-CG	12.58	126.38	113.80
1	A	177	ASP	CA-C-O	12.53	135.43	121.39
1	A	245	VAL	N-CA-CB	-12.49	93.55	112.67
1	A	240	CYS	CA-C-O	12.38	130.35	118.34
1	A	183	VAL	CB-CA-C	12.29	127.44	111.70
1	A	424	SER	CA-C-O	-11.94	107.67	121.16
1	A	401	ASP	CA-CB-CG	11.89	124.50	112.60
1	A	154	ASN	CA-CB-CG	11.74	124.34	112.60
1	A	298	ASN	O-C-N	11.74	130.21	121.88
1	A	202	GLY	O-C-N	11.53	136.77	123.51
1	A	189	ASP	CA-CB-CG	-11.44	101.16	112.60
1	A	424	SER	O-C-N	11.16	137.22	123.16
1	A	245	VAL	CB-CA-C	11.15	121.74	110.70
1	A	2	THR	N-CA-C	10.88	125.15	109.48
1	A	294	GLU	CB-CG-CD	10.86	131.06	112.60
1	A	418	SER	CA-C-O	-10.78	108.63	120.38
1	A	325	PRO	CA-C-O	-10.70	109.78	121.23
1	A	132	VAL	CA-C-O	-10.70	110.89	121.58
1	A	445	VAL	CA-C-N	10.64	142.26	121.41
1	A	445	VAL	C-N-CA	10.64	142.26	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	THR	CA-CB-OG1	-10.55	93.77	109.60
1	A	461	ARG	NE-CZ-NH2	-10.52	109.73	119.20
1	A	41	THR	CA-CB-OG1	-10.50	93.84	109.60
1	A	65	VAL	N-CA-CB	-10.44	93.92	111.98
1	A	98	ASP	CA-CB-CG	-10.42	102.18	112.60
1	A	328	TYR	O-C-N	-10.16	111.44	123.13
1	A	449	GLY	CA-C-O	-10.03	108.16	119.10
1	A	188	TYR	CA-C-O	10.03	131.18	120.55
1	A	382	TYR	O-C-N	-9.92	110.73	122.93
1	A	450	ASN	CA-C-N	9.77	133.98	122.85
1	A	450	ASN	C-N-CA	9.77	133.98	122.85
1	A	415	SER	O-C-N	9.75	135.56	122.59
1	A	132	VAL	O-C-N	9.75	132.66	122.62
1	A	363	ALA	O-C-N	9.73	132.59	122.09
1	A	244	ASN	CA-CB-CG	-9.70	102.90	112.60
1	A	68	GLN	OE1-CD-NE2	-9.52	113.08	122.60
1	A	373	ILE	CA-CB-CG2	9.45	126.57	110.50
1	A	69	LEU	CA-C-N	9.38	129.11	119.64
1	A	69	LEU	C-N-CA	9.38	129.11	119.64
1	A	60	ILE	CA-CB-CG2	9.23	126.19	110.50
1	A	156	GLU	N-CA-C	-9.21	101.46	112.89
1	A	225	VAL	CA-C-O	-9.16	112.23	121.49
1	A	7	ARG	NE-CZ-NH2	-9.15	110.97	119.20
1	A	105	SER	CA-C-O	-9.00	109.06	120.31
1	A	340	ASP	CA-C-O	8.99	127.26	119.71
1	A	255	TYR	CA-C-O	-8.98	111.19	121.07
1	A	452	PRO	O-C-N	8.90	134.65	122.64
1	A	232	LEU	CB-CA-C	8.87	126.01	111.83
1	A	160	GLN	OE1-CD-NE2	-8.80	113.80	122.60
1	A	282	ASP	CA-C-O	-8.80	109.12	119.15
1	A	178	THR	CA-C-N	8.79	132.93	120.28
1	A	178	THR	C-N-CA	8.79	132.93	120.28
1	A	475	CYS	CA-C-O	-8.78	111.18	120.40
1	A	186	GLU	O-C-N	8.78	131.11	122.07
1	A	244	ASN	CA-C-O	-8.76	107.65	119.12
1	A	149	PHE	CA-CB-CG	-8.74	105.06	113.80
1	A	471	GLY	N-CA-C	-8.70	92.56	113.18
1	A	100	LEU	N-CA-C	-8.70	101.77	112.38
1	A	168	ASP	CA-C-N	8.68	135.21	120.72
1	A	168	ASP	C-N-CA	8.68	135.21	120.72
1	A	87	ILE	CA-C-O	-8.60	108.47	119.39
1	A	409	LEU	CA-C-O	-8.47	111.59	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ALA	CA-C-O	-8.46	110.55	120.10
1	A	130	SER	CA-C-O	-8.43	110.28	119.97
1	A	388	TYR	N-CA-CB	-8.41	96.66	111.39
1	A	201	ASP	CA-CB-CG	-8.39	104.21	112.60
1	A	239	THR	N-CA-C	8.38	122.00	111.69
1	A	374	SER	CB-CA-C	-8.36	96.92	110.79
1	A	216	TRP	N-CA-C	8.35	125.01	113.16
1	A	68	GLN	CG-CD-OE1	8.34	137.49	120.80
1	A	109	GLU	CB-CG-CD	8.28	126.67	112.60
1	A	201	ASP	O-C-N	8.27	133.79	122.46
1	A	96	THR	N-CA-CB	-8.24	96.99	111.08
1	A	96	THR	CA-C-O	-8.22	111.83	121.11
1	A	162	GLU	CA-C-O	8.21	128.17	119.14
1	A	369	ARG	CD-NE-CZ	8.11	135.76	124.40
1	A	362	ILE	O-C-N	8.09	129.72	121.87
1	A	201	ASP	CA-C-O	-8.08	109.82	119.27
1	A	143	GLN	OE1-CD-NE2	8.06	130.66	122.60
1	A	256	TYR	CA-C-O	-8.05	111.43	119.08
1	A	105	SER	O-C-N	8.04	133.16	122.30
1	A	185	ASN	CB-CG-ND2	-8.03	104.35	116.40
1	A	308	ILE	CA-C-O	-8.03	109.90	119.85
1	A	250	LEU	N-CA-CB	-8.02	97.95	110.06
1	A	264	SER	CA-C-O	-8.02	112.34	121.40
1	A	47	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	39	GLY	CA-C-N	-7.93	112.81	120.34
1	A	39	GLY	C-N-CA	-7.93	112.81	120.34
1	A	57	PHE	CA-CB-CG	-7.91	105.89	113.80
1	A	340	ASP	O-C-N	-7.90	114.90	121.38
1	A	394	ILE	CA-C-O	-7.88	112.14	121.28
1	A	349	LEU	CA-C-O	-7.86	109.97	119.49
1	A	355	ASP	CA-CB-CG	-7.85	104.75	112.60
1	A	130	SER	O-C-N	7.84	131.91	122.27
