



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:41 AM UTC

PDB ID : 1JDA / pdb_00001jda
Title : MALTOTETRAOSE-FORMING EXO-AMYLASE
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Deposited on : 1997-06-16
Resolution : 2.20 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

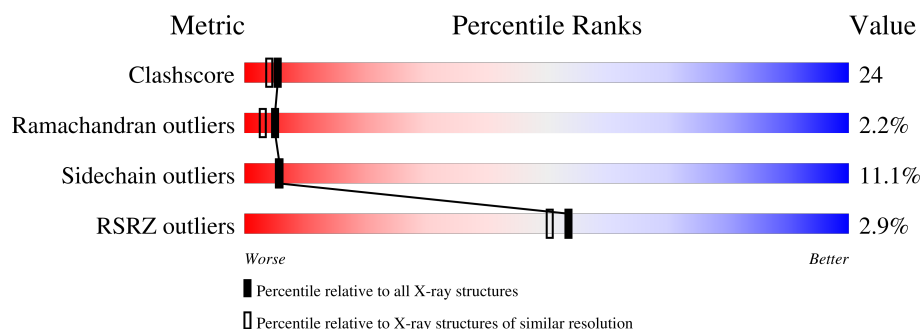
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	429	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3502 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 1,4-ALPHA MALTOTETRAHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3297	2070	597	620	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLN	GLU	engineered mutation	UNP P13507
A	334	ASP	SER	conflict	UNP P13507

- 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		

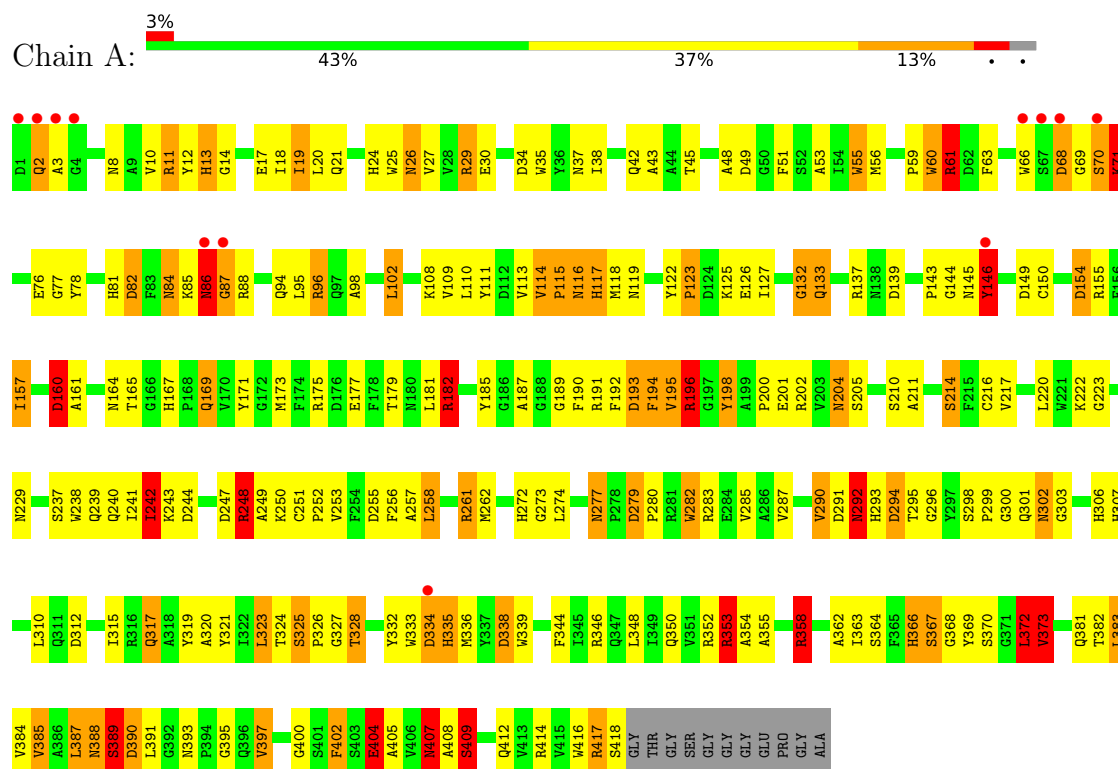
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total	O	0	0
			203	203		

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: 1,4-ALPHA MALTOTETRAHYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.70Å 171.00Å 46.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 94.8 (10.00-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 2.20Å)	Xtriage
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.174 , (Not available) 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3502	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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	1.43	12/3402 (0.4%)	2.50	213/4631 (4.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	PHE	C-N	-7.44	1.23	1.33
1	A	248	ARG	CD-NE	-7.20	1.36	1.46
1	A	255	ASP	C-O	6.65	1.30	1.23
1	A	248	ARG	NE-CZ	-6.50	1.25	1.33
1	A	82	ASP	CA-CB	5.76	1.64	1.53
1	A	296	GLY	C-O	5.60	1.28	1.23
1	A	146	TYR	N-CA	5.57	1.51	1.45
1	A	114	VAL	N-CA	-5.51	1.39	1.46
1	A	51	PHE	N-CA	5.40	1.52	1.45
1	A	196	ARG	CD-NE	-5.21	1.39	1.46
1	A	253	VAL	N-CA	5.19	1.52	1.46
1	A	339	TRP	C-N	-5.09	1.27	1.33

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ARG	CD-NE-CZ	37.65	177.11	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ARG	CD-NE-CZ	18.73	150.62	124.40
1	A	146	TYR	CB-CA-C	16.80	136.02	109.97
1	A	366	HIS	CA-C-N	15.87	142.12	120.38
1	A	366	HIS	C-N-CA	15.87	142.12	120.38
1	A	63	PHE	CA-CB-CG	11.92	125.72	113.80
1	A	346	ARG	NE-CZ-NH1	11.63	133.13	121.50
1	A	84	ASN	CA-CB-CG	11.55	124.15	112.60
1	A	194	PHE	CA-C-N	11.50	142.68	121.97
1	A	194	PHE	C-N-CA	11.50	142.68	121.97
1	A	417	ARG	CA-C-N	10.78	141.10	121.70
