



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 PM UTC

PDB ID : 1GOH / pdb_00001goh
Title : NOVEL THIOETHER BOND REVEALED BY A 1.7 ANGSTROMS CRYSTAL STRUCTURE OF GALACTOSE OXIDASE
Authors : Ito, N.; Phillips, S.E.V.; Knowles, P.F.
Deposited on : 1993-09-30
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

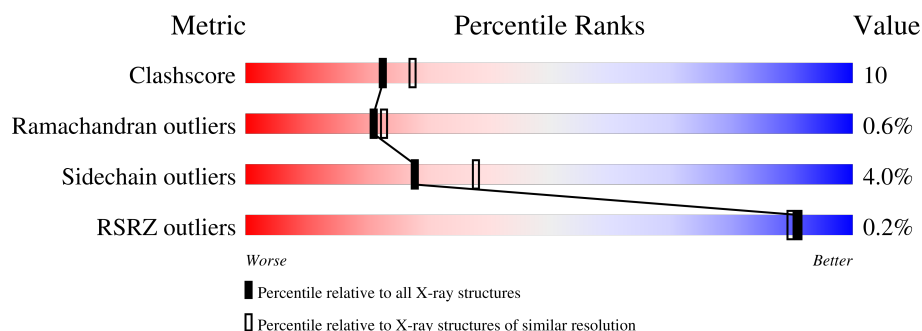
1 Overall quality at a glance

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	639	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5141 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 GALACTOSE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			4830	3017	840	954	19			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is water.

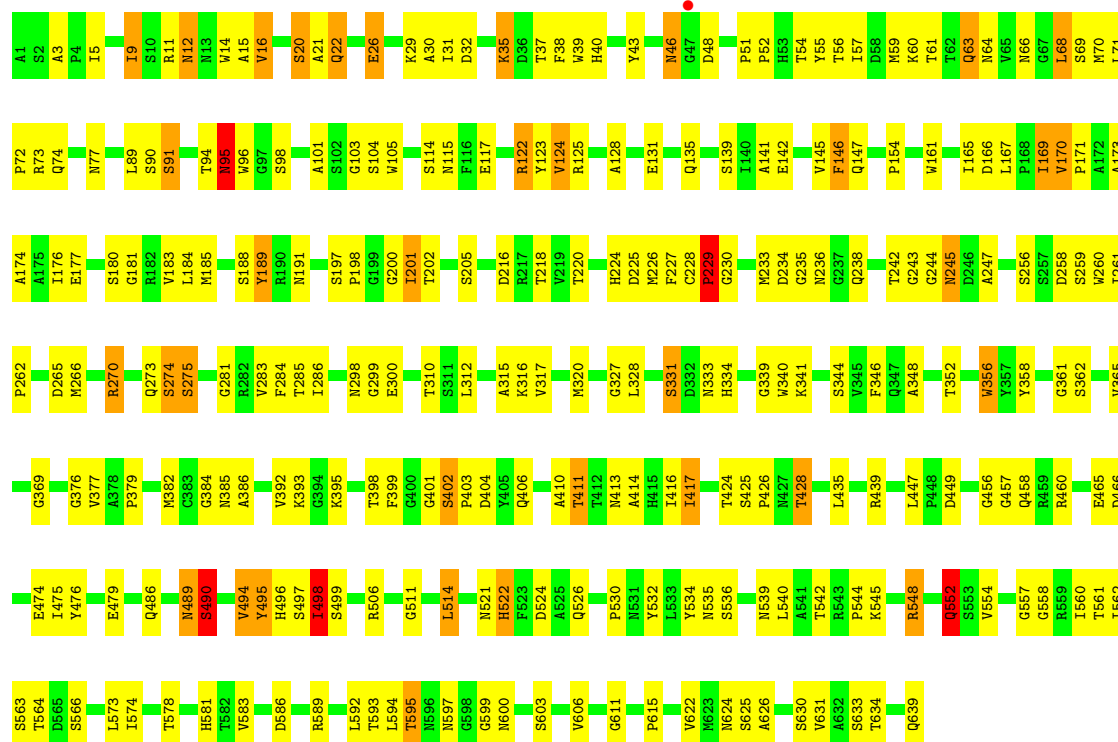
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	310	Total	O	0	0
			310	310		