1	A	200	ILE	CB-CG1-CD1	-7.82	97.39	113.80
1	A	265	THR	CA-C-N	-7.77	110.40	122.37
1	A	265	THR	C-N-CA	-7.77	110.40	122.37
1	A	397	ARG	CA-C-O	-7.76	110.74	120.28
1	A	250	LEU	CB-CA-C	7.74	122.61	109.53
1	A	364	SER	O-C-N	-7.71	111.82	122.46
1	A	393	THR	CA-C-O	-7.71	112.12	121.06
1	A	298	ASN	CA-C-O	-7.69	112.36	120.28
1	A	181	ASP	CA-C-N	-7.65	109.80	120.74
1	A	181	ASP	C-N-CA	-7.65	109.80	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	GLU	N-CA-CB	7.64	123.08	110.39
1	A	435	THR	CA-C-O	-7.64	112.05	120.38
1	A	33	ALA	N-CA-C	-7.60	102.97	111.71
1	A	318	ILE	CA-CB-CG2	7.59	123.41	110.50
1	A	467	GLU	O-C-N	7.59	129.98	122.09
1	A	304	TYR	CA-C-O	-7.58	110.73	119.60
1	A	436	GLU	O-C-N	-7.56	112.99	122.82
1	A	461	ARG	CA-C-O	-7.53	112.23	120.36
1	A	149	PHE	CA-C-O	7.51	129.34	120.70
1	A	437	VAL	O-C-N	7.46	131.35	122.17
1	A	117	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	222	ALA	CA-C-O	7.44	128.44	120.55
1	A	35	GLN	OE1-CD-NE2	-7.43	115.17	122.60
1	A	26	THR	O-C-N	7.40	131.15	122.19
1	A	232	LEU	N-CA-CB	-7.40	99.92	110.58
1	A	460	PRO	O-C-N	-7.40	113.96	123.06
1	A	453	VAL	O-C-N	-7.40	114.88	121.61
1	A	370	ASN	CB-CG-ND2	7.38	127.48	116.40
1	A	74	ALA	CA-C-O	7.38	128.42	119.49
1	A	31	ASN	CA-CB-CG	-7.38	105.22	112.60
1	A	226	TYR	O-C-N	7.37	131.88	122.89
1	A	12	TYR	CA-C-O	-7.36	112.58	120.46
1	A	151	PHE	CA-C-O	-7.33	112.94	120.71
1	A	423	LEU	CA-C-O	7.29	128.59	120.43
1	A	289	LEU	O-C-N	-7.28	114.79	122.94
1	A	332	GLU	CA-C-O	-7.23	110.49	119.38
1	A	179	THR	O-C-N	-7.21	113.79	122.22
1	A	1	ALA	CA-C-N	7.20	130.44	120.65
1	A	1	ALA	C-N-CA	7.20	130.44	120.65
1	A	438	ILE	O-C-N	7.17	131.54	122.57
1	A	146	PHE	N-CA-C	7.17	121.21	109.24
1	A	2	THR	CB-CA-C	-7.15	98.40	109.62
1	A	369	ARG	NE-CZ-NH1	-7.13	114.36	121.50
1	A	277	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	A	103	LEU	CB-CA-C	7.11	122.19	110.81
1	A	323	GLY	CA-C-N	7.11	127.43	122.60
1	A	323	GLY	C-N-CA	7.11	127.43	122.60
1	A	389	LYS	CA-C-O	-7.10	112.05	120.43
1	A	211	VAL	CB-CA-C	7.10	121.41	110.83
1	A	298	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	A	470	ALA	O-C-N	7.08	132.01	122.59
1	A	396	MET	CA-C-O	-7.08	113.16	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	PRO	O-C-N	7.07	130.72	122.23
1	A	225	VAL	CA-CB-CG1	7.05	122.38	110.40
1	A	222	ALA	N-CA-C	7.04	118.95	111.28
1	A	18	ARG	N-CA-C	7.01	121.92	112.88
1	A	62	ILE	CA-C-O	-7.00	112.08	121.32
1	A	455	MET	O-C-N	-6.99	114.10	123.19
1	A	275	MET	CA-C-O	-6.99	111.93	119.97
1	A	229	GLY	CA-C-O	6.99	127.79	120.94
1	A	291	THR	CA-C-O	-6.99	112.89	120.92
1	A	388	TYR	O-C-N	-6.97	115.68	123.48
1	A	153	GLN	CB-CA-C	6.96	123.27	110.11
1	A	417	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	225	VAL	O-C-N	6.94	130.91	122.58
1	A	260	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	A	314	VAL	CA-C-O	-6.93	112.98	120.47
1	A	202	GLY	CA-C-O	-6.93	113.57	121.68
1	A	216	TRP	CB-CG-CD1	-6.93	116.50	126.90
1	A	244	ASN	O-C-N	6.93	132.64	122.39
1	A	26	THR	CA-CB-OG1	-6.92	99.22	109.60
1	A	369	ARG	NH1-CZ-NH2	6.92	128.29	119.30
1	A	60	ILE	CA-CB-CG1	-6.91	98.65	110.40
1	A	369	ARG	N-CA-C	-6.91	103.67	111.07
1	A	397	ARG	CD-NE-CZ	-6.90	114.73	124.40
1	A	40	GLY	CA-C-O	-6.89	114.46	121.90
1	A	179	THR	CA-C-O	6.87	127.86	120.10
1	A	36	LYS	CA-C-O	-6.85	113.45	121.46
1	A	363	ALA	CA-C-O	-6.84	113.65	120.70
1	A	415	SER	CA-CB-OG	-6.84	97.42	111.10
1	A	199	SER	CA-C-N	-6.84	112.60	122.45
1	A	199	SER	C-N-CA	-6.84	112.60	122.45
1	A	183	VAL	N-CA-CB	-6.81	103.47	110.62
1	A	413	GLY	O-C-N	-6.81	116.05	122.86
1	A	135	SER	CA-C-N	-6.81	109.47	120.64
1	A	135	SER	C-N-CA	-6.81	109.47	120.64
1	A	58	THR	CA-CB-OG1	-6.81	99.39	109.60
1	A	389	LYS	N-CA-CB	-6.80	98.95	110.99
1	A	332	GLU	O-C-N	6.78	131.52	122.43
1	A	46	ILE	CB-CG1-CD1	6.78	128.03	113.80
1	A	212	GLN	CB-CG-CD	6.75	124.08	112.60
1	A	107	LEU	CA-C-O	6.75	128.08	121.00