1	A	417	ARG	C-N-CA	10.78	141.10	121.70
1	A	196	ARG	NE-CZ-NH1	10.68	132.18	121.50
1	A	11	ARG	NE-CZ-NH1	10.68	132.18	121.50
1	A	346	ARG	CD-NE-CZ	10.45	139.02	124.40
1	A	416	TRP	CA-C-N	10.14	140.90	121.54
1	A	416	TRP	C-N-CA	10.14	140.90	121.54
1	A	242	ILE	CA-CB-CG2	9.77	127.11	110.50
1	A	8	ASN	CA-CB-CG	9.61	122.21	112.60
1	A	146	TYR	CA-CB-CG	9.50	131.00	113.90
1	A	353	ARG	CD-NE-CZ	9.38	137.53	124.40
1	A	248	ARG	NE-CZ-NH1	9.32	130.82	121.50
1	A	283	ARG	NE-CZ-NH2	-9.30	110.83	119.20
1	A	29	ARG	NE-CZ-NH1	9.26	130.76	121.50
1	A	335	HIS	CA-C-N	8.84	132.65	120.63
1	A	335	HIS	C-N-CA	8.84	132.65	120.63
1	A	354	ALA	CA-C-O	-8.63	110.04	119.97
1	A	196	ARG	CD-NE-CZ	8.59	136.42	124.40
1	A	20	LEU	CA-C-O	-8.52	111.10	120.38
1	A	358	ARG	NE-CZ-NH1	8.38	129.88	121.50
1	A	390	ASP	CA-CB-CG	8.14	120.74	112.60
1	A	393	ASN	OD1-CG-ND2	-8.12	114.48	122.60
1	A	229	ASN	CA-CB-CG	-8.12	104.48	112.60
1	A	193	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	242	ILE	CB-CA-C	7.84	123.04	112.22
1	A	82	ASP	CB-CA-C	-7.83	93.61	110.45
1	A	34	ASP	CA-CB-CG	7.79	120.39	112.60
1	A	402	PHE	CA-C-N	7.78	135.34	122.73
1	A	402	PHE	C-N-CA	7.78	135.34	122.73
1	A	229	ASN	OD1-CG-ND2	7.57	130.17	122.60
1	A	60	TRP	CA-C-O	7.56	129.35	120.58
1	A	182	ARG	NE-CZ-NH2	-7.56	112.39	119.20
1	A	94	GLN	OE1-CD-NE2	-7.54	115.06	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	GLU	CB-CG-CD	7.49	125.32	112.60
1	A	291	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	290	VAL	N-CA-C	-7.32	105.97	111.90
1	A	339	TRP	CA-C-N	7.28	132.71	120.91
1	A	339	TRP	C-N-CA	7.28	132.71	120.91
1	A	293	HIS	CA-CB-CG	-7.28	106.53	113.80
1	A	353	ARG	NE-CZ-NH1	7.26	128.76	121.50
1	A	160	ASP	CA-CB-CG	-7.19	105.41	112.60
1	A	117	HIS	CA-CB-CG	-7.19	106.61	113.80
1	A	119	ASN	CA-C-N	7.14	130.18	120.54
1	A	119	ASN	C-N-CA	7.14	130.18	120.54
1	A	373	VAL	CB-CA-C	7.12	119.81	110.12
1	A	198	TYR	CA-C-O	-7.12	113.61	121.23
1	A	283	ARG	NE-CZ-NH1	7.10	128.60	121.50
1	A	334	ASP	CA-CB-CG	-6.99	105.61	112.60
1	A	282	TRP	CA-C-N	6.97	129.62	120.28
1	A	282	TRP	C-N-CA	6.97	129.62	120.28
1	A	110	LEU	CA-C-O	-6.96	112.84	120.43
1	A	25	TRP	N-CA-C	6.96	119.71	111.71
1	A	296	GLY	N-CA-C	6.92	122.05	112.57
1	A	139	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	338	ASP	O-C-N	6.89	131.40	122.03
1	A	190	PHE	CA-CB-CG	-6.87	106.93	113.80
1	A	49	ASP	CA-C-N	-6.83	111.83	122.69
1	A	49	ASP	C-N-CA	-6.83	111.83	122.69
1	A	291	ASP	O-C-N	6.82	130.71	123.42
