



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 02:32 PM EDT

PDB ID : 6TAA
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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

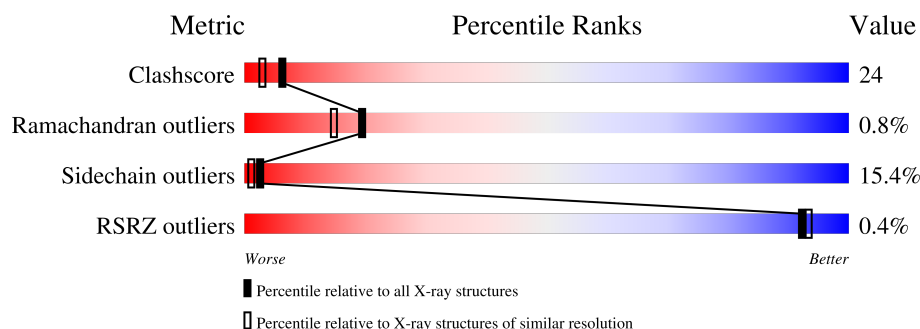
1 Overall quality at a glance

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 (three-letter code: CA) (formula: Ca).

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

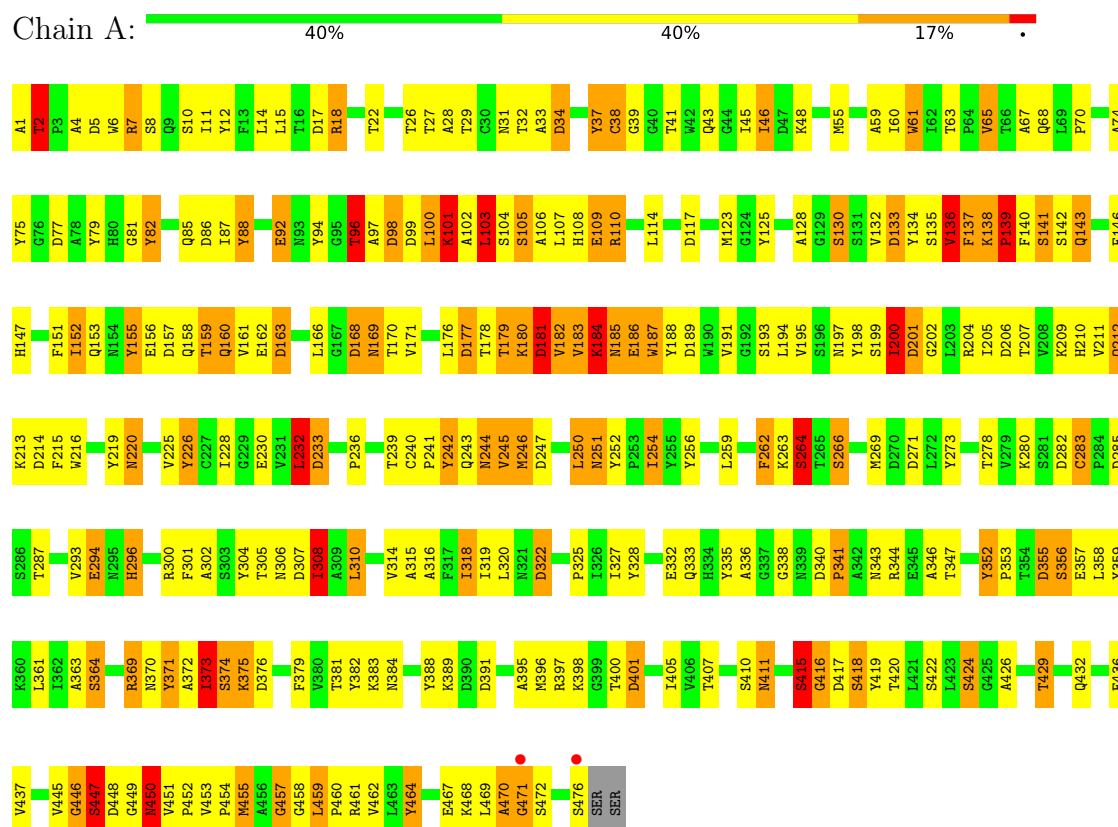
- Molecule 3 is water.