1	A	155	TYR	O-C-N	6.72	132.24	122.43
1	A	228	ILE	O-C-N	-6.71	116.09	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	VAL	O-C-N	-6.70	115.32	121.89
1	A	71	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	A	277	ASN	CB-CG-ND2	6.67	126.41	116.40
1	A	278	THR	CA-CB-OG1	-6.63	99.65	109.60
1	A	291	THR	CA-CB-OG1	-6.63	99.65	109.60
1	A	474	ILE	CA-C-O	-6.62	114.20	121.29
1	A	447	SER	CA-C-O	6.62	129.98	120.51
1	A	373	ILE	CB-CG1-CD1	-6.62	99.90	113.80
1	A	409	LEU	CA-C-N	-6.61	110.32	121.75
1	A	409	LEU	C-N-CA	-6.61	110.32	121.75
1	A	67	ALA	CA-C-O	-6.60	112.92	120.58
1	A	46	ILE	O-C-N	-6.59	115.35	121.94
1	A	139	PRO	N-CA-CB	-6.55	95.40	102.60
1	A	325	PRO	CB-CA-C	-6.53	103.41	111.64
1	A	328	TYR	CA-C-N	6.53	134.01	121.54
1	A	328	TYR	C-N-CA	6.53	134.01	121.54
1	A	304	TYR	O-C-N	6.52	131.62	122.36
1	A	158	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	103	LEU	CA-C-N	6.51	131.11	120.63
1	A	103	LEU	C-N-CA	6.51	131.11	120.63
1	A	88	TYR	CA-C-O	6.50	127.17	119.56
1	A	46	ILE	N-CA-C	-6.50	103.54	110.36
1	A	390	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	419	TYR	CA-C-N	-6.49	113.52	122.93
1	A	419	TYR	C-N-CA	-6.49	113.52	122.93
1	A	243	GLN	CA-C-N	-6.48	108.99	121.94
1	A	243	GLN	C-N-CA	-6.48	108.99	121.94
1	A	321	ASN	O-C-N	6.47	130.62	122.65
1	A	474	ILE	CA-C-N	-6.46	113.64	123.07
1	A	474	ILE	C-N-CA	-6.46	113.64	123.07
1	A	279	VAL	CA-C-N	-6.46	111.12	120.29
1	A	279	VAL	C-N-CA	-6.46	111.12	120.29
1	A	128	ALA	CB-CA-C	6.45	120.67	109.65
1	A	101	LYS	O-C-N	6.43	130.99	122.30
1	A	469	LEU	CA-C-O	-6.42	113.37	120.69
1	A	184	LYS	CB-CA-C	-6.41	100.19	110.84
1	A	228	ILE	CB-CA-C	6.40	119.86	110.77
1	A	15	LEU	CA-C-O	-6.39	113.27	120.43
1	A	452	PRO	CA-C-N	-6.39	117.16	123.04
1	A	452	PRO	C-N-CA	-6.39	117.16	123.04
1	A	80	HIS	CA-C-N	6.39	132.50	121.07
1	A	80	HIS	C-N-CA	6.39	132.50	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	SER	N-CA-C	-6.38	97.22	110.80
1	A	186	GLU	CG-CD-OE1	6.37	133.05	118.40
1	A	316	ALA	O-C-N	-6.36	114.44	122.27
1	A	429	THR	CA-CB-CG2	6.35	121.29	110.50
1	A	96	THR	OG1-CB-CG2	6.34	121.98	109.30
1	A	379	PHE	O-C-N	6.34	128.86	122.08
1	A	193	SER	CA-C-O	-6.33	113.21	120.24
1	A	63	THR	CA-CB-CG2	6.32	121.24	110.50
1	A	308	ILE	N-CA-CB	6.32	124.31	111.05
1	A	392	THR	CA-CB-OG1	-6.32	100.12	109.60
1	A	43	GLN	CB-CG-CD	6.30	123.32	112.60
1	A	382	TYR	CA-C-O	6.30	128.06	120.81
1	A	347	THR	O-C-N	-6.30	115.44	122.12
1	A	437	VAL	CA-C-O	-6.30	111.39	119.39
1	A	63	THR	CA-C-N	6.30	126.32	119.90
1	A	63	THR	C-N-CA	6.30	126.32	119.90
1	A	253	PRO	O-C-N	-6.28	115.02	122.24
1	A	66	THR	CA-C-N	6.26	130.26	121.24
1	A	66	THR	C-N-CA	6.26	130.26	121.24
1	A	163	ASP	N-CA-CB	-6.26	101.97	110.67
1	A	462	VAL	CA-CB-CG2	6.25	121.03	110.40
1	A	213	LYS	O-C-N	6.25	128.59	122.09
1	A	415	SER	N-CA-CB	6.25	121.05	110.49
1	A	467	GLU	CA-C-O	-6.25	114.22	120.90
1	A	92	GLU	CA-C-O	-6.24	111.70	119.38
1	A	393	THR	CA-CB-OG1	-6.24	100.25	109.60
1	A	153	GLN	CB-CG-CD	6.23	123.19	112.60
1	A	63	THR	CA-CB-OG1	-6.22	100.26	109.60
1	A	243	GLN	O-C-N	6.22	130.71	122.43
1	A	426	ALA	CA-C-O	6.22	127.15	120.24
1	A	405	ILE	O-C-N	-6.22	116.13	123.03
1	A	442	THR	O-C-N	-6.21	115.11	123.19
1	A	364	SER	CB-CA-C	6.21	122.96	109.99
1	A	306	ASN	O-C-N	-6.20	113.81	122.37
1	A	282	ASP	N-CA-CB	-6.20	101.30	110.53
1	A	183	VAL	N-CA-C	-6.20	103.79	110.23
1	A	386	PRO	O-C-N	-6.18	116.48	123.03
1	A	436	GLU	N-CA-C	-6.18	99.10	108.67
1	A	71	GLN	CG-CD-NE2	6.16	125.64	116.40
1	A	309	ALA	N-CA-C	-6.16	104.49	111.14
1	A	432	GLN	CA-C-N	6.16	130.87	122.19
1	A	432	GLN	C-N-CA	6.16	130.87	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	SER	CA-CB-OG	-6.15	98.79	111.10
1	A	152	ILE	CA-CB-CG1	-6.15	99.95	110.40
1	A	370	ASN	CB-CG-OD1	-6.14	108.53	120.80
1	A	475	CYS	CA-C-N	-6.12	110.69	121.70
1	A	475	CYS	C-N-CA	-6.12	110.69	121.70
1	A	69	LEU	CB-CA-C	6.11	119.59	109.56
