



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 1GOF / pdb_00001gof
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 : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

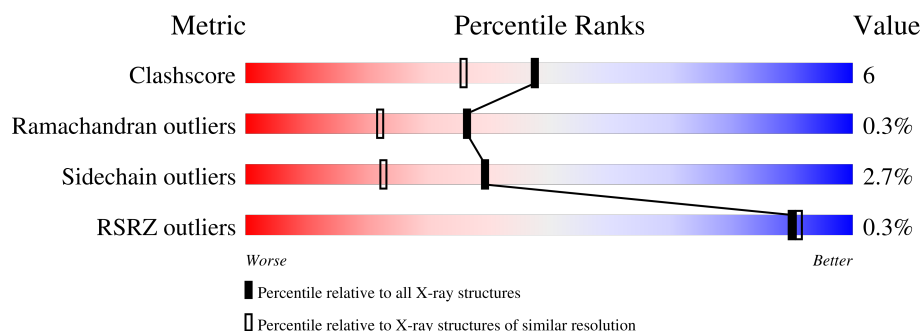
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5156 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			

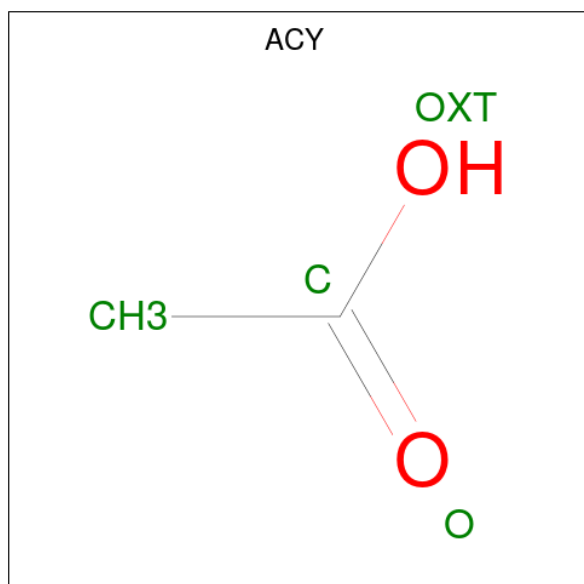
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

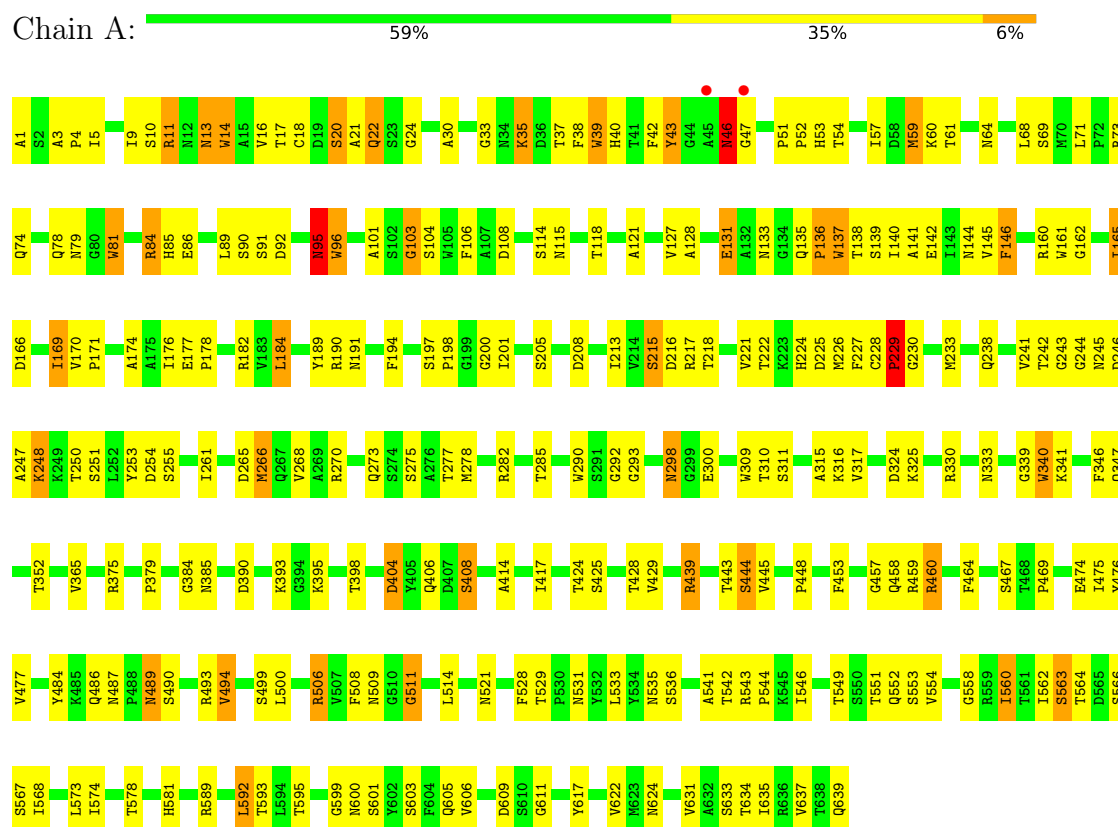
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	316	Total	O	0	0
			316	316		

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



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 – 1.70 10.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.70) 72.4 (10.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.70Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available) 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.1	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	5156	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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: CU, ACY, 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	1.39	6/4959 (0.1%)	2.38	290/6765 (4.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	PRO	C-N	-6.17	1.26	1.34
1	A	542	THR	CA-CB	5.47	1.61	1.53
1	A	5	ILE	CA-CB	5.24	1.61	1.54
1	A	609	ASP	N-CA	5.05	1.52	1.46
1	A	246	ASP	CA-C	5.01	1.59	1.53
1	A	508	PHE	CA-C	5.01	1.58	1.52

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	CD-NE-CZ	22.99	156.59	124.40
1	A	200	GLY	CA-C-O	13.76	134.10	119.10
1	A	200	GLY	N-CA-C	13.30	132.50	115.21
1	A	114	SER	N-CA-CB	12.57	129.94	110.84
1	A	216	ASP	CA-CB-CG	11.48	124.08	112.60
1	A	316	LYS	O-C-N	10.71	135.65	123.01
1	A	103	GLY	CA-C-O	-10.60	111.67	120.79
1	A	144	ASN	OD1-CG-ND2	10.25	132.85	122.60
1	A	118	THR	O-C-N	9.50	134.73	122.95
1	A	101	ALA	CA-C-O	-9.35	111.22	121.23
1	A	460	ARG	NE-CZ-NH2	-9.34	110.80	119.20
1	A	104	SER	O-C-N	9.25	134.00	123.27