1	A	369	TYR	CA-CB-CG	-6.82	101.63	113.90
1	A	388	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	A	86	ASN	CA-C-N	6.79	134.71	121.41
1	A	86	ASN	C-N-CA	6.79	134.71	121.41
1	A	346	ARG	NH1-CZ-NH2	-6.74	110.54	119.30
1	A	146	TYR	N-CA-CB	-6.72	101.77	111.25
1	A	336	MET	CA-C-O	-6.72	113.98	120.90
1	A	384	VAL	CA-C-O	-6.69	113.43	120.39
1	A	196	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	A	405	ALA	CA-C-N	6.55	132.14	122.71
1	A	405	ALA	C-N-CA	6.55	132.14	122.71
1	A	324	THR	CA-CB-CG2	6.55	121.63	110.50
1	A	369	TYR	CA-C-O	-6.54	113.96	121.68
1	A	292	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	192	PHE	O-C-N	6.48	130.62	123.04
1	A	181	LEU	N-CA-CB	-6.47	100.25	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	LEU	CA-C-O	-6.47	113.61	120.80
1	A	185	TYR	CA-C-N	6.46	134.08	121.41
1	A	185	TYR	C-N-CA	6.46	134.08	121.41
1	A	277	ASN	O-C-N	6.45	126.92	121.31
1	A	367	SER	N-CA-C	6.42	119.10	111.33
1	A	204	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	A	169	GLN	OE1-CD-NE2	6.36	128.96	122.60
1	A	13	HIS	CA-CB-CG	-6.36	107.44	113.80
1	A	48	ALA	CA-C-N	6.35	131.32	120.72
1	A	48	ALA	C-N-CA	6.35	131.32	120.72
1	A	190	PHE	O-C-N	6.34	131.00	123.27
1	A	279	ASP	CB-CA-C	6.33	117.09	109.31
1	A	414	ARG	CD-NE-CZ	6.32	133.24	124.40
1	A	262	MET	CA-C-N	6.29	129.22	120.29
1	A	262	MET	C-N-CA	6.29	129.22	120.29
1	A	241	ILE	CA-C-N	6.27	129.32	120.42
1	A	241	ILE	C-N-CA	6.27	129.32	120.42
1	A	96	ARG	CD-NE-CZ	-6.25	115.66	124.40
1	A	223	GLY	O-C-N	6.23	128.00	121.77
1	A	383	LEU	N-CA-CB	-6.22	100.44	111.08
1	A	11	ARG	NH1-CZ-NH2	-6.21	111.22	119.30
1	A	298	SER	O-C-N	6.18	126.27	121.88
1	A	258	LEU	CA-C-N	6.18	128.56	120.28
1	A	258	LEU	C-N-CA	6.18	128.56	120.28
1	A	116	ASN	OD1-CG-ND2	6.18	128.78	122.60
1	A	302	ASN	CA-CB-CG	6.18	118.78	112.60
1	A	139	ASP	N-CA-C	-6.16	105.02	112.54
1	A	84	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	A	408	ALA	CA-C-N	6.11	133.22	121.54
1	A	408	ALA	C-N-CA	6.11	133.22	121.54
1	A	115	PRO	N-CA-C	6.11	121.50	113.86
1	A	397	VAL	N-CA-CB	-6.08	101.20	111.23
1	A	328	THR	CA-C-O	-6.04	113.95	119.62
1	A	257	ALA	N-CA-C	-6.03	104.63	111.14
1	A	287	VAL	N-CA-CB	6.02	119.44	112.15
1	A	327	GLY	N-CA-C	-6.00	101.78	112.58
1	A	30	GLU	CA-C-O	-6.00	114.13	120.55
1	A	249	ALA	CA-C-N	5.98	130.62	122.07
1	A	249	ALA	C-N-CA	5.98	130.62	122.07
1	A	256	PHE	N-CA-CB	5.97	120.30	110.39
1	A	407	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	222	LYS	CA-C-O	-5.94	113.03	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	GLY	CA-C-O	-5.92	115.82	121.62