1	A	448	ASP	CA-CB-CG	-6.11	106.49	112.60
1	A	301	PHE	O-C-N	6.11	128.36	122.07
1	A	81	GLY	CA-C-O	-6.11	111.50	119.44
1	A	464	TYR	O-C-N	6.10	126.59	121.83
1	A	252	TYR	O-C-N	-6.10	114.97	120.71
1	A	358	LEU	N-CA-C	-6.09	104.55	112.23
1	A	364	SER	CA-CB-OG	-6.09	98.91	111.10
1	A	27	THR	CA-CB-OG1	-6.09	100.47	109.60
1	A	295	ASN	CA-C-O	6.08	127.41	121.14
1	A	143	GLN	CG-CD-NE2	-6.08	107.29	116.40
1	A	352	TYR	CA-CB-CG	6.08	124.84	113.90
1	A	463	LEU	N-CA-CB	-6.05	100.54	110.52
1	A	172	SER	CA-C-N	-6.04	114.60	123.30
1	A	172	SER	C-N-CA	-6.04	114.60	123.30
1	A	13	PHE	CA-C-O	-6.04	113.67	120.43
1	A	350	SER	N-CA-C	-6.03	105.41	112.89
1	A	4	ALA	CA-C-O	-6.00	114.15	120.63
1	A	459	LEU	N-CA-C	5.99	117.44	109.83
1	A	366	ASN	O-C-N	5.98	128.97	122.15
1	A	159	THR	N-CA-CB	-5.98	101.08	110.30
1	A	22	THR	CA-CB-CG2	5.98	120.66	110.50
1	A	387	ILE	CB-CG1-CD1	5.96	126.32	113.80
1	A	418	SER	CA-C-N	5.96	131.98	121.80
1	A	418	SER	C-N-CA	5.96	131.98	121.80
1	A	96	THR	CA-CB-OG1	-5.95	100.68	109.60
1	A	199	SER	CA-C-O	-5.95	114.59	122.44
1	A	205	ILE	O-C-N	5.94	129.42	123.18
1	A	67	ALA	CA-C-N	5.94	134.01	122.07
1	A	67	ALA	C-N-CA	5.94	134.01	122.07
1	A	293	VAL	CA-C-O	-5.92	113.39	120.78
1	A	24	GLY	CA-C-N	-5.92	111.82	120.75
1	A	24	GLY	C-N-CA	-5.92	111.82	120.75
1	A	274	ASN	CA-C-O	-5.92	114.61	120.82
1	A	33	ALA	CB-CA-C	5.89	121.53	110.63
1	A	184	LYS	O-C-N	5.89	129.33	122.20
1	A	387	ILE	O-C-N	-5.89	116.31	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ASP	CB-CA-C	5.88	118.50	109.50
1	A	213	LYS	N-CA-C	5.88	118.17	111.11
1	A	461	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	A	73	THR	CA-CB-OG1	-5.87	100.79	109.60
1	A	403	SER	CA-C-N	5.87	129.82	121.42
1	A	403	SER	C-N-CA	5.87	129.82	121.42
1	A	322	ASP	N-CA-CB	-5.86	101.73	110.17
1	A	96	THR	N-CA-C	5.86	119.09	109.72
1	A	81	GLY	CA-C-N	-5.84	113.30	122.65
1	A	81	GLY	C-N-CA	-5.84	113.30	122.65
1	A	193	SER	O-C-N	5.84	129.82	122.23
1	A	336	ALA	N-CA-CB	-5.83	103.09	111.54
1	A	309	ALA	CA-C-N	-5.82	112.48	120.28
1	A	309	ALA	C-N-CA	-5.82	112.48	120.28
1	A	469	LEU	N-CA-C	-5.82	100.51	109.76
1	A	205	ILE	CB-CG1-CD1	-5.81	101.59	113.80
1	A	129	GLY	CA-C-O	5.81	126.50	119.65
1	A	204	ARG	CD-NE-CZ	5.80	132.52	124.40
1	A	297	ASP	O-C-N	5.80	129.21	122.19
1	A	401	ASP	CB-CA-C	5.79	119.03	109.70
1	A	45	ILE	CB-CG1-CD1	-5.79	101.64	113.80
1	A	469	LEU	O-C-N	-5.77	116.29	123.04
1	A	420	THR	CB-CA-C	5.76	119.75	109.38
1	A	283	CYS	CA-CB-SG	5.76	127.64	114.40
1	A	388	TYR	CA-CB-CG	-5.76	103.54	113.90
1	A	69	LEU	N-CA-C	-5.74	103.00	109.60
1	A	157	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	233	ASP	CA-CB-CG	-5.72	106.88	112.60
1	A	315	ALA	N-CA-CB	5.71	118.61	110.16
1	A	358	LEU	CD1-CG-CD2	-5.71	98.24	110.80
1	A	244	ASN	CA-C-N	-5.70	115.74	122.36
1	A	244	ASN	C-N-CA	-5.70	115.74	122.36
1	A	64	PRO	N-CA-CB	5.70	108.27	103.25
1	A	433	GLN	O-C-N	5.70	129.71	123.22
1	A	366	ASN	N-CA-CB	5.68	118.57	110.16
1	A	398	LYS	O-C-N	-5.68	116.46	123.44
1	A	264	SER	CA-CB-OG	-5.67	99.76	111.10
1	A	16	THR	CA-C-O	5.67	126.75	120.63
1	A	104	SER	CA-C-O	5.67	126.30	119.61
1	A	153	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	333	GLN	CB-CG-CD	5.66	122.22	112.60
1	A	110	ARG	NE-CZ-NH2	5.65	124.29	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	VAL	CA-CB-CG1	5.65	120.01	110.40
1	A	457	GLY	CA-C-N	5.65	132.49	121.41
1	A	457	GLY	C-N-CA	5.65	132.49	121.41
1	A	95	GLY	CA-C-N	5.64	131.67	122.81
1	A	95	GLY	C-N-CA	5.64	131.67	122.81
1	A	232	LEU	CA-C-N	5.64	131.23	121.64
1	A	232	LEU	C-N-CA	5.64	131.23	121.64
1	A	70	PRO	CA-C-O	5.63	126.35	118.86
1	A	321	ASN	CA-C-N	-5.62	112.11	120.94
1	A	321	ASN	C-N-CA	-5.62	112.11	120.94
1	A	380	VAL	CB-CA-C	5.62	120.51	111.29
1	A	39	GLY	N-CA-C	5.61	123.83	115.64
1	A	98	ASP	CA-C-N	5.60	127.72	120.44
1	A	98	ASP	C-N-CA	5.60	127.72	120.44
1	A	283	CYS	N-CA-C	-5.58	103.14	110.39
1	A	239	THR	N-CA-CB	-5.57	101.90	110.20