1	A	622	VAL	CA-C-O	-9.22	109.15	121.32
1	A	493	ARG	NE-CZ-NH2	-9.14	110.97	119.20
1	A	384	GLY	N-CA-C	-9.10	98.59	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ASN	CA-C-O	-8.93	111.09	120.55
1	A	208	ASP	CA-CB-CG	-8.92	103.68	112.60
1	A	408	SER	N-CA-CB	-8.78	95.41	111.13
1	A	101	ALA	O-C-N	8.73	132.76	123.42
1	A	460	ARG	NH1-CZ-NH2	8.65	130.54	119.30
1	A	81	TRP	O-C-N	8.63	133.65	122.95
1	A	566	SER	O-C-N	8.54	132.55	123.42
1	A	605	GLN	CA-C-O	-8.51	111.69	120.71
1	A	511	GLY	O-C-N	8.45	130.94	122.91
1	A	310	THR	O-C-N	8.43	133.17	123.31
1	A	631	VAL	N-CA-C	-8.38	97.99	109.55
1	A	606	VAL	N-CA-CB	-8.33	99.55	111.21
1	A	133	ASN	OD1-CG-ND2	8.15	130.75	122.60
1	A	578	THR	CA-CB-OG1	-8.13	97.40	109.60
1	A	265	ASP	CA-CB-CG	8.08	120.68	112.60
1	A	3	ALA	O-C-N	8.06	130.64	122.17
1	A	541	ALA	CA-C-O	7.96	131.20	121.81
1	A	221	VAL	O-C-N	7.91	129.86	121.87
1	A	146	PHE	CA-CB-CG	-7.86	105.94	113.80
1	A	300	GLU	CB-CG-CD	-7.67	99.55	112.60
1	A	201	ILE	O-C-N	7.64	131.53	123.05
1	A	593	THR	CB-CA-C	7.63	122.92	109.72
1	A	553	SER	O-C-N	-7.62	114.36	123.27
1	A	633	SER	N-CA-CB	7.61	122.95	110.69
1	A	190	ARG	NE-CZ-NH1	7.57	129.07	121.50
1	A	38	PHE	N-CA-C	7.55	120.84	108.99
1	A	184	LEU	O-C-N	-7.50	114.79	123.27
1	A	246	ASP	O-C-N	7.50	131.84	122.84
1	A	18	CYS	CA-C-O	-7.42	112.76	121.44
1	A	136	PRO	N-CA-C	7.40	124.26	114.27
1	A	38	PHE	CA-CB-CG	7.40	121.20	113.80
1	A	293	GLY	N-CA-C	-7.40	104.92	111.95
1	A	104	SER	CA-C-O	-7.39	112.48	121.06
1	A	115	ASN	CA-C-O	-7.31	112.41	120.38
1	A	390	ASP	O-C-N	-7.28	114.83	123.28
1	A	128	ALA	CA-C-O	-7.26	112.99	120.54
1	A	24	GLY	N-CA-C	-7.26	106.05	114.69
1	A	230	GLY	N-CA-C	-7.23	99.59	112.54
1	A	131	GLU	N-CA-C	-7.23	97.91	109.76
1	A	543	ARG	CD-NE-CZ	7.21	134.49	124.40
1	A	460	ARG	CA-CB-CG	-7.21	99.69	114.10
1	A	558	GLY	CA-C-O	7.20	131.96	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ASP	CA-C-O	-7.14	112.82	120.46
1	A	261	ILE	CA-C-O	7.11	123.92	119.51
1	A	459	ARG	NE-CZ-NH1	7.09	128.59	121.50
1	A	330	ARG	NE-CZ-NH1	7.08	128.58	121.50