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: GALACTOSE OXIDASE

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.00Å 89.40Å 86.70Å 90.00° 117.80° 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) 76.5 (10.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.19Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.156 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5141	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: NA

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	1.28	4/4959 (0.1%)	2.13	193/6765 (2.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	SER	N-CA	5.39	1.52	1.45
1	A	202	THR	CA-CB	5.09	1.61	1.53
1	A	611	GLY	N-CA	5.09	1.52	1.45
1	A	167	LEU	CA-CB	5.03	1.60	1.54

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ARG	CD-NE-CZ	16.79	147.91	124.40
1	A	122	ARG	CD-NE-CZ	11.68	140.75	124.40
1	A	188	SER	O-C-N	11.47	131.72	123.11
1	A	557	GLY	CA-C-N	10.17	129.76	120.10
1	A	557	GLY	C-N-CA	10.17	129.76	120.10
1	A	333	ASN	CA-CB-CG	9.98	122.58	112.60
1	A	66	ASN	CA-CB-CG	9.84	122.44	112.60
1	A	3	ALA	O-C-N	9.54	130.39	121.71
1	A	216	ASP	CA-CB-CG	9.36	121.96	112.60
1	A	64	ASN	CA-CB-CG	-9.01	103.59	112.60
1	A	146	PHE	CA-CB-CG	-8.31	105.49	113.80
1	A	315	ALA	O-C-N	7.87	131.45	122.55
1	A	449	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	597	ASN	CA-CB-CG	7.65	120.25	112.60
1	A	586	ASP	CA-C-O	-7.56	111.85	120.24
1	A	631	VAL	N-CA-C	-7.49	99.05	109.45
1	A	26	GLU	CA-CB-CG	7.48	129.06	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	ASP	O-C-N	7.36	132.98	123.11
1	A	169	ILE	CA-C-O	-7.35	114.43	121.64
1	A	169	ILE	O-C-N	7.30	131.06	122.95
1	A	489	ASN	OD1-CG-ND2	7.16	129.76	122.60
1	A	361	GLY	O-C-N	7.13	130.67	122.61
1	A	247	ALA	CA-C-O	-7.11	111.22	119.61
1	A	274	SER	CA-C-O	-7.10	113.14	121.16
1	A	20	SER	O-C-N	7.07	131.31	123.25
1	A	435	LEU	O-C-N	7.03	130.81	122.79
1	A	265	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	104	SER	O-C-N	6.88	131.25	123.27
1	A	593	THR	CB-CA-C	6.85	121.42	110.19
1	A	283	VAL	CA-C-O	6.84	127.57	120.39
1	A	273	GLN	OE1-CD-NE2	-6.80	115.80	122.60
1	A	384	GLY	N-CA-C	-6.73	102.02	112.85
1	A	54	THR	N-CA-CB	-6.71	99.11	111.13
1	A	544	PRO	N-CA-C	-6.70	100.96	111.34
1	A	238	GLN	OE1-CD-NE2	6.60	129.20	122.60
1	A	198	PRO	N-CA-C	-6.56	106.15	114.35
1	A	361	GLY	CA-C-O	-6.47	113.53	121.68
1	A	218	THR	CA-C-N	-6.42	114.73	123.14
1	A	218	THR	C-N-CA	-6.42	114.73	123.14
1	A	600	ASN	OD1-CG-ND2	6.36	128.96	122.60
1	A	344	SER	O-C-N	6.36	130.10	122.85
1	A	586	ASP	O-C-N	6.34	130.48	122.23
1	A	456	GLY	CA-C-O	-6.34	114.47	122.01
1	A	286	ILE	O-C-N	6.32	129.95	123.00
1	A	460	ARG	CD-NE-CZ	-6.31	115.56	124.40
1	A	115	ASN	CB-CA-C	6.30	120.15	109.75
1	A	188	SER	CA-C-O	-6.26	115.69	120.19
1	A	456	GLY	O-C-N	6.25	129.55	122.67
1	A	339	GLY	N-CA-C	-6.24	102.29	111.03
1	A	20	SER	N-CA-CB	6.21	122.04	111.66
1	A	382	MET	CB-CA-C	6.21	119.16	109.84