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

3 Residue-property plots

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 7.68 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.70-2.10) 87.2 (7.68-2.10)	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)	0.27 , 80.2	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	1.33	8/3781 (0.2%)	2.49	243/5164 (4.7%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	GLU	CD-OE1	15.63	1.42	1.25
1	A	92	GLU	CD-OE2	-12.74	1.11	1.25
1	A	138	LYS	CE-NZ	-12.61	1.17	1.49
1	A	169	ASN	CG-OD1	8.74	1.43	1.24
1	A	181	ASP	CB-CG	8.38	1.69	1.51
1	A	471	GLY	N-CA	5.50	1.54	1.46
1	A	138	LYS	CB-CG	5.30	1.66	1.52
1	A	39	GLY	C-O	5.12	1.31	1.23

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	ARG	NE-CZ-NH2	-21.14	109.73	120.30
1	A	7	ARG	NE-CZ-NH2	-18.67	110.97	120.30
1	A	461	ARG	NE-CZ-NH1	14.15	127.38	120.30
1	A	401	ASP	CB-CG-OD1	13.90	130.81	118.30
1	A	369	ARG	NE-CZ-NH1	-11.87	114.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ASP	CB-CG-OD2	-11.61	107.85	118.30
1	A	322	ASP	CB-CG-OD2	-11.33	108.10	118.30
1	A	133	ASP	CB-CG-OD1	10.67	127.90	118.30
1	A	242	TYR	CB-CG-CD2	-10.63	114.62	121.00
1	A	256	TYR	CB-CG-CD2	-10.60	114.64	121.00
1	A	157	ASP	CB-CG-OD2	-10.39	108.95	118.30
1	A	204	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	371	TYR	CB-CG-CD2	-9.76	115.14	121.00
1	A	94	TYR	CB-CG-CD2	-9.68	115.19	121.00
1	A	34	ASP	CB-CG-OD2	-9.57	109.69	118.30
1	A	445	VAL	C-N-CA	9.51	142.26	122.30
1	A	117	ASP	CB-CG-OD1	9.49	126.84	118.30
1	A	12	TYR	CB-CG-CD1	9.15	126.49	121.00
1	A	417	ASP	CB-CG-OD2	9.00	126.40	118.30
1	A	271	ASP	CB-CG-OD1	8.83	126.24	118.30
1	A	17	ASP	CB-CG-OD2	8.79	126.21	118.30
1	A	202	GLY	O-C-N	8.79	136.77	122.70
1	A	369	ARG	CD-NE-CZ	8.68	135.76	123.60
1	A	183	VAL	CB-CA-C	8.44	127.44	111.40
1	A	232	LEU	CB-CA-C	8.32	126.01	110.20
1	A	397	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	424	SER	O-C-N	8.25	137.22	123.20
1	A	471	GLY	N-CA-C	-8.22	92.56	113.10
1	A	226	TYR	CB-CG-CD2	8.16	125.89	121.00
1	A	245	VAL	N-CA-CB	-8.16	93.55	111.50
1	A	369	ARG	NH1-CZ-NH2	8.09	128.29	119.40
1	A	216	TRP	CB-CG-CD1	-8.08	116.50	127.00
1	A	65	VAL	N-CA-CB	-7.99	93.92	111.50
1	A	110	ARG	NE-CZ-NH2	7.97	124.29	120.30
1	A	68	GLN	CG-CD-OE1	7.94	137.49	121.60
1	A	273	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	A	88	TYR	CB-CG-CD1	-7.87	116.28	121.00
1	A	256	TYR	CB-CG-CD1	7.86	125.72	121.00
1	A	373	ILE	CA-CB-CG2	7.83	126.57	110.90
1	A	155	TYR	CB-CG-CD1	-7.82	116.31	121.00
1	A	214	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	388	TYR	N-CA-CB	-7.74	96.66	110.60
1	A	233	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	225	VAL	CA-CB-CG1	7.65	122.38	110.90
1	A	60	ILE	CA-CB-CG2	7.64	126.19	110.90
1	A	33	ALA	CB-CA-C	7.62	121.53	110.10
1	A	169	ASN	OD1-CG-ND2	-7.59	104.43	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	CYS	CA-CB-SG	7.58	127.64	114.00
1	A	397	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	252	TYR	CB-CG-CD1	-7.52	116.49	121.00
1	A	177	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	382	TYR	O-C-N	-7.48	110.73	122.70
1	A	452	PRO	O-C-N	7.47	134.65	122.70
1	A	12	TYR	CB-CG-CD2	-7.46	116.53	121.00
1	A	186	GLU	CG-CD-OE1	7.38	133.05	118.30
1	A	177	ASP	CA-C-O	7.30	135.43	120.10
1	A	415	SER	O-C-N	7.27	135.56	123.20
1	A	429	THR	CA-CB-OG1	-7.25	93.77	109.00
1	A	41	THR	CA-CB-OG1	-7.22	93.84	109.00
1	A	307	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	94	TYR	CB-CG-CD1	7.16	125.29	121.00
1	A	18	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	201	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	128	ALA	CB-CA-C	7.05	120.67	110.10
1	A	328	TYR	O-C-N	-7.04	111.44	122.70
1	A	415	SER	N-CA-CB	7.03	121.05	110.50
1	A	96	THR	N-CA-CB	-7.01	96.99	110.30