1	A	368	GLY	N-CA-C	5.90	125.28	115.66
1	A	409	SER	N-CA-CB	5.88	120.43	110.49
1	A	414	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	A	210	SER	N-CA-C	5.85	121.08	113.88
1	A	59	PRO	CA-C-N	5.84	129.66	121.24
1	A	59	PRO	C-N-CA	5.84	129.66	121.24
1	A	37	ASN	CA-C-O	5.84	126.61	120.42
1	A	21	GLN	N-CA-C	-5.82	100.77	109.15
1	A	350	GLN	O-C-N	5.82	128.38	122.09
1	A	400	GLY	CA-C-O	-5.78	118.15	122.37
1	A	300	GLY	CA-C-N	5.77	132.56	121.54
1	A	300	GLY	C-N-CA	5.77	132.56	121.54
1	A	358	ARG	CD-NE-CZ	5.76	132.47	124.40
1	A	165	THR	CA-C-N	5.74	132.66	121.41
1	A	165	THR	C-N-CA	5.74	132.66	121.41
1	A	366	HIS	CA-CB-CG	-5.73	108.07	113.80
1	A	126	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	325	SER	CA-C-N	5.72	126.99	119.84
1	A	325	SER	C-N-CA	5.72	126.99	119.84
1	A	292	ASN	CA-C-N	5.71	128.50	120.28
1	A	292	ASN	C-N-CA	5.71	128.50	120.28
1	A	363	ILE	CA-C-N	5.70	131.49	122.94
1	A	363	ILE	C-N-CA	5.70	131.49	122.94
1	A	149	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	56	MET	CA-C-O	5.68	126.50	120.64
1	A	248	ARG	N-CA-C	5.66	119.36	112.23
1	A	45	THR	CA-CB-CG2	5.63	120.08	110.50
1	A	290	VAL	CB-CA-C	5.59	116.67	111.30
1	A	53	ALA	CA-C-O	-5.55	115.34	121.33
1	A	181	LEU	CB-CA-C	5.54	120.87	110.63
1	A	366	HIS	CA-C-O	5.54	126.38	120.46
1	A	10	VAL	CB-CA-C	5.53	118.79	111.21
1	A	274	LEU	CA-C-O	-5.52	114.70	120.55
1	A	292	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	45	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	389	SER	CA-CB-OG	5.46	122.03	111.10
1	A	250	LYS	CA-C-O	-5.44	115.23	121.54
1	A	324	THR	CA-CB-OG1	-5.43	101.45	109.60
1	A	217	VAL	CA-C-O	5.43	126.71	120.90
1	A	261	ARG	CD-NE-CZ	5.43	132.00	124.40
1	A	272	HIS	CA-CB-CG	-5.42	108.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	VAL	CA-C-N	-5.42	118.44	122.18
1	A	217	VAL	C-N-CA	-5.42	118.44	122.18
1	A	86	ASN	CA-C-O	5.41	128.15	121.99
1	A	26	ASN	CA-C-O	-5.40	113.35	119.78
1	A	182	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	362	ALA	CA-C-N	5.39	130.95	122.33
1	A	362	ALA	C-N-CA	5.39	130.95	122.33
1	A	146	TYR	CA-C-N	5.38	125.30	119.76
1	A	146	TYR	C-N-CA	5.38	125.30	119.76
1	A	238	TRP	CA-C-N	5.34	127.44	120.28
1	A	238	TRP	C-N-CA	5.34	127.44	120.28
1	A	29	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
1	A	194	PHE	N-CA-CB	-5.32	103.24	111.65
1	A	20	LEU	O-C-N	5.32	129.57	123.29
1	A	201	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	204	ASN	N-CA-C	-5.32	105.56	111.36