1	A	406	GLN	O-C-N	6.21	130.24	123.10
1	A	498	ILE	O-C-N	6.20	130.02	123.02
1	A	114	SER	N-CA-CB	6.19	120.25	110.84
1	A	417	ILE	CA-C-N	-6.17	114.31	123.00
1	A	417	ILE	C-N-CA	-6.17	114.31	123.00
1	A	498	ILE	CA-C-O	-6.16	115.53	121.63
1	A	458	GLN	CA-C-O	6.13	128.33	121.40
1	A	535	ASN	N-CA-C	-6.08	100.99	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	SER	O-C-N	6.06	130.07	123.10
1	A	114	SER	CA-C-O	-6.05	113.79	120.33
1	A	561	THR	O-C-N	6.05	130.50	123.30
1	A	224	HIS	N-CA-CB	-6.05	100.64	110.81
1	A	457	GLY	CA-C-N	6.05	132.01	122.21
1	A	457	GLY	C-N-CA	6.05	132.01	122.21
1	A	26	GLU	CB-CG-CD	6.05	122.88	112.60
1	A	377	VAL	CA-C-O	-6.02	113.99	120.85
1	A	499	SER	N-CA-CB	6.02	121.90	111.13
1	A	524	ASP	N-CA-CB	-6.01	101.75	111.24
1	A	35	LYS	CA-CB-CG	5.99	126.07	114.10
1	A	327	GLY	CA-C-N	5.94	129.05	120.38
1	A	327	GLY	C-N-CA	5.94	129.05	120.38
1	A	548	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	A	333	ASN	O-C-N	5.91	129.59	122.85
1	A	589	ARG	O-C-N	5.90	130.46	123.27
1	A	376	GLY	CA-C-O	5.89	127.38	122.13
1	A	416	ILE	CA-C-O	-5.89	114.23	120.48
1	A	594	LEU	O-C-N	5.87	130.05	123.19
1	A	476	TYR	CA-C-O	-5.81	114.10	120.43
1	A	170	VAL	N-CA-C	-5.79	102.29	107.56
1	A	399	PHE	N-CA-C	5.78	117.89	108.76
1	A	633	SER	N-CA-C	-5.78	100.29	109.59
1	A	16	VAL	CA-C-N	5.74	132.03	122.73
1	A	16	VAL	C-N-CA	5.74	132.03	122.73
1	A	245	ASN	CA-C-O	-5.74	114.47	120.55
1	A	202	THR	CA-C-N	-5.72	114.13	122.19
1	A	202	THR	C-N-CA	-5.72	114.13	122.19
1	A	404	ASP	CA-CB-CG	-5.71	106.89	112.60
1	A	245	ASN	O-C-N	5.70	128.16	122.12
1	A	236	ASN	OD1-CG-ND2	5.69	128.29	122.60
1	A	489	ASN	N-CA-CB	5.68	119.24	110.60
1	A	552	GLN	CB-CA-C	5.63	120.32	110.64
1	A	615	PRO	CA-C-O	5.63	128.98	121.95
1	A	369	GLY	O-C-N	5.58	127.52	122.88
1	A	564	THR	CA-CB-OG1	-5.57	101.24	109.60
1	A	46	ASN	O-C-N	5.56	129.71	122.42
1	A	101	ALA	O-C-N	5.55	129.69	123.48
1	A	147	GLN	O-C-N	5.54	130.06	123.24
1	A	124	VAL	CA-C-N	5.54	131.54	121.89
1	A	124	VAL	C-N-CA	5.54	131.54	121.89
1	A	243	GLY	CA-C-N	-5.54	116.11	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	GLY	C-N-CA	-5.54	116.11	121.31
1	A	131	GLU	O-C-N	5.52	130.22	123.21
1	A	230	GLY	N-CA-C	-5.50	101.88	111.62
1	A	331	SER	CA-C-O	-5.47	112.87	119.49
1	A	128	ALA	CA-C-O	-5.47	114.85	120.54
1	A	352	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	633	SER	N-CA-CB	5.46	119.47	110.69
1	A	95	ASN	O-C-N	5.43	129.51	123.05
1	A	413	ASN	O-C-N	5.42	129.58	122.97
1	A	447	LEU	CA-C-N	5.40	125.47	119.32
1	A	447	LEU	C-N-CA	5.40	125.47	119.32
1	A	495	TYR	CA-C-O	5.40	126.84	120.96
1	A	386	ALA	CB-CA-C	5.39	118.45	110.14
1	A	606	VAL	N-CA-C	-5.39	104.00	108.63
1	A	266	MET	N-CA-C	-5.38	103.43	110.53
1	A	312	LEU	O-C-N	5.37	126.20	121.37
1	A	522	HIS	O-C-N	5.37	130.21	123.12
1	A	14	TRP	CA-C-O	5.36	127.23	121.55
1	A	310	THR	O-C-N	5.36	129.58	123.31
1	A	183	VAL	CA-C-O	-5.35	114.39	120.65
1	A	205	SER	CA-C-N	5.35	130.96	122.94
1	A	205	SER	C-N-CA	5.35	130.96	122.94