1	A	605	GLN	O-C-N	7.06	132.17	123.21
1	A	118	THR	CA-CB-OG1	-7.04	99.03	109.60
1	A	581	HIS	CE1-NE2-CD2	7.03	116.03	109.00
1	A	277	THR	CA-CB-OG1	-7.00	99.10	109.60
1	A	81	TRP	CA-C-O	-6.98	112.97	120.92
1	A	457	GLY	CA-C-O	6.98	131.15	122.78
1	A	213	ILE	O-C-N	6.93	130.50	122.81
1	A	64	ASN	CA-CB-CG	-6.91	105.69	112.60
1	A	560	ILE	CA-C-O	6.86	128.35	120.67
1	A	37	THR	O-C-N	6.85	131.91	123.21
1	A	424	THR	CA-CB-OG1	-6.83	99.35	109.60
1	A	324	ASP	CA-CB-CG	-6.80	105.80	112.60
1	A	309	TRP	CA-C-O	-6.74	113.03	120.38
1	A	486	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	A	141	ALA	CA-C-O	6.67	127.57	120.70
1	A	241	VAL	CA-C-N	-6.61	113.02	122.94
1	A	241	VAL	C-N-CA	-6.61	113.02	122.94
1	A	393	LYS	CA-C-N	6.56	133.06	120.66
1	A	393	LYS	C-N-CA	6.56	133.06	120.66
1	A	564	THR	CA-CB-OG1	-6.53	99.80	109.60
1	A	490	SER	O-C-N	6.51	129.89	122.20
1	A	611	GLY	N-CA-C	-6.50	106.60	114.66
1	A	352	THR	O-C-N	6.50	129.01	122.12
1	A	544	PRO	N-CA-C	-6.47	101.70	111.41
1	A	347	GLN	CA-C-O	-6.47	113.53	120.46
1	A	46	ASN	N-CA-C	-6.46	103.68	113.89
1	A	270	ARG	O-C-N	6.45	130.60	123.25
1	A	247	ALA	CA-C-O	-6.44	112.99	120.20
1	A	47	GLY	N-CA-C	-6.41	101.93	112.83
1	A	136	PRO	CB-CA-C	-6.41	101.36	111.04
1	A	600	ASN	CA-C-O	6.40	128.90	121.28
1	A	282	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	A	198	PRO	N-CA-C	-6.33	106.44	114.35
1	A	20	SER	N-CA-CB	6.32	122.69	111.69
1	A	489	ASN	OD1-CG-ND2	6.32	128.92	122.60
1	A	182	ARG	CA-CB-CG	-6.29	101.51	114.10
1	A	425	SER	CA-C-O	6.29	124.30	119.46
1	A	3	ALA	CA-C-O	-6.24	114.76	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	ASP	O-C-N	6.23	131.29	123.19
1	A	57	ILE	O-C-N	6.21	129.88	123.18
1	A	245	ASN	N-CA-CB	6.18	119.20	110.12
1	A	292	GLY	CA-C-O	-6.17	112.17	119.02
1	A	20	SER	CB-CA-C	-6.15	96.55	110.07
1	A	128	ALA	O-C-N	6.14	130.36	123.05
1	A	213	ILE	CB-CA-C	-6.14	103.17	111.15
1	A	169	ILE	CA-C-O	-6.13	115.64	121.64
1	A	476	TYR	CA-C-O	-6.10	113.78	120.43
1	A	218	THR	CA-CB-OG1	-6.06	100.51	109.60