1	A	254	ILE	CA-CB-CG1	-5.56	100.95	110.40
1	A	105	SER	CA-CB-OG	5.56	122.21	111.10
1	A	169	ASN	CB-CG-OD1	5.55	131.90	120.80
1	A	446	GLY	O-C-N	5.54	129.91	122.70
1	A	108	HIS	O-C-N	5.54	127.99	122.12
1	A	401	ASP	O-C-N	-5.54	116.22	122.97
1	A	159	THR	CA-C-N	5.53	128.72	120.31
1	A	159	THR	C-N-CA	5.53	128.72	120.31
1	A	68	GLN	CA-C-O	-5.53	115.19	121.72
1	A	474	ILE	N-CA-C	5.53	115.66	110.30
1	A	117	ASP	N-CA-CB	-5.53	101.72	110.06
1	A	151	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	249	VAL	O-C-N	5.52	129.25	123.02
1	A	33	ALA	O-C-N	-5.51	115.77	122.22
1	A	226	TYR	CA-C-O	-5.51	114.99	121.16
1	A	136	VAL	O-C-N	-5.50	114.53	122.12
1	A	172	SER	CA-C-O	-5.49	114.80	121.28
1	A	122	HIS	N-CA-C	5.49	116.61	108.60
1	A	301	PHE	CA-C-O	-5.48	115.06	120.82
1	A	244	ASN	N-CA-CB	5.48	119.30	110.42
1	A	10	SER	CA-CB-OG	-5.48	100.14	111.10
1	A	256	TYR	O-C-N	5.47	124.70	120.38
1	A	390	ASP	CA-C-O	-5.47	115.33	121.40
1	A	162	GLU	N-CA-C	5.46	120.21	113.50
1	A	330	GLY	N-CA-C	-5.45	107.41	113.79
1	A	473	LYS	CB-CG-CD	5.45	123.83	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	LEU	O-C-N	-5.45	115.99	121.27
1	A	454	PRO	CB-CA-C	5.44	116.35	111.40
1	A	285	ASP	CB-CA-C	5.43	118.81	111.70
1	A	228	ILE	CA-CB-CG2	5.43	119.73	110.50
1	A	379	PHE	CA-C-N	-5.43	112.20	121.97
1	A	379	PHE	C-N-CA	-5.43	112.20	121.97
1	A	447	SER	N-CA-C	-5.43	99.24	110.80
1	A	153	GLN	CA-CB-CG	5.42	124.94	114.10
1	A	473	LYS	CA-C-N	-5.41	113.93	120.70
1	A	473	LYS	C-N-CA	-5.41	113.93	120.70
1	A	471	GLY	O-C-N	5.41	129.73	122.70
1	A	379	PHE	CA-C-O	-5.41	115.12	121.07
1	A	347	THR	CA-C-N	5.41	127.79	120.38
1	A	347	THR	C-N-CA	5.41	127.79	120.38
1	A	363	ALA	N-CA-CB	5.40	117.91	110.07
1	A	368	ILE	CA-C-O	5.40	126.58	120.85
1	A	401	ASP	CB-CG-OD1	5.40	130.81	118.40
1	A	12	TYR	O-C-N	5.39	129.92	123.13
1	A	274	ASN	CA-CB-CG	-5.39	107.21	112.60
1	A	160	GLN	CA-CB-CG	5.39	124.87	114.10
1	A	268	SER	CA-C-O	-5.39	114.82	120.58
1	A	239	THR	CA-C-N	5.37	126.80	120.09
1	A	239	THR	C-N-CA	5.37	126.80	120.09
1	A	366	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	401	ASP	CA-C-O	5.36	127.04	121.15
1	A	216	TRP	CB-CG-CD2	5.35	134.29	126.80
1	A	415	SER	CA-C-O	-5.35	112.86	120.51
1	A	452	PRO	CA-C-O	-5.35	110.86	120.60
1	A	156	GLU	N-CA-CB	5.35	119.11	110.40
1	A	458	GLY	CA-C-O	-5.34	111.28	120.57
1	A	464	TYR	CA-C-O	-5.33	114.58	119.76
1	A	440	CYS	CA-C-N	5.33	131.77	122.81
1	A	440	CYS	C-N-CA	5.33	131.77	122.81
1	A	65	VAL	CB-CA-C	5.32	118.83	110.95
1	A	6	TRP	CA-C-N	5.32	127.94	120.28
1	A	6	TRP	C-N-CA	5.32	127.94	120.28
1	A	239	THR	CA-C-O	5.32	126.14	120.24
1	A	319	ILE	O-C-N	-5.31	116.50	121.87
1	A	137	PHE	N-CA-CB	-5.31	102.16	109.97
1	A	314	VAL	CA-CB-CG1	5.30	119.41	110.40
1	A	318	ILE	CB-CG1-CD1	-5.29	102.69	113.80
1	A	448	ASP	N-CA-CB	-5.29	102.83	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	TYR	CA-CB-CG	5.29	123.43	113.90
1	A	219	TYR	O-C-N	5.29	127.51	122.07
1	A	140	PHE	O-C-N	-5.28	116.11	122.71
1	A	110	ARG	CA-C-N	5.28	129.46	120.91
1	A	110	ARG	C-N-CA	5.28	129.46	120.91
1	A	370	ASN	CB-CA-C	5.26	119.23	110.81
1	A	122	HIS	N-CA-CB	-5.26	103.37	111.46
1	A	381	THR	N-CA-CB	5.25	118.54	110.61
1	A	46	ILE	CA-CB-CG2	-5.24	101.59	110.50
1	A	260	ASN	O-C-N	5.24	128.72	122.27
1	A	422	SER	N-CA-CB	5.24	119.04	110.39
1	A	260	ASN	CA-C-O	-5.24	113.94	119.97
1	A	327	ILE	O-C-N	5.24	128.91	123.26
1	A	49	LEU	CA-C-O	-5.23	115.00	120.55
1	A	264	SER	O-C-N	5.23	129.50	123.17
1	A	72	THR	N-CA-CB	5.23	118.52	110.21
1	A	162	GLU	N-CA-CB	-5.23	102.84	110.53
1	A	95	GLY	CA-C-O	5.22	125.28	120.79
1	A	257	PRO	CA-C-N	5.22	127.54	120.65
1	A	257	PRO	C-N-CA	5.22	127.54	120.65
1	A	78	ALA	N-CA-C	-5.21	105.63	112.72
1	A	308	ILE	O-C-N	5.21	128.88	122.05
1	A	372	ALA	CA-C-N	-5.21	111.99	120.64
1	A	372	ALA	C-N-CA	-5.21	111.99	120.64
1	A	406	VAL	O-C-N	5.21	128.72	123.20
1	A	133	ASP	O-C-N	5.20	129.08	122.84