1	A	189	TYR	CA-C-N	5.34	131.79	122.81
1	A	189	TYR	C-N-CA	5.34	131.79	122.81
1	A	465	GLU	CA-C-O	5.34	126.13	120.36
1	A	552	GLN	CB-CG-CD	5.34	121.68	112.60
1	A	634	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	630	SER	CA-C-N	-5.34	113.89	121.85
1	A	630	SER	C-N-CA	-5.34	113.89	121.85
1	A	625	SER	O-C-N	5.33	128.46	122.22
1	A	259	SER	CA-C-N	5.33	129.85	122.77
1	A	259	SER	C-N-CA	5.33	129.85	122.77
1	A	64	ASN	OD1-CG-ND2	5.32	127.92	122.60
1	A	131	GLU	N-CA-C	-5.32	101.03	109.59
1	A	3	ALA	CA-C-O	-5.31	115.21	120.26
1	A	165	ILE	CB-CG1-CD1	5.31	124.95	113.80
1	A	68	LEU	CA-CB-CG	5.31	134.88	116.30
1	A	105	TRP	O-C-N	5.30	129.40	123.19
1	A	181	GLY	N-CA-C	-5.30	108.31	115.36
1	A	258	ASP	CA-C-N	-5.29	113.57	122.29
1	A	258	ASP	C-N-CA	-5.29	113.57	122.29
1	A	595	THR	CB-CA-C	5.27	118.73	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LEU	CA-C-O	-5.27	114.94	121.11
1	A	233	MET	N-CA-C	-5.26	100.60	108.96
1	A	300	GLU	CB-CG-CD	-5.25	103.68	112.60
1	A	428	THR	CA-CB-OG1	-5.23	101.75	109.60
1	A	300	GLU	N-CA-CB	5.22	121.24	111.52
1	A	356	TRP	CA-C-N	-5.22	115.36	122.93
1	A	356	TRP	C-N-CA	-5.22	115.36	122.93
1	A	229	PRO	N-CA-CB	-5.21	97.78	103.25
1	A	216	ASP	CB-CA-C	5.20	119.07	109.71
1	A	622	VAL	CA-C-O	-5.20	114.80	121.40
1	A	589	ARG	CA-C-N	-5.19	115.96	123.28
1	A	589	ARG	C-N-CA	-5.19	115.96	123.28
1	A	521	ASN	CA-C-N	-5.19	115.49	122.86
1	A	521	ASN	C-N-CA	-5.19	115.49	122.86
1	A	526	GLN	O-C-N	5.18	129.89	123.15
1	A	411	THR	CA-CB-CG2	5.17	119.30	110.50
1	A	270	ARG	N-CA-CB	-5.17	102.70	111.69
1	A	385	ASN	CA-C-N	-5.17	114.74	122.39
1	A	385	ASN	C-N-CA	-5.17	114.74	122.39
1	A	497	SER	CA-C-N	5.16	130.02	122.69
1	A	497	SER	C-N-CA	5.16	130.02	122.69
1	A	358	TYR	N-CA-CB	-5.16	102.26	111.08
1	A	392	VAL	CB-CA-C	5.15	118.77	112.02
1	A	91	SER	N-CA-C	-5.15	107.05	113.38
1	A	544	PRO	CA-C-O	-5.15	115.52	121.95
1	A	205	SER	O-C-N	-5.14	117.62	123.48
1	A	22	GLN	N-CA-CB	5.13	118.54	110.23
1	A	275	SER	N-CA-C	-5.13	101.40	109.50
1	A	447	LEU	N-CA-CB	-5.11	103.72	109.49
1	A	548	ARG	N-CA-C	5.10	117.47	108.75
1	A	154	PRO	N-CA-C	-5.10	103.11	111.21
1	A	234	ASP	CA-C-O	5.09	127.36	122.01
1	A	530	PRO	CB-CA-C	5.09	117.64	110.98
1	A	135	GLN	O-C-N	5.08	127.95	121.34
1	A	599	GLY	O-C-N	5.08	127.90	122.41
1	A	578	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	242	THR	N-CA-C	5.07	117.67	109.40
1	A	315	ALA	N-CA-C	-5.06	99.08	108.24
1	A	583	VAL	N-CA-CB	-5.06	105.01	110.53
1	A	176	ILE	CA-C-O	-5.06	115.16	120.57
1	A	220	THR	O-C-N	5.05	127.45	122.10
1	A	402	SER	CA-C-N	5.04	124.65	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	SER	C-N-CA	5.04	124.65	119.05
1	A	362	SER	O-C-N	5.04	128.82	122.37
1	A	200	GLY	CA-C-O	5.03	124.69	119.06
1	A	490	SER	CA-CB-OG	-5.02	101.06	111.10
1	A	9	ILE	CB-CG1-CD1	-5.01	103.28	113.80
1	A	201	ILE	O-C-N	5.01	128.61	123.05
1	A	315	ALA	CA-C-N	5.00	127.96	120.95
1	A	315	ALA	C-N-CA	5.00	127.96	120.95