1	A	328	THR	O-C-N	5.29	128.16	121.12
1	A	291	ASP	N-CA-CB	5.29	119.76	111.56
1	A	387	LEU	CB-CA-C	5.28	118.74	110.19
1	A	154	ASP	O-C-N	5.26	129.07	122.65
1	A	404	GLU	CA-CB-CG	5.23	124.55	114.10
1	A	395	GLY	O-C-N	-5.22	116.88	122.73
1	A	18	ILE	CA-C-O	-5.21	115.58	120.22
1	A	61	ARG	NE-CZ-NH2	-5.21	114.52	119.20
1	A	251	CYS	CB-CA-C	-5.20	100.34	108.91
1	A	179	THR	CA-C-O	5.19	125.92	120.42
1	A	55	TRP	CA-CB-CG	5.16	123.40	113.60
1	A	77	GLY	N-CA-C	5.15	121.84	114.64
1	A	175	ARG	CD-NE-CZ	5.12	131.57	124.40
1	A	335	HIS	N-CA-CB	5.12	117.64	110.12
1	A	113	VAL	O-C-N	5.11	128.70	123.18
1	A	310	LEU	CA-C-O	-5.11	114.87	120.69
1	A	114	VAL	CA-C-N	5.10	124.71	119.56
1	A	114	VAL	C-N-CA	5.10	124.71	119.56
1	A	307	HIS	N-CA-CB	5.09	118.14	110.30
1	A	385	VAL	N-CA-CB	-5.09	105.05	111.46
1	A	2	GLN	N-CA-C	-5.06	101.72	109.76
1	A	82	ASP	CB-CG-OD1	-5.05	106.78	118.40
1	A	229	ASN	O-C-N	5.04	128.12	122.22
1	A	294	ASP	CA-C-O	5.02	126.64	120.56
1	A	114	VAL	O-C-N	5.02	126.82	121.10
1	A	45	THR	O-C-N	5.02	127.25	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ALA	CB-CA-C	5.01	118.88	110.92
1	A	214	SER	N-CA-CB	-5.00	103.48	110.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain
1	A	353	ARG	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	3297	0	3014	150	0
2	A	2	0	0	0	0
3	A	203	0	0	12	0
All	All	3502	0	3014	150	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 (150) 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:370:SER:O	1:A:389:SER:HB2	1.24	1.24
1:A:71:LYS:HD3	1:A:302:ASN:OD1	1.61	1.01
1:A:277:ASN:HD22	1:A:279:ASP:H	1.07	1.01
1:A:370:SER:O	1:A:389:SER:CB	2.10	0.99
1:A:145:ASN:HD21	1:A:154:ASP:HB3	1.24	0.98
1:A:116:ASN:HD22	1:A:117:HIS:HD2	1.06	0.98
1:A:86:ASN:C	1:A:86:ASN:OD1	2.11	0.94
1:A:334:ASP:OD1	1:A:338:ASP:OD2	1.87	0.92
1:A:11:ARG:HH22	1:A:204:ASN:ND2	1.68	0.92
1:A:11:ARG:HH12	1:A:204:ASN:HD22	0.92	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:PRO:HD3	1:A:334:ASP:OD2	1.70	0.91
1:A:11:ARG:HH12	1:A:204:ASN:ND2	1.68	0.90
1:A:17:GLU:OE2	1:A:108:LYS:HE2	1.74	0.87
1:A:11:ARG:NH1	1:A:204:ASN:HD22	1.70	0.87
1:A:26:ASN:HD22	1:A:29:ARG:HH11	1.26	0.82
1:A:61:ARG:HD2	1:A:84:ASN:HB3	1.60	0.82
1:A:70:SER:O	1:A:71:LYS:HB2	1.79	0.79
1:A:116:ASN:HD22	1:A:117:HIS:CD2	1.96	0.79
1:A:277:ASN:ND2	1:A:279:ASP:H	1.79	0.79
1:A:211:ALA:HB1	1:A:214:SER:OG	1.83	0.78
1:A:143:PRO:HB2	1:A:146:TYR:HE1	1.48	0.78
1:A:409:SER:O	1:A:412:GLN:HG3	1.84	0.78