1	A	106	PHE	CA-C-O	-6.04	115.15	121.55
1	A	429	VAL	CA-CB-CG2	6.02	120.64	110.40
1	A	213	ILE	N-CA-C	6.01	116.82	108.89
1	A	229	PRO	N-CA-CB	-6.00	96.95	103.25
1	A	635	ILE	N-CA-CB	-6.00	101.60	111.44
1	A	224	HIS	CA-CB-CG	5.99	119.79	113.80
1	A	33	GLY	N-CA-C	-5.98	106.83	115.27
1	A	133	ASN	CA-CB-CG	-5.96	106.64	112.60
1	A	458	GLN	OE1-CD-NE2	5.96	128.56	122.60
1	A	417	ILE	CA-C-O	-5.96	113.93	120.72
1	A	404	ASP	CA-C-O	-5.94	114.40	121.11
1	A	459	ARG	CD-NE-CZ	5.93	132.71	124.40
1	A	176	ILE	O-C-N	-5.92	115.96	122.83
1	A	91	SER	N-CA-C	-5.92	106.10	113.38
1	A	177	GLU	N-CA-C	-5.91	97.90	108.47
1	A	528	PHE	O-C-N	5.90	130.25	123.29
1	A	457	GLY	CA-C-N	5.90	131.77	122.21
1	A	457	GLY	C-N-CA	5.90	131.77	122.21
1	A	633	SER	N-CA-C	-5.90	100.09	109.59
1	A	221	VAL	CA-C-O	-5.90	114.26	120.57
1	A	589	ARG	CD-NE-CZ	-5.90	116.14	124.40
1	A	144	ASN	O-C-N	5.89	130.81	123.15
1	A	141	ALA	O-C-N	-5.87	115.75	122.09
1	A	238	GLN	OE1-CD-NE2	5.87	128.47	122.60
1	A	54	THR	N-CA-CB	-5.86	100.63	111.53
1	A	96	TRP	CA-CB-CG	-5.86	102.46	113.60
1	A	138	THR	CA-CB-OG1	-5.86	100.81	109.60
1	A	340	TRP	CA-C-N	-5.86	111.91	120.75
1	A	340	TRP	C-N-CA	-5.86	111.91	120.75
1	A	316	LYS	CA-C-N	-5.83	110.27	120.29
1	A	316	LYS	C-N-CA	-5.83	110.27	120.29
1	A	375	ARG	CD-NE-CZ	-5.83	116.24	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	THR	CA-CB-OG1	-5.80	100.90	109.60
1	A	567	SER	O-C-N	5.78	129.94	122.89
1	A	487	ASN	O-C-N	5.77	127.90	121.43
1	A	315	ALA	N-CA-C	-5.77	97.13	107.98
1	A	637	VAL	N-CA-CB	5.77	117.96	111.21
1	A	13	ASN	N-CA-C	5.75	120.03	113.19
1	A	443	THR	CA-CB-OG1	-5.75	100.98	109.60
1	A	563	SER	N-CA-CB	5.75	121.83	111.37
1	A	552	GLN	CB-CG-CD	5.72	122.33	112.60
1	A	592	LEU	CA-C-N	-5.72	115.11	123.00
1	A	592	LEU	C-N-CA	-5.72	115.11	123.00
1	A	595	THR	N-CA-C	-5.72	99.41	108.73
1	A	22	GLN	CA-CB-CG	-5.72	102.66	114.10
1	A	79	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	310	THR	CA-C-O	-5.72	113.97	120.32
1	A	395	LYS	O-C-N	5.71	129.73	123.27
1	A	217	ARG	CB-CG-CD	5.70	124.42	111.30