There are no chirality outliers.

There are no planarity outliers.

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	4830	0	4604	99	1
2	A	1	0	0	0	0
3	A	310	0	0	6	1
All	All	5141	0	4604	99	2

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 10.

All (99) 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:22:GLN:HE21	1:A:46:ASN:HB2	1.32	0.93
1:A:35:LYS:HE3	1:A:71:LEU:HD21	1.58	0.82
1:A:22:GLN:NE2	1:A:46:ASN:HB2	1.92	0.82
1:A:417:ILE:HG12	1:A:428:THR:HG22	1.69	0.74
1:A:298:ASN:HD22	1:A:317:VAL:H	1.36	0.74
1:A:122:ARG:HD3	1:A:123:TYR:CE1	2.22	0.73
1:A:379:PRO:HD2	3:A:769:HOH:O	1.93	0.67
1:A:60:LYS:HA	1:A:122:ARG:HH21	1.60	0.65
1:A:73:ARG:HD3	1:A:77:ASN:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:HB3	1:A:498:ILE:HD13	1.78	0.64
1:A:32:ASP:OD2	1:A:37:THR:OG1	2.11	0.64
1:A:475:ILE:HD12	1:A:486:GLN:CD	2.24	0.62
1:A:298:ASN:ND2	1:A:317:VAL:H	1.96	0.61
1:A:340:TRP:CG	1:A:341:LYS:H	2.20	0.60
1:A:35:LYS:HE2	1:A:74:GLN:HG3	1.85	0.59
1:A:189:TYR:CD1	1:A:197:SER:HB2	2.38	0.58
1:A:552:GLN:HG3	3:A:961:HOH:O	2.04	0.57
1:A:495:TYR:O	1:A:496:HIS:HB2	2.04	0.57
1:A:30:ALA:HB3	1:A:55:TYR:OH	2.05	0.57
1:A:9:ILE:HD12	1:A:145:VAL:HG12	1.85	0.57
1:A:56:THR:HG21	1:A:125:ARG:HH21	1.70	0.56
1:A:21:ALA:HA	1:A:40:HIS:O	2.06	0.56
1:A:30:ALA:O	1:A:142:GLU:HA	2.05	0.56
1:A:71:LEU:HD12	1:A:72:PRO:HD2	1.87	0.55
1:A:171:PRO:HD2	1:A:511:GLY:HA2	1.89	0.55
1:A:174:ALA:HA	1:A:184:LEU:O	2.06	0.55
1:A:103:GLY:HA3	1:A:166:ASP:O	2.08	0.53
1:A:146:PHE:N	1:A:146:PHE:CD1	2.73	0.53
1:A:22:GLN:NE2	1:A:43:TYR:O	2.42	0.53
1:A:11:ARG:NH1	1:A:31:ILE:HA	2.23	0.52
1:A:170:VAL:HB	1:A:514:LEU:HD13	1.92	0.52
1:A:573:LEU:HG	1:A:592:LEU:HD11	1.92	0.52
1:A:59:MET:C	1:A:61:THR:H	2.18	0.52
1:A:38:PHE:HB3	1:A:141:ALA:HA	1.92	0.51
1:A:5:ILE:HD12	1:A:490:SER:HB3	1.93	0.51
1:A:548:ARG:O	1:A:562:ILE:HA	2.11	0.51
1:A:95:ASN:HD22	1:A:95:ASN:N	2.08	0.51
1:A:439:ARG:NH2	1:A:474:GLU:HG3	2.25	0.51
1:A:16:VAL:HG12	1:A:57:ILE:HG12	1.92	0.51
1:A:560:ILE:O	1:A:603:SER:HA	2.10	0.50
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.47	0.50
1:A:227:PHE:O	1:A:244:GLY:HA3	2.11	0.50
1:A:328:LEU:HA	1:A:331:SER:OG	2.11	0.50
1:A:228:CYS:N	1:A:229:PRO:HD3	2.26	0.50
1:A:174:ALA:CB	1:A:498:ILE:HD13	2.42	0.49
1:A:522:HIS:HD2	3:A:820:HOH:O	1.94	0.49
1:A:317:VAL:O	1:A:320:MET:HG2	2.13	0.48
1:A:539:ASN:HB3	3:A:893:HOH:O	2.13	0.48