1	A	239	THR	CA-CB-OG1	5.18	117.37	109.60
1	A	244	ASN	OD1-CG-ND2	5.17	127.77	122.60
1	A	53	GLN	CA-CB-CG	-5.16	103.77	114.10
1	A	25	SER	CA-CB-OG	-5.16	100.78	111.10
1	A	11	ILE	N-CA-C	5.16	116.01	108.53
1	A	183	VAL	CA-CB-CG1	5.16	119.17	110.40
1	A	93	ASN	O-C-N	-5.16	116.19	122.22
1	A	426	ALA	CB-CA-C	5.15	120.13	110.70
1	A	7	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	A	197	ASN	CA-C-N	-5.15	114.26	122.29
1	A	197	ASN	C-N-CA	-5.15	114.26	122.29
1	A	33	ALA	N-CA-CB	5.14	118.14	110.22
1	A	5	ASP	N-CA-C	5.14	118.70	112.23
1	A	405	ILE	CB-CG1-CD1	-5.14	103.01	113.80
1	A	72	THR	CA-C-O	-5.13	115.09	120.58
1	A	307	ASP	N-CA-CB	-5.12	101.82	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	THR	O-C-N	-5.11	116.96	122.79
1	A	2	THR	OG1-CB-CG2	5.10	119.50	109.30
1	A	404	GLN	OE1-CD-NE2	5.10	127.70	122.60
1	A	464	TYR	CA-CB-CG	5.08	123.04	113.90
1	A	66	THR	CA-C-O	5.08	127.76	121.87
1	A	450	ASN	CA-C-O	-5.08	115.27	121.05
1	A	178	THR	CA-C-O	5.07	125.60	119.11
1	A	17	ASP	CA-C-O	-5.07	114.37	120.10
1	A	216	TRP	CA-CB-CG	-5.06	103.98	113.60
1	A	451	VAL	N-CA-C	5.06	112.56	107.55
1	A	140	PHE	CA-C-O	5.05	129.15	122.63
1	A	177	ASP	O-C-N	-5.05	116.47	122.63
1	A	362	ILE	CA-C-O	-5.05	115.70	120.95
1	A	85	GLN	O-C-N	5.04	128.30	122.25
1	A	163	ASP	CA-C-O	5.04	124.36	118.97
1	A	201	ASP	CA-C-N	-5.04	110.79	121.22
1	A	201	ASP	C-N-CA	-5.04	110.79	121.22
1	A	243	GLN	N-CA-C	-5.04	106.83	112.87
1	A	384	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	101	LYS	N-CA-CB	5.03	117.98	110.19
1	A	80	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	65	VAL	O-C-N	-5.02	117.31	122.23
1	A	94	TYR	CA-C-O	5.01	125.53	119.31
1	A	116	VAL	CB-CA-C	5.01	118.22	110.50
1	A	58	THR	CA-CB-CG2	5.01	119.02	110.50
1	A	206	ASP	CA-C-O	5.01	127.70	121.94
1	A	56	GLY	N-CA-C	-5.00	108.33	115.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3686	0	3478	180	0
2	A	2	0	0	0	0
3	A	239	0	0	15	0
All	All	3927	0	3478	180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (180) 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:205:ILE:HD12	1:A:246:MET:CE	1.67	1.22
1:A:96:THR:HG23	1:A:98:ASP:H	1.19	1.04
1:A:96:THR:CG2	1:A:98:ASP:H	1.71	1.02
1:A:96:THR:HG22	1:A:99:ASP:H	1.27	1.00
1:A:206:ASP:OD2	1:A:207:THR:HG23	1.66	0.95
1:A:296:HIS:H	1:A:296:HIS:CD2	1.80	0.95
1:A:205:ILE:HD12	1:A:246:MET:HE2	1.46	0.92
1:A:280:LYS:HG3	1:A:383:LYS:HG2	1.54	0.88
1:A:296:HIS:H	1:A:296:HIS:HD2	1.22	0.86
1:A:374:SER:HB3	1:A:375:LYS:HD3	1.58	0.86
1:A:177:ASP:OD1	1:A:179:THR:HB	1.75	0.86
1:A:46:ILE:HD11	1:A:103:LEU:N	1.92	0.85
1:A:178:THR:O	1:A:184:LYS:HD2	1.77	0.84
1:A:96:THR:CG2	1:A:98:ASP:HB2	2.07	0.82
1:A:446:GLY:O	1:A:447:SER:HB3	1.80	0.81
1:A:96:THR:HG21	1:A:98:ASP:HB2	1.59	0.81
1:A:133:ASP:O	1:A:136:VAL:HG23	1.80	0.81
1:A:77:ASP:OD2	3:A:585:HOH:O	2.00	0.80
1:A:96:THR:CG2	1:A:98:ASP:N	2.44	0.80
1:A:205:ILE:CD1	1:A:246:MET:CE	2.57	0.79
1:A:70:PRO:O	3:A:589:HOH:O	2.01	0.77
1:A:205:ILE:HD12	1:A:246:MET:HE1	1.65	0.74
1:A:180:LYS:HD3	1:A:183:VAL:HG23	1.70	0.74
1:A:180:LYS:HG3	1:A:182:VAL:HG23	1.70	0.73
1:A:240:CYS:N	1:A:241:PRO:CD	2.52	0.73
1:A:31:ASN:OD1	1:A:31:ASN:C	2.32	0.72
1:A:134:TYR:CE1	1:A:143:GLN:HB3	2.24	0.72
1:A:158:GLN:O	1:A:162:GLU:HG3	1.90	0.71
1:A:446:GLY:O	1:A:447:SER:CB	2.37	0.71
1:A:96:THR:HG22	1:A:98:ASP:N	2.07	0.70
1:A:371:TYR:O	1:A:374:SER:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ALA:O	1:A:105:SER:HB3	1.92	0.70
1:A:38:CYS:O	3:A:579:HOH:O	2.11	0.68
1:A:96:THR:HG22	1:A:99:ASP:N	2.06	0.68
1:A:302:ALA:HA	1:A:305:THR:O	1.95	0.67
1:A:178:THR:O	1:A:184:LYS:CD	2.42	0.66
1:A:296:HIS:CD2	1:A:296:HIS:N	2.57	0.66
1:A:107:LEU:HD13	1:A:114:LEU:HB2	1.78	0.66
1:A:181:ASP:O	1:A:185:ASN:HB2	1.95	0.65
1:A:177:ASP:O	1:A:183:VAL:HG11	1.97	0.65
1:A:107:LEU:CD1	1:A:114:LEU:HB2	2.27	0.65
1:A:159:THR:O	1:A:163:ASP:HB2	1.98	0.64
1:A:470:ALA:C	1:A:472:SER:H	2.06	0.63