1	A	486	GLN	CA-C-N	-5.70	112.39	120.49
1	A	486	GLN	C-N-CA	-5.70	112.39	120.49
1	A	581	HIS	CG-CD2-NE2	-5.70	101.50	107.20
1	A	46	ASN	O-C-N	5.70	128.44	122.23
1	A	35	LYS	CA-CB-CG	5.69	125.49	114.10
1	A	178	PRO	O-C-N	5.69	129.06	122.23
1	A	340	TRP	O-C-N	5.69	131.56	122.11
1	A	593	THR	N-CA-C	-5.68	99.92	109.07
1	A	170	VAL	N-CA-C	-5.68	102.39	107.56
1	A	118	THR	CA-C-O	-5.68	114.44	120.92
1	A	222	THR	CA-CB-OG1	-5.67	101.09	109.60
1	A	339	GLY	N-CA-C	-5.66	103.84	111.54
1	A	270	ARG	N-CA-CB	-5.65	102.23	111.66
1	A	127	VAL	CA-C-O	5.64	126.56	120.53
1	A	43	TYR	N-CA-CB	5.63	120.45	111.56
1	A	551	THR	O-C-N	5.62	129.44	123.42
1	A	509	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	268	VAL	O-C-N	5.61	129.26	123.20
1	A	417	ILE	CA-C-N	-5.60	114.90	123.07
1	A	417	ILE	C-N-CA	-5.60	114.90	123.07
1	A	17	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	509	ASN	CA-C-N	-5.56	111.15	121.15
1	A	509	ASN	C-N-CA	-5.56	111.15	121.15
1	A	589	ARG	CA-C-N	-5.54	115.47	123.28
1	A	589	ARG	C-N-CA	-5.54	115.47	123.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	ASN	CB-CA-C	5.53	123.95	111.78
1	A	352	THR	CA-CB-OG1	-5.53	101.30	109.60
1	A	108	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	617	TYR	CA-C-O	-5.53	114.56	120.92
1	A	245	ASN	O-C-N	5.53	127.98	122.12
1	A	506	ARG	CD-NE-CZ	5.52	132.12	124.40
1	A	546	ILE	N-CA-C	-5.51	99.30	107.51
1	A	69	SER	CA-C-O	5.50	127.55	121.11
1	A	273	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	A	95	ASN	O-C-N	5.50	129.59	123.05
1	A	266	MET	CA-C-O	5.45	128.20	121.87
1	A	333	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	233	MET	N-CA-C	-5.44	100.30	108.96
1	A	278	MET	CA-C-O	-5.42	115.01	121.89
1	A	346	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	428	THR	OG1-CB-CG2	-5.41	98.47	109.30
1	A	499	SER	N-CA-CB	5.41	120.81	111.13
1	A	47	GLY	O-C-N	5.41	129.33	122.68
1	A	85	HIS	CA-CB-CG	-5.40	108.40	113.80
1	A	460	ARG	CD-NE-CZ	-5.40	116.83	124.40
1	A	325	LYS	O-C-N	-5.40	115.37	122.39