1	A	271	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	374	SER	CB-CA-C	-6.94	96.92	110.10
1	A	332	GLU	N-CA-CB	6.93	123.08	110.60
1	A	449	GLY	CA-C-O	-6.91	108.16	120.60
1	A	75	TYR	CB-CG-CD1	6.87	125.12	121.00
1	A	371	TYR	CB-CG-CD1	6.86	125.12	121.00
1	A	157	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	364	SER	O-C-N	-6.80	111.82	122.70
1	A	364	SER	CB-CA-C	6.77	122.96	110.10
1	A	462	VAL	CA-CB-CG2	6.76	121.03	110.90
1	A	419	TYR	CB-CG-CD2	-6.71	116.97	121.00
1	A	426	ALA	CB-CA-C	6.68	120.13	110.10
1	A	376	ASP	CB-CG-OD1	-6.67	112.29	118.30
1	A	252	TYR	CB-CG-CD2	6.66	125.00	121.00
1	A	355	ASP	CB-CG-OD1	-6.66	112.31	118.30
1	A	464	TYR	CB-CG-CD1	-6.61	117.03	121.00
1	A	171	VAL	CG1-CB-CG2	-6.61	100.33	110.90
1	A	34	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	322	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	139	PRO	N-CA-CB	-6.55	95.40	102.60
1	A	105	SER	O-C-N	6.54	133.16	122.70
1	A	370	ASN	CB-CG-OD1	-6.54	108.53	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	A	250	LEU	CB-CA-C	6.53	122.61	110.20
1	A	18	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	60	ILE	CA-CB-CG1	-6.50	98.65	111.00
1	A	389	LYS	N-CA-CB	-6.47	98.95	110.60
1	A	153	GLN	CB-CA-C	6.44	123.27	110.40
1	A	417	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	125	TYR	CB-CG-CD1	-6.41	117.15	121.00
1	A	459	LEU	CA-CB-CG	6.41	130.04	115.30
1	A	37	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	A	204	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	429	THR	CA-CB-CG2	6.35	121.29	112.40
1	A	328	TYR	CA-C-N	6.34	131.16	117.20
1	A	397	ARG	CD-NE-CZ	-6.33	114.73	123.60
1	A	63	THR	CA-CB-CG2	6.31	121.24	112.40
1	A	103	LEU	CB-CA-C	6.31	122.19	110.20
1	A	182	VAL	CG1-CB-CG2	6.31	121.00	110.90
1	A	138	LYS	CD-CE-NZ	6.26	126.09	111.70
1	A	318	ILE	CA-CB-CG2	6.25	123.41	110.90
1	A	294	GLU	CB-CG-CD	6.25	131.06	114.20
1	A	140	PHE	C-N-CA	6.23	137.28	121.70
1	A	450	ASN	CA-CB-CG	-6.23	99.69	113.40
1	A	201	ASP	O-C-N	6.23	133.79	123.20
1	A	250	LEU	N-CA-CB	-6.23	97.95	110.40
1	A	132	VAL	O-C-N	6.22	132.66	122.70
1	A	244	ASN	O-C-N	6.21	132.64	122.70
1	A	163	ASP	CA-CB-CG	6.19	127.02	113.40
1	A	363	ALA	O-C-N	6.18	132.59	122.70
1	A	347	THR	CA-CB-CG2	-6.16	103.77	112.40
1	A	181	ASP	CA-CB-CG	-6.15	99.88	113.40
1	A	391	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	315	ALA	N-CA-CB	6.08	118.61	110.10
1	A	437	VAL	CA-CB-CG1	6.07	120.01	110.90
1	A	436	GLU	O-C-N	-6.07	112.99	122.70
1	A	88	TYR	CB-CG-CD2	6.06	124.64	121.00
1	A	335	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	A	352	TYR	CA-CB-CG	6.02	124.84	113.40
1	A	451	VAL	CA-C-O	6.00	132.71	120.10
1	A	132	VAL	CG1-CB-CG2	6.00	120.50	110.90
1	A	300	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	184	LYS	CA-C-N	-5.99	104.03	117.20
1	A	155	TYR	O-C-N	5.96	132.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	244	ASN	CA-C-O	-5.93	107.65	120.10
1	A	395	ALA	CB-CA-C	5.93	118.99	110.10
1	A	216	TRP	CB-CG-CD2	5.92	134.29	126.60
1	A	424	SER	CA-C-O	-5.92	107.67	120.10
1	A	22	THR	CA-CB-CG2	5.90	120.66	112.40
1	A	200	ILE	CB-CG1-CD1	-5.90	97.39	113.90
1	A	308	ILE	N-CA-CB	5.88	124.31	110.80
1	A	146	PHE	CB-CG-CD1	5.86	124.90	120.80
1	A	469	LEU	CA-C-N	5.85	130.07	117.20
1	A	470	ALA	CA-C-N	-5.85	104.50	116.20
1	A	188	TYR	CB-CG-CD1	5.84	124.50	121.00
1	A	110	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	200	ILE	CG1-CB-CG2	-5.83	98.56	111.40
1	A	152	ILE	CA-CB-CG1	-5.82	99.95	111.00
1	A	103	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	82	TYR	CB-CG-CD1	5.79	124.47	121.00
1	A	242	TYR	CG-CD1-CE1	-5.77	116.68	121.30
1	A	461	ARG	CA-C-N	5.76	129.88	117.20
1	A	130	SER	O-C-N	5.76	131.91	122.70
1	A	33	ALA	N-CA-CB	5.74	118.14	110.10
1	A	226	TYR	O-C-N	5.74	131.88	122.70
1	A	123	MET	CG-SD-CE	5.71	109.33	100.20
1	A	422	SER	N-CA-CB	5.70	119.04	110.50