1:A:166:LEU:HD21	1:A:210:HIS:CE1	2.33	0.63
1:A:96:THR:HG23	1:A:98:ASP:N	2.04	0.63
1:A:82:TYR:OH	1:A:296:HIS:HE1	1.83	0.61
1:A:134:TYR:CD1	1:A:143:GLN:HB3	2.36	0.61
1:A:358:LEU:CD2	1:A:358:LEU:N	2.63	0.61
1:A:8:SER:HB2	1:A:373:ILE:CD1	2.31	0.60
1:A:156:GLU:HB3	3:A:606:HOH:O	2.02	0.60
1:A:98:ASP:O	1:A:101:LYS:HB2	2.00	0.60
1:A:8:SER:HB2	1:A:373:ILE:HD11	1.84	0.59
1:A:155:TYR:HA	1:A:161:VAL:CG2	2.32	0.59
1:A:31:ASN:OD1	1:A:32:THR:N	2.36	0.58
1:A:322:ASP:OD1	1:A:398:LYS:NZ	2.31	0.58
1:A:147:HIS:CE1	1:A:177:ASP:HA	2.38	0.58
1:A:156:GLU:OE1	3:A:606:HOH:O	2.17	0.58
1:A:1:ALA:O	1:A:226:TYR:N	2.36	0.58
1:A:88:TYR:OH	1:A:186:GLU:OE2	2.19	0.58
1:A:242:TYR:C	1:A:244:ASN:N	2.62	0.58
1:A:10:SER:HB3	1:A:325:PRO:HG2	1.87	0.57
1:A:240:CYS:N	1:A:241:PRO:HD2	2.19	0.57
1:A:2:THR:HB	1:A:5:ASP:H	1.70	0.57
1:A:155:TYR:HA	1:A:161:VAL:HG23	1.86	0.57
1:A:450:ASN:HD22	1:A:450:ASN:N	2.00	0.57
1:A:46:ILE:HD11	1:A:103:LEU:CA	2.34	0.56
1:A:308:ILE:HG22	1:A:358:LEU:HD21	1.86	0.56
1:A:100:LEU:HD13	1:A:198:TYR:CD1	2.41	0.56
1:A:67:ALA:HB3	1:A:86:ASP:HB3	1.85	0.56
1:A:338:GLY:O	1:A:343:ASN:HB3	2.05	0.56
1:A:55:MET:HG3	1:A:359:TYR:CE2	2.41	0.56
1:A:470:ALA:C	1:A:472:SER:N	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PHE:HE2	1:A:405:ILE:HD12	1.70	0.56
1:A:467:GLU:CG	1:A:468:LYS:N	2.69	0.55
1:A:230:GLU:OE2	1:A:232:LEU:HD12	2.07	0.55
1:A:178:THR:HA	1:A:183:VAL:HG12	1.89	0.55
1:A:177:ASP:C	1:A:183:VAL:HG11	2.33	0.54
1:A:411:ASN:C	1:A:411:ASN:HD22	2.15	0.54
1:A:85:GLN:O	1:A:137:PHE:HA	2.06	0.54
1:A:361:LEU:C	1:A:361:LEU:HD13	2.33	0.54
1:A:96:THR:CG2	1:A:98:ASP:CB	2.83	0.54
1:A:278:THR:HA	3:A:644:HOH:O	2.08	0.54
1:A:180:LYS:HG2	1:A:180:LYS:O	2.08	0.54
1:A:333:GLN:NE2	1:A:353:PRO:HG2	2.23	0.54
1:A:99:ASP:C	1:A:101:LYS:N	2.66	0.53
1:A:178:THR:HA	1:A:183:VAL:CG1	2.38	0.53
1:A:205:ILE:HD12	1:A:246:MET:HE3	1.79	0.53
1:A:37:TYR:CE1	1:A:79:TYR:HA	2.43	0.53
1:A:371:TYR:O	1:A:372:ALA:C	2.51	0.53
1:A:10:SER:CB	1:A:325:PRO:HG2	2.39	0.53
1:A:108:HIS:NE2	1:A:201:ASP:OD2	2.28	0.52
1:A:400:THR:O	1:A:401:ASP:C	2.52	0.52
1:A:27:THR:O	1:A:28:ALA:C	2.53	0.52
1:A:352:TYR:N	1:A:353:PRO:CD	2.73	0.52
1:A:109:GLU:HG3	1:A:109:GLU:O	2.10	0.51
1:A:220:ASN:OD1	1:A:246:MET:HA	2.11	0.51
1:A:180:LYS:HG3	1:A:182:VAL:H	1.76	0.51
1:A:358:LEU:N	1:A:358:LEU:HD22	2.26	0.51
1:A:106:ALA:O	1:A:110:ARG:HG3	2.11	0.51
1:A:158:GLN:HE21	1:A:162:GLU:CD	2.18	0.50
1:A:251:ASN:ND2	1:A:254:ILE:H	2.09	0.50
1:A:280:LYS:HG3	1:A:383:LYS:CG	2.34	0.50
1:A:98:ASP:O	1:A:101:LYS:CB	2.60	0.50
1:A:187:TRP:HA	1:A:187:TRP:CE3	2.48	0.49
1:A:48:LYS:HE2	1:A:352:TYR:CE2	2.47	0.49
1:A:206:ASP:OD2	1:A:207:THR:CG2	2.50	0.49
1:A:6:TRP:CD1	1:A:226:TYR:HB3	2.48	0.48
1:A:180:LYS:HG2	1:A:183:VAL:H	1.77	0.48
1:A:308:ILE:HD13	3:A:649:HOH:O	2.13	0.48
1:A:319:ILE:HA	1:A:325:PRO:HB3	1.96	0.48
1:A:11:ILE:HA	1:A:59:ALA:O	2.14	0.48
1:A:429:THR:H	1:A:432:GLN:NE2	2.12	0.48
1:A:205:ILE:CD1	1:A:246:MET:HE1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PHE:CE2	1:A:405:ILE:HD12	2.49	0.47
1:A:239:THR:C	1:A:241:PRO:HD2	2.39	0.47
1:A:374:SER:C	1:A:375:LYS:HD3	2.39	0.47
1:A:180:LYS:C	1:A:182:VAL:N	2.72	0.47
1:A:308:ILE:H	1:A:308:ILE:HG13	1.62	0.47
1:A:114:LEU:HD23	1:A:200:ILE:HG22	1.96	0.47
1:A:181:ASP:O	1:A:185:ASN:CB	2.62	0.47
1:A:415:SER:O	1:A:457:GLY:HA2	2.15	0.46
1:A:134:TYR:O	1:A:141:SER:HA	2.16	0.46
1:A:1:ALA:HA	1:A:201:ASP:O	2.16	0.46
1:A:453:VAL:HA	1:A:454:PRO:HD3	1.64	0.46
1:A:319:ILE:O	1:A:369:ARG:HD2	2.16	0.46
1:A:312:LYS:NZ	3:A:649:HOH:O	2.41	0.45
1:A:206:ASP:O	1:A:207:THR:C	2.58	0.45
1:A:99:ASP:C	1:A:101:LYS:H	2.24	0.45
1:A:240:CYS:HB2	1:A:241:PRO:HD3	1.98	0.45
1:A:242:TYR:C	1:A:244:ASN:H	2.22	0.45
1:A:333:GLN:HE22	1:A:356:SER:HB3	1.82	0.45
1:A:34:ASP:HA	3:A:512:HOH:O	2.17	0.45
1:A:97:ALA:O	1:A:101:LYS:HD3	2.17	0.45
1:A:55:MET:HG3	1:A:359:TYR:CZ	2.52	0.45
1:A:205:ILE:HD13	1:A:205:ILE:HG21	1.78	0.45