1	A	92	ASP	CB-CA-C	5.40	118.09	109.02
1	A	140	ILE	CA-C-O	-5.40	114.90	120.25
1	A	477	VAL	CA-CB-CG1	-5.40	101.22	110.40
1	A	266	MET	O-C-N	-5.40	116.64	122.79
1	A	11	ARG	CG-CD-NE	-5.38	100.16	112.00
1	A	53	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	86	GLU	OE1-CD-OE2	5.38	135.80	122.90
1	A	226	MET	N-CA-C	5.37	119.39	113.21
1	A	633	SER	CA-CB-OG	-5.37	100.36	111.10
1	A	22	GLN	N-CA-CB	5.37	118.16	110.06
1	A	266	MET	CA-CB-CG	-5.36	103.38	114.10
1	A	365	VAL	N-CA-C	-5.36	101.28	108.35
1	A	290	TRP	O-C-N	-5.36	116.44	122.12
1	A	509	ASN	N-CA-CB	-5.35	101.69	110.68
1	A	601	SER	O-C-N	5.34	129.66	123.30
1	A	1	ALA	CA-C-N	-5.34	114.33	122.23
1	A	1	ALA	C-N-CA	-5.34	114.33	122.23
1	A	121	ALA	CA-C-O	-5.32	115.53	121.23
1	A	222	THR	CB-CA-C	5.32	118.97	110.09
1	A	298	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	160	ARG	CD-NE-CZ	-5.32	116.95	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	SER	CA-CB-OG	-5.32	100.47	111.10
1	A	86	GLU	CA-C-O	-5.31	114.23	120.60
1	A	531	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	16	VAL	CA-C-N	5.29	130.87	122.94
1	A	16	VAL	C-N-CA	5.29	130.87	122.94
1	A	39	TRP	CA-C-O	5.29	127.08	121.16
1	A	544	PRO	CA-C-O	-5.29	115.31	122.08
1	A	53	HIS	CA-C-O	-5.27	115.16	121.11
1	A	106	PHE	CA-CB-CG	-5.26	108.54	113.80
1	A	121	ALA	O-C-N	5.26	129.04	123.42
1	A	634	THR	CA-CB-OG1	-5.25	101.72	109.60
1	A	218	THR	CA-C-N	-5.25	116.68	123.19
1	A	218	THR	C-N-CA	-5.25	116.68	123.19
1	A	106	PHE	N-CA-CB	-5.25	102.33	110.04
1	A	551	THR	CA-C-N	-5.25	114.10	122.29
1	A	551	THR	C-N-CA	-5.25	114.10	122.29
1	A	494	VAL	O-C-N	-5.25	116.01	122.57
1	A	531	ASN	CA-C-O	-5.24	113.15	119.49
1	A	599	GLY	O-C-N	5.23	128.06	122.41
1	A	521	ASN	O-C-N	5.23	129.16	123.04
1	A	261	ILE	N-CA-CB	-5.19	106.87	112.37
1	A	385	ASN	CB-CG-ND2	5.19	124.19	116.40
1	A	406	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	A	568	ILE	CB-CA-C	5.18	118.80	110.82
1	A	273	GLN	CB-CG-CD	5.17	121.38	112.60
1	A	233	MET	CA-CB-CG	-5.16	103.78	114.10