1:A:132:GLY:O	1:A:133:GLN:HG2	1.84	0.77
1:A:160:ASP:OD1	1:A:160:ASP:N	2.14	0.77
1:A:317:GLN:H	1:A:317:GLN:HE21	1.31	0.76
1:A:145:ASN:HD21	1:A:154:ASP:CB	2.01	0.73
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.21	0.73
1:A:216:CYS:O	1:A:252:PRO:HD2	1.88	0.73
1:A:319:TYR:OH	1:A:335:HIS:CD2	2.42	0.73
1:A:86:ASN:OD1	1:A:87:GLY:N	2.22	0.73
1:A:24:HIS:HD2	1:A:26:ASN:H	1.38	0.72
1:A:292:ASN:ND2	1:A:294:ASP:H	1.89	0.70
1:A:358:ARG:HG3	3:A:530:HOH:O	1.91	0.69
1:A:407:ASN:C	1:A:407:ASN:HD22	2.02	0.67
1:A:82:ASP:HB3	1:A:84:ASN:H	1.60	0.67
1:A:24:HIS:HE1	3:A:489:HOH:O	1.77	0.66
1:A:11:ARG:NH2	1:A:204:ASN:ND2	2.41	0.65
1:A:85:LYS:NZ	1:A:177:GLU:OE2	2.26	0.65
1:A:292:ASN:ND2	1:A:295:THR:H	1.94	0.65
1:A:154:ASP:OD2	1:A:196:ARG:HD3	1.97	0.65
1:A:145:ASN:ND2	1:A:155:ARG:H	1.94	0.65
1:A:277:ASN:HD22	1:A:279:ASP:N	1.87	0.65
1:A:71:LYS:CD	1:A:302:ASN:OD1	2.43	0.64
1:A:61:ARG:HD3	1:A:82:ASP:HB2	1.78	0.64
1:A:388:ASN:ND2	1:A:412:GLN:HB3	2.12	0.64
1:A:3:ALA:HB2	1:A:13:HIS:CE1	2.34	0.62
1:A:143:PRO:HD2	3:A:578:HOH:O	1.99	0.62
1:A:84:ASN:OD1	1:A:86:ASN:HB3	2.01	0.61
1:A:332:TYR:HB3	1:A:335:HIS:CD2	2.35	0.61
1:A:402:PHE:CD1	1:A:417:ARG:HB2	2.35	0.61
1:A:319:TYR:OH	1:A:335:HIS:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:HB2	3:A:662:HOH:O	2.01	0.61
1:A:11:ARG:HH22	1:A:204:ASN:HD21	1.46	0.60
1:A:144:GLY:O	1:A:146:TYR:N	2.32	0.60
1:A:258:LEU:HB2	1:A:273:GLY:HA3	1.84	0.60
1:A:42:GLN:HG3	3:A:597:HOH:O	2.02	0.59
1:A:3:ALA:HB1	1:A:13:HIS:NE2	2.18	0.59
1:A:3:ALA:CB	1:A:13:HIS:CE1	2.86	0.59
1:A:167:HIS:HD2	1:A:169:GLN:H	1.49	0.58
1:A:38:ILE:O	1:A:42:GLN:HG2	2.03	0.58
1:A:332:TYR:HB3	1:A:335:HIS:HD2	1.69	0.57
1:A:61:ARG:CD	1:A:84:ASN:HB3	2.31	0.57
1:A:182:ARG:HD2	1:A:211:ALA:HB2	1.85	0.57
1:A:116:ASN:ND2	1:A:117:HIS:HD2	1.90	0.56
1:A:390:ASP:O	1:A:391:LEU:C	2.48	0.56
1:A:325:SER:HB2	1:A:326:PRO:CD	2.36	0.56
1:A:299:PRO:CD	1:A:334:ASP:OD2	2.51	0.55
1:A:312:ASP:HA	1:A:315:ILE:HG13	1.88	0.55
1:A:292:ASN:HD21	1:A:294:ASP:HB2	1.71	0.55
1:A:292:ASN:HD22	1:A:294:ASP:H	1.54	0.55
1:A:19:ILE:HD13	1:A:328:THR:CG2	2.38	0.54
1:A:61:ARG:HB3	1:A:84:ASN:O	2.08	0.54
1:A:321:TYR:HB2	1:A:387:LEU:HD11	1.90	0.54
1:A:402:PHE:HD1	1:A:417:ARG:HB2	1.73	0.54
1:A:122:TYR:CD1	1:A:123:PRO:HD2	2.43	0.53
1:A:335:HIS:HE1	3:A:522:HOH:O	1.92	0.53
1:A:87:GLY:O	1:A:88:ARG:HB2	2.09	0.53
1:A:333:TRP:HD1	1:A:334:ASP:OD1	1.92	0.53
1:A:88:ARG:NH1	3:A:564:HOH:O	2.41	0.53
1:A:355:ALA:CB	1:A:381:GLN:HB2	2.39	0.53