1:A:180:LYS:CD	1:A:183:VAL:HG23	2.44	0.44
1:A:14:LEU:HD11	1:A:45:ILE:HD11	1.98	0.44
1:A:470:ALA:HB3	1:A:471:GLY:H	1.39	0.44
1:A:152:ILE:HG12	1:A:160:GLN:O	2.16	0.44
1:A:450:ASN:OD1	3:A:714:HOH:O	2.21	0.44
1:A:405:ILE:HG12	1:A:464:TYR:HD1	1.83	0.44
1:A:320:LEU:HD13	1:A:407:THR:OG1	2.18	0.43
1:A:233:ASP:HB3	1:A:239:THR:OG1	2.19	0.43
1:A:158:GLN:O	1:A:158:GLN:HG3	2.17	0.43
1:A:18:ARG:O	1:A:346:ALA:HA	2.18	0.43
1:A:259:LEU:O	1:A:263:LYS:HB3	2.18	0.43
1:A:2:THR:HB	1:A:5:ASP:CB	2.48	0.43
1:A:151:PHE:CZ	1:A:168:ASP:HA	2.54	0.43
1:A:450:ASN:CG	3:A:714:HOH:O	2.61	0.43
1:A:382:TYR:CD1	1:A:382:TYR:C	2.97	0.43
1:A:55:MET:HE3	1:A:55:MET:HB2	1.81	0.43
1:A:74:ALA:HB3	1:A:170:THR:CG2	2.49	0.43
1:A:333:GLN:NE2	3:A:657:HOH:O	2.50	0.42
1:A:418:SER:HA	1:A:455:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLU:OE2	1:A:301:PHE:N	2.40	0.42
1:A:374:SER:CB	1:A:375:LYS:HD3	2.39	0.42
1:A:228:ILE:HD13	1:A:228:ILE:HG21	1.78	0.42
1:A:264:SER:HB3	1:A:266:SER:H	1.85	0.42
1:A:333:GLN:HE22	1:A:353:PRO:HG2	1.83	0.42
1:A:467:GLU:HG3	1:A:468:LYS:HG2	2.01	0.42
1:A:96:THR:C	1:A:98:ASP:N	2.77	0.42
1:A:156:GLU:HA	3:A:606:HOH:O	2.20	0.42
1:A:355:ASP:N	1:A:355:ASP:OD1	2.50	0.42
1:A:262:PHE:O	1:A:310:LEU:HG	2.20	0.42
1:A:209:LYS:HG2	3:A:526:HOH:O	2.19	0.41
1:A:212:GLN:H	1:A:212:GLN:HE21	1.67	0.41
1:A:96:THR:HG22	1:A:98:ASP:CA	2.50	0.41
1:A:264:SER:C	1:A:266:SER:N	2.77	0.41
1:A:415:SER:HB2	1:A:416:GLY:H	1.20	0.41
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.90	0.41
1:A:264:SER:C	1:A:266:SER:H	2.29	0.41
1:A:177:ASP:O	1:A:183:VAL:CG1	2.67	0.41
1:A:180:LYS:HB3	3:A:617:HOH:O	2.22	0.40
1:A:340:ASP:HA	1:A:341:PRO:HA	1.81	0.40
1:A:448:ASP:N	1:A:448:ASP:OD1	2.47	0.40
1:A:96:THR:CG2	1:A:98:ASP:CA	3.00	0.40
1:A:4:ALA:HA	1:A:7:ARG:NH1	2.36	0.40
1:A:133:ASP:C	1:A:135:SER:H	2.29	0.40
1:A:138:LYS:HA	1:A:139:PRO:HA	1.77	0.40
1:A:429:THR:H	1:A:432:GLN:HE21	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	474/478 (99%)	450 (95%)	20 (4%)	4 (1%)	16 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	GLY
1	A	447	SER
1	A	416	GLY
1	A	415	SER

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	397/399 (100%)	329 (83%)	68 (17%)	2 1

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	15	LEU
1	A	29	THR
1	A	43	GLN
1	A	61	TRP
1	A	65	VAL
1	A	87	ILE
1	A	96	THR
1	A	100	LEU
1	A	101	LYS
1	A	103	LEU
1	A	109	GLU
1	A	130	SER
1	A	135	SER
1	A	136	VAL
1	A	139	PRO
1	A	141	SER

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Mol	Chain	Res	Type
1	A	142	SER
1	A	143	GLN
1	A	159	THR
1	A	161	VAL
1	A	169	ASN
1	A	179	THR
1	A	180	LYS
1	A	181	ASP
1	A	184	LYS
1	A	187	TRP
1	A	193	SER
1	A	195	VAL
1	A	199	SER
1	A	200	ILE
1	A	212	GLN
1	A	213	LYS
1	A	232	LEU
1	A	245	VAL
1	A	246	MET
1	A	250	LEU
1	A	251	ASN
1	A	264	SER
1	A	266	SER
1	A	283	CYS
1	A	296	HIS
1	A	308	ILE
1	A	310	LEU
1	A	318	ILE
1	A	327	ILE
1	A	334	HIS
1	A	341	PRO
1	A	356	SER
1	A	357	GLU
1	A	361	LEU
1	A	364	SER
1	A	373	ILE
1	A	375	LYS
1	A	381	THR
1	A	383	LYS
1	A	384	ASN
1	A	396	MET
1	A	410	SER

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Mol	Chain	Res	Type
1	A	411	ASN
1	A	420	THR
1	A	424	SER
1	A	443	VAL
1	A	447	SER
1	A	450	ASN
1	A	459	LEU
1	A	474	ILE
1	A	476	SER

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

Mol	Chain	Res	Type
1	A	9	GLN
1	A	85	GLN
1	A	143	GLN
1	A	147	HIS
1	A	197	ASN
1	A	212	GLN
1	A	251	ASN
1	A	277	ASN
1	A	296	HIS
1	A	321	ASN
1	A	333	GLN
1	A	370	ASN
1	A	384	ASN
1	A	411	ASN
1	A	432	GLN
1	A	450	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	476/478 (99%)	-0.31	1 (0%) 91 92	4, 14, 25, 40	12 (2%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	GLY	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	479	1/1	0.98	0.02	14,14,14,14	0
2	CA	A	480	1/1	0.98	0.11	9,9,9,9	1

6.5 Other polymers [i](#)

There are no such residues in this entry.