1	A	269	MET	CG-SD-CE	5.68	109.30	100.20
1	A	314	VAL	CA-CB-CG1	5.67	119.41	110.90
1	A	293	VAL	CA-CB-CG2	-5.64	102.44	110.90
1	A	391	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	219	TYR	CB-CG-CD1	5.58	124.35	121.00
1	A	304	TYR	O-C-N	5.58	131.62	122.70
1	A	363	ALA	N-CA-CB	5.58	117.91	110.10
1	A	137	PHE	CB-CG-CD1	-5.57	116.90	120.80
1	A	179	THR	O-C-N	-5.57	113.79	122.70
1	A	117	ASP	OD1-CG-OD2	-5.56	112.73	123.30
1	A	189	ASP	CA-CB-CG	-5.56	101.16	113.40
1	A	197	ASN	CA-CB-CG	5.56	125.64	113.40
1	A	306	ASN	O-C-N	-5.55	113.81	122.70
1	A	87	ILE	CA-C-O	-5.54	108.47	120.10
1	A	332	GLU	O-C-N	5.51	131.52	122.70
1	A	181	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	183	VAL	CA-CB-CG1	5.51	119.17	110.90
1	A	7	ARG	NH1-CZ-NH2	5.50	125.45	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	TYR	CD1-CE1-CZ	-5.49	114.86	119.80
1	A	201	ASP	C-N-CA	-5.48	110.79	122.30
1	A	388	TYR	CD1-CE1-CZ	5.48	124.73	119.80
1	A	418	SER	CA-C-O	-5.46	108.63	120.10
1	A	460	PRO	O-C-N	-5.46	113.96	122.70
1	A	245	VAL	CB-CA-C	5.44	121.74	111.40
1	A	344	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	168	ASP	C-N-CA	5.41	135.21	121.70
1	A	437	VAL	O-C-N	5.41	131.35	122.70
1	A	308	ILE	CB-CA-C	-5.39	100.81	111.60
1	A	455	MET	O-C-N	-5.38	114.10	122.70
1	A	262	PHE	CG-CD2-CE2	5.36	126.70	120.80
1	A	388	TYR	CG-CD2-CE2	5.34	125.57	121.30
1	A	254	ILE	CA-CB-CG1	-5.29	100.95	111.00
1	A	26	THR	O-C-N	5.28	131.15	122.70
1	A	226	TYR	CA-CB-CG	5.28	123.43	113.40
1	A	188	TYR	CA-C-O	5.28	131.18	120.10
1	A	211	VAL	CB-CA-C	5.27	121.41	111.40
1	A	105	SER	CA-C-O	-5.26	109.06	120.10
1	A	186	GLU	O-C-N	5.26	131.11	122.70
1	A	195	VAL	CA-CB-CG2	5.25	118.78	110.90
1	A	153	GLN	CA-CB-CG	5.25	124.94	113.40
1	A	2	THR	N-CA-C	5.24	125.15	111.00
1	A	232	LEU	N-CA-CB	-5.24	99.92	110.40
1	A	282	ASP	CA-C-O	-5.23	109.12	120.10
1	A	160	GLN	CA-CB-CG	5.21	124.87	113.40
1	A	247	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	460	PRO	CA-C-N	5.21	128.66	117.20
1	A	96	THR	OG1-CB-CG2	5.21	121.98	110.00
1	A	215	PHE	CA-CB-CG	5.20	126.38	113.90
1	A	216	TRP	N-CA-C	5.19	125.01	111.00
1	A	388	TYR	CA-CB-CG	-5.19	103.54	113.40
1	A	470	ALA	O-C-N	5.18	132.01	123.20
1	A	38	CYS	CA-CB-SG	-5.18	104.67	114.00
1	A	328	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	101	LYS	O-C-N	5.18	130.99	122.70
1	A	458	GLY	CA-C-O	-5.18	111.28	120.60
1	A	194	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	282	ASP	N-CA-CB	-5.17	101.30	110.60
1	A	316	ALA	O-C-N	-5.16	114.44	122.70
1	A	61	TRP	CH2-CZ2-CE2	5.15	122.55	117.40
1	A	169	ASN	CB-CG-OD1	5.15	131.90	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ASN	CB-CG-ND2	-5.15	104.35	116.70
1	A	155	TYR	CD1-CG-CD2	5.14	123.55	117.90
1	A	225	VAL	O-C-N	5.13	130.91	122.70
1	A	226	TYR	CG-CD2-CE2	5.13	125.40	121.30
1	A	216	TRP	CA-CB-CG	-5.11	103.98	113.70
1	A	293	VAL	CG1-CB-CG2	5.11	119.08	110.90
1	A	191	VAL	CA-CB-CG1	5.11	118.56	110.90
1	A	92	GLU	CG-CD-OE1	-5.11	108.09	118.30
1	A	136	VAL	O-C-N	-5.11	114.53	122.70
1	A	401	ASP	CB-CG-OD2	-5.11	113.71	118.30
1	A	415	SER	N-CA-C	-5.10	97.22	111.00
1	A	184	LYS	CB-CA-C	-5.10	100.19	110.40
1	A	415	SER	CA-CB-OG	-5.10	97.42	111.20
1	A	98	ASP	CA-CB-CG	-5.10	102.18	113.40
1	A	243	GLN	C-N-CA	-5.09	108.99	121.70
1	A	464	TYR	CA-CB-CG	5.08	123.04	113.40
1	A	186	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	A	88	TYR	CD1-CE1-CZ	-5.07	115.24	119.80
1	A	352	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	A	81	GLY	CA-C-O	-5.05	111.50	120.60
1	A	457	GLY	CA-C-N	5.05	126.31	116.20
1	A	46	ILE	CB-CG1-CD1	5.05	128.03	113.90
1	A	401	ASP	CA-CB-CG	5.04	124.50	113.40
1	A	426	ALA	N-CA-CB	-5.03	103.06	110.10
1	A	236	PRO	O-C-N	5.01	130.72	122.70
1	A	264	SER	CB-CA-C	-5.01	100.58	110.10
1	A	336	ALA	N-CA-CB	-5.01	103.09	110.10
1	A	243	GLN	O-C-N	5.00	130.71	122.70