1:A:167:HIS:CD2	1:A:169:GLN:HB3	2.43	0.53
1:A:404:GLU:OE1	1:A:407:ASN:HB2	2.09	0.53
1:A:191:ARG:NH1	1:A:193:ASP:HB2	2.23	0.52
1:A:11:ARG:NH1	1:A:204:ASN:ND2	2.42	0.52
1:A:114:VAL:O	1:A:114:VAL:HG12	2.08	0.52
1:A:43:ALA:HB2	1:A:102:LEU:HD13	1.91	0.52
1:A:303:GLY:HA2	3:A:562:HOH:O	2.10	0.52
1:A:323:LEU:O	1:A:352:ARG:HD2	2.10	0.52
1:A:122:TYR:CG	1:A:123:PRO:HD2	2.46	0.51
1:A:244:ASP:O	1:A:248:ARG:HG3	2.10	0.51
1:A:26:ASN:ND2	1:A:29:ARG:HH11	2.01	0.51
1:A:2:GLN:O	1:A:14:GLY:HA3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HD23	1:A:242:ILE:HD12	1.92	0.51
1:A:29:ARG:NH2	1:A:76:GLU:OE2	2.24	0.50
1:A:61:ARG:HD3	1:A:82:ASP:CB	2.42	0.50
1:A:366:HIS:HB2	1:A:373:VAL:HG22	1.92	0.50
1:A:143:PRO:HB2	1:A:146:TYR:CE1	2.38	0.50
1:A:195:VAL:CG1	1:A:220:LEU:HB2	2.41	0.50
1:A:81:HIS:HD2	3:A:495:HOH:O	1.94	0.50
1:A:279:ASP:OD1	1:A:280:PRO:HD2	2.11	0.50
1:A:200:PRO:HB2	1:A:248:ARG:HB2	1.94	0.49
1:A:319:TYR:O	1:A:323:LEU:HB2	2.12	0.49
1:A:320:ALA:HA	1:A:348:LEU:HD13	1.95	0.49
1:A:387:LEU:O	1:A:388:ASN:C	2.56	0.49
1:A:137:ARG:NH2	1:A:146:TYR:O	2.33	0.48
1:A:167:HIS:CD2	1:A:169:GLN:H	2.30	0.48
1:A:292:ASN:HD22	1:A:292:ASN:C	2.22	0.48
1:A:19:ILE:HD13	1:A:328:THR:HG22	1.95	0.48
1:A:43:ALA:CB	1:A:102:LEU:HD13	2.44	0.48
1:A:373:VAL:HA	1:A:385:VAL:O	2.13	0.48
1:A:195:VAL:HG11	1:A:220:LEU:HB2	1.96	0.47
1:A:115:PRO:HG2	1:A:198:TYR:CZ	2.49	0.46
1:A:108:LYS:HZ2	1:A:108:LYS:HG3	1.61	0.46
1:A:417:ARG:CG	3:A:544:HOH:O	2.63	0.46
1:A:111:TYR:CD2	1:A:187:ALA:HB2	2.50	0.46
1:A:202:ARG:O	1:A:205:SER:HB2	2.16	0.46
1:A:69:GLY:O	1:A:70:SER:C	2.58	0.45
1:A:325:SER:HB2	1:A:326:PRO:HD2	1.99	0.45
1:A:145:ASN:ND2	1:A:154:ASP:HB3	2.09	0.45
1:A:118:MET:HE3	1:A:118:MET:HB2	1.72	0.45
1:A:382:THR:O	1:A:417:ARG:HB3	2.17	0.45
1:A:292:ASN:HD22	1:A:294:ASP:N	2.13	0.45
1:A:42:GLN:CG	3:A:597:HOH:O	2.63	0.45
1:A:145:ASN:HD21	1:A:155:ARG:H	1.65	0.44
1:A:323:LEU:HD12	1:A:323:LEU:HA	1.88	0.44
1:A:60:TRP:HB3	1:A:82:ASP:O	2.18	0.44
1:A:127:ILE:HG23	1:A:173:MET:HE1	1.99	0.44
1:A:115:PRO:HG2	1:A:198:TYR:CE2	2.53	0.43
1:A:292:ASN:ND2	1:A:294:ASP:N	2.62	0.43
1:A:261:ARG:NE	1:A:261:ARG:HA	2.32	0.43
1:A:344:PHE:CZ	1:A:348:LEU:HD11	2.53	0.43
1:A:171:TYR:CD1	1:A:171:TYR:C	2.96	0.43
1:A:194:PHE:CD2	1:A:194:PHE:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:HD2	1:A:211:ALA:CB	2.49	0.43
1:A:118:MET:O	1:A:161:ALA:HB1	2.20	0.42
1:A:191:ARG:HH11	1:A:193:ASP:HB2	1.85	0.42
1:A:35:TRP:CE3	1:A:38:ILE:HD12	2.54	0.42
1:A:96:ARG:HH11	1:A:96:ARG:HD3	1.66	0.42