1:A:522:HIS:CD2	3:A:820:HOH:O	2.66	0.48
1:A:94:THR:HB	1:A:95:ASN:HD22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TYR:HB2	1:A:201:ILE:HG23	1.96	0.48
1:A:225:ASP:CG	1:A:245:ASN:HD22	2.23	0.47
1:A:285:THR:O	1:A:299:GLY:HA2	2.14	0.47
1:A:401:GLY:O	1:A:411:THR:HG22	2.15	0.47
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.96	0.46
1:A:61:THR:O	1:A:122:ARG:HA	2.15	0.46
1:A:226:MET:HE1	1:A:260:TRP:CH2	2.50	0.46
1:A:39:TRP:O	1:A:139:SER:HA	2.14	0.46
1:A:177:GLU:HB2	1:A:180:SER:OG	2.15	0.46
1:A:235:GLY:HA3	1:A:281:GLY:HA3	1.96	0.46
1:A:624:ASN:OD1	1:A:626:ALA:HB3	2.15	0.46
1:A:275:SER:HA	1:A:284:PHE:O	2.16	0.45
1:A:51:PRO:HA	1:A:52:PRO:C	2.41	0.45
1:A:554:VAL:HG22	1:A:558:GLY:HA3	1.98	0.44
1:A:59:MET:HE2	1:A:124:VAL:HG23	1.98	0.44
1:A:298:ASN:ND2	1:A:316:LYS:HA	2.32	0.44
1:A:334:HIS:CE1	1:A:581:HIS:HB3	2.53	0.44
1:A:356:TRP:O	1:A:365:VAL:HA	2.17	0.44
1:A:123:TYR:CD1	1:A:123:TYR:N	2.84	0.43
1:A:298:ASN:HD22	1:A:317:VAL:N	2.11	0.43
1:A:402:SER:HB2	1:A:403:PRO:HD2	2.00	0.43
1:A:94:THR:HB	1:A:95:ASN:ND2	2.34	0.43
1:A:506:ARG:HD3	3:A:819:HOH:O	2.18	0.43
1:A:117:GLU:OE2	1:A:490:SER:HB2	2.19	0.43
1:A:173:ALA:O	1:A:185:MET:HA	2.18	0.43
1:A:425:SER:HA	1:A:426:PRO:HD2	1.81	0.42
1:A:554:VAL:CG2	1:A:558:GLY:HA3	2.49	0.42
1:A:70:MET:HE1	1:A:72:PRO:HG3	2.01	0.42
1:A:35:LYS:HE3	1:A:71:LEU:CD2	2.41	0.42
1:A:534:TYR:CE1	1:A:540:LEU:HD23	2.55	0.42
1:A:393:LYS:HB2	1:A:395:LYS:HG2	2.00	0.42
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.55	0.42
1:A:466:ASP:OD2	1:A:522:HIS:HE1	2.02	0.42
1:A:26:GLU:OE1	1:A:29:LYS:HE2	2.20	0.41
1:A:43:TYR:HA	1:A:48:ASP:OD1	2.21	0.41
1:A:59:MET:O	1:A:61:THR:HG22	2.19	0.41
1:A:122:ARG:HD3	1:A:123:TYR:HE1	1.81	0.41
1:A:346:PHE:CE2	1:A:348:ALA:HB2	2.56	0.41
1:A:479:GLU:H	1:A:479:GLU:CD	2.27	0.41
1:A:15:ALA:HB2	1:A:60:LYS:HZ2	1.86	0.41
1:A:61:THR:HG23	1:A:63:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:VAL:O	1:A:495:TYR:C	2.61	0.41
1:A:59:MET:O	1:A:60:LYS:HB2	2.21	0.41
1:A:270:ARG:HH11	1:A:270:ARG:HD3	1.63	0.40
1:A:398:THR:O	1:A:414:ALA:HA	2.21	0.40
1:A:95:ASN:N	1:A:95:ASN:ND2	2.69	0.40
1:A:261:ILE:HA	1:A:262:PRO:HD3	1.85	0.40
1:A:410:ALA:HB1	1:A:439:ARG:C	2.47	0.40
1:A:424:THR:O	1:A:426:PRO:HD3	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:ND2	1:A:548:ARG:NH1[3_545]	2.15	0.05
3:A:836:HOH:O	3:A:958:HOH:O[2_656]	2.17	0.03