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	3477	172	0
2	A	2	0	0	0	0
3	A	239	0	0	13	0
All	All	3927	0	3477	172	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 24.

All (172) 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:205:ILE:HD12	1:A:246:MET:HE2	1.44	0.99
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: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: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: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
1:A:102:ALA:O	1:A:105:SER:HB3	1.92	0.70
1:A:205:ILE:HD12	1:A:246:MET:HE1	1.68	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:ASN:OD1	1:A:31:ASN:C	2.32	0.67
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: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:470:ALA:C	1:A:472:SER:H	2.06	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: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:205:ILE:HD12	1:A:246:MET:HE3	1.77	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:379:PHE:HE2	1:A:405:ILE:HD12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:85:GLN:O	1:A:137:PHE:HA	2.06	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:178:THR:HA	1:A:183:VAL:CG1	2.38	0.53
1:A:242:TYR:C	1:A:244:ASN:N	2.62	0.53
1:A:37:TYR:CE1	1:A:79:TYR:HA	2.43	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: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:470:ALA:C	1:A:472:SER:N	2.63	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: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:177:ASP:C	1:A:183:VAL:HG11	2.33	0.50
1:A:361:LEU:C	1:A:361:LEU:HD13	2.33	0.49
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:411:ASN:C	1:A:411:ASN:HD22	2.15	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:371:TYR:O	1:A:372:ALA:C	2.51	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:379:PHE:CE2	1:A:405:ILE:HD12	2.49	0.47
1:A:400:THR:O	1:A:401:ASP:C	2.52	0.47
1:A:27:THR:O	1:A:28:ALA:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:ASP:C	1:A:101:LYS:N	2.66	0.45
1:A:240:CYS:HB2	1:A:241:PRO:HD3	1.98	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:355:ASP:N	1:A:355:ASP:OD1	2.50	0.44
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:239:THR:C	1:A:241:PRO:HD2	2.39	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: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:374:SER:C	1:A:375:LYS:HD3	2.39	0.42
1:A:418:SER:HA	1:A:455:MET:O	2.19	0.42
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:156:GLU:HA	3:A:606:HOH:O	2.20	0.42
1:A:180:LYS:C	1:A:182:VAL:N	2.72	0.42
1:A:242:TYR:C	1:A:244:ASN:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:SER:OG	1:A:198:TYR:O	2.31	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:206:ASP:O	1:A:207:THR:C	2.58	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:285:ASP:OD1	1:A:287:THR:OG1	2.26	0.41
1:A:99:ASP:C	1:A:101:LYS:H	2.24	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: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