1:A:66:TRP:CE3	1:A:66:TRP:O	2.73	0.42
1:A:78:TYR:O	1:A:117:HIS:HE1	2.02	0.42
1:A:372:LEU:HA	3:A:480:HOH:O	2.21	0.41
1:A:3:ALA:HB1	1:A:13:HIS:CE1	2.55	0.41
1:A:11:ARG:NH2	1:A:204:ASN:HD21	2.14	0.41
1:A:17:GLU:CD	1:A:108:LYS:HE2	2.42	0.41
1:A:243:LYS:NZ	1:A:247:ASP:OD1	2.44	0.41
1:A:237:SER:H	1:A:240:GLN:HE21	1.68	0.41
1:A:409:SER:O	1:A:412:GLN:CG	2.63	0.40
1:A:150:CYS:O	1:A:164:ASN:HB2	2.22	0.40
1:A:282:TRP:O	1:A:285:VAL:HG22	2.22	0.40
1:A:306:HIS:O	1:A:306:HIS:ND1	2.54	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	416/429 (97%)	386 (93%)	21 (5%)	9 (2%)	5 3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	71	LYS
1	A	87	GLY
1	A	133	GLN

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Mol	Chain	Res	Type
1	A	68	ASP
1	A	123	PRO
1	A	132	GLY
1	A	301	GLN
1	A	157	ILE

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	333/337 (99%)	296 (89%)	37 (11%)	6 6

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	19	ILE
1	A	27	VAL
1	A	55	TRP
1	A	61	ARG
1	A	68	ASP
1	A	71	LYS
1	A	86	ASN
1	A	95	LEU
1	A	102	LEU
1	A	109	VAL
1	A	125	LYS
1	A	146	TYR
1	A	157	ILE
1	A	160	ASP
1	A	195	VAL
1	A	196	ARG
1	A	239	GLN
1	A	242	ILE
1	A	248	ARG
1	A	290	VAL

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Mol	Chain	Res	Type
1	A	292	ASN
1	A	317	GLN
1	A	323	LEU
1	A	353	ARG
1	A	358	ARG
1	A	364	SER
1	A	367	SER
1	A	372	LEU
1	A	373	VAL
1	A	383	LEU
1	A	389	SER
1	A	397	VAL
1	A	404	GLU
1	A	407	ASN
1	A	409	SER
1	A	418	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	24	HIS
1	A	26	ASN
1	A	42	GLN
1	A	81	HIS
1	A	97	GLN
1	A	117	HIS
1	A	145	ASN
1	A	167	HIS
1	A	180	ASN
1	A	204	ASN
1	A	229	ASN
1	A	240	GLN
1	A	264	ASN
1	A	275	ASN
1	A	277	ASN
1	A	292	ASN
1	A	305	GLN
1	A	307	HIS
1	A	317	GLN
1	A	335	HIS
1	A	366	HIS

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Mol	Chain	Res	Type
1	A	381	GLN
1	A	388	ASN
1	A	407	ASN
1	A	410	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	418/429 (97%)	0.29	12 (2%) 53 50	8, 19, 39, 62	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	SER	5.2
1	A	68	ASP	4.8
1	A	146	TYR	3.9
1	A	67	SER	3.3
1	A	4	GLY	3.1
1	A	334	ASP	3.1
1	A	1	ASP	3.1
1	A	66	TRP	2.6
1	A	2	GLN	2.4
1	A	87	GLY	2.4
1	A	86	ASN	2.3
1	A	3	ALA	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 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($\text{\AA}^2$)	Q<0.9
2	CA	A	455	1/1	0.77	0.09	58,58,58,58	0
2	CA	A	454	1/1	0.94	0.11	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.