1	A	14	TRP	CA-C-N	5.16	130.04	122.77
1	A	14	TRP	C-N-CA	5.16	130.04	122.77
1	A	333	ASN	O-C-N	5.16	128.71	122.94
1	A	275	SER	N-CA-C	-5.14	101.37	109.50
1	A	566	SER	CA-CB-OG	5.14	121.37	111.10
1	A	379	PRO	CA-C-N	5.13	128.14	120.90
1	A	379	PRO	C-N-CA	5.13	128.14	120.90
1	A	311	SER	CA-C-O	-5.13	115.42	121.16
1	A	316	LYS	CA-C-O	-5.12	115.22	121.05
1	A	278	MET	O-C-N	5.10	128.76	122.84
1	A	273	GLN	CG-CD-NE2	5.09	124.04	116.40
1	A	293	GLY	O-C-N	5.08	128.16	122.87
1	A	16	VAL	N-CA-C	5.08	115.79	108.48
1	A	250	THR	CA-C-N	5.08	130.55	122.94
1	A	250	THR	C-N-CA	5.08	130.55	122.94
1	A	464	PHE	O-C-N	5.08	128.37	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LEU	O-C-N	5.07	129.79	123.19
1	A	165	ILE	CB-CA-C	-5.07	104.14	111.19
1	A	444	SER	N-CA-CB	-5.07	103.70	111.56
1	A	490	SER	N-CA-CB	-5.07	103.25	110.80
1	A	311	SER	N-CA-CB	-5.07	102.52	109.97
1	A	404	ASP	CA-CB-CG	-5.07	107.53	112.60
1	A	622	VAL	CA-C-N	5.06	130.53	122.94
1	A	622	VAL	C-N-CA	5.06	130.53	122.94
1	A	137	TRP	O-C-N	5.06	128.60	122.68
1	A	475	ILE	CA-CB-CG1	-5.06	101.80	110.40
1	A	486	GLN	CG-CD-NE2	5.06	123.98	116.40
1	A	500	LEU	O-C-N	5.05	129.13	123.27
1	A	243	GLY	O-C-N	5.03	127.98	122.60
1	A	445	VAL	CA-C-N	-5.03	115.88	122.37
1	A	445	VAL	C-N-CA	-5.03	115.88	122.37
1	A	535	ASN	N-CA-C	-5.03	102.57	110.17
1	A	59	MET	N-CA-C	-5.03	107.10	113.18
1	A	484	TYR	O-C-N	5.03	129.19	123.31
1	A	162	GLY	O-C-N	5.02	126.79	121.77
1	A	225	ASP	N-CA-C	-5.01	99.16	107.99
1	A	73	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	A	242	THR	N-CA-C	5.01	117.56	109.40
1	A	144	ASN	CA-C-O	-5.00	115.58	121.44

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	4603	53	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	6	0	0
5	A	316	0	0	1	0
All	All	5156	0	4609	53	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 6.

All (53) 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	1.33	0.93
1:A:22:GLN:NE2	1:A:46:ASN:HB2	1.98	0.79
1:A:35:LYS:HE3	1:A:71:LEU:HD21	1.67	0.74
1:A:298:ASN:HD22	1:A:317:VAL:H	1.