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	474/478 (99%)	450 (95%)	20 (4%)	4 (1%)	19 15

All (4) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	336 (85%)	61 (15%)	2 1

All (61) 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	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
1	A	142	SER
1	A	143	GLN
1	A	159	THR
1	A	169	ASN
1	A	176	LEU
1	A	180	LYS
1	A	181	ASP
1	A	184	LYS
1	A	187	TRP

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Mol	Chain	Res	Type
1	A	193	SER
1	A	199	SER
1	A	200	ILE
1	A	212	GLN
1	A	213	LYS
1	A	220	ASN
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	341	PRO
1	A	356	SER
1	A	357	GLU
1	A	364	SER
1	A	373	ILE
1	A	375	LYS
1	A	381	THR
1	A	384	ASN
1	A	396	MET
1	A	410	SER
1	A	411	ASN
1	A	420	THR
1	A	424	SER
1	A	447	SER
1	A	450	ASN
1	A	459	LEU
1	A	476	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	93	ASN

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Mol	Chain	Res	Type
1	A	143	GLN
1	A	212	GLN
1	A	251	ASN
1	A	277	ASN
1	A	296	HIS
1	A	321	ASN
1	A	331	GLN
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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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%)	-0.49	2 (0%) 92 93	4, 14, 26, 40	12 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	GLY	3.0
1	A	476	SER	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	480	1/1	0.98	0.11	9,9,9,9	1
2	CA	A	479	1/1	0.99	0.03	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.