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	637/639 (100%)	605 (95%)	28 (4%)	4 (1%)	21	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	514	LEU
1	A	494	VAL
1	A	229	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	526/526 (100%)	505 (96%)	21 (4%)	28	38

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	63	GLN
1	A	68	LEU
1	A	69	SER
1	A	91	SER
1	A	95	ASN
1	A	98	SER
1	A	229	PRO
1	A	256	SER
1	A	274	SER
1	A	490	SER
1	A	498	ILE
1	A	532	TYR
1	A	536	SER
1	A	542	THR
1	A	545	LYS
1	A	552	GLN
1	A	563	SER
1	A	574	ILE
1	A	595	THR
1	A	639	GLN

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

Mol	Chain	Res	Type
1	A	22	GLN
1	A	46	ASN
1	A	74	GLN
1	A	78	GLN

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Mol	Chain	Res	Type
1	A	95	ASN
1	A	238	GLN
1	A	298	ASN
1	A	355	ASN
1	A	372	GLN
1	A	413	ASN
1	A	522	HIS
1	A	552	GLN
1	A	597	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 1 ligands modelled in this entry, 1 is 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 ⓘ

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	639/639 (100%)	-0.99	1 (0%) 91 90	6, 21, 65, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLY	2.1

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	NA	A	702	1/1	0.97	0.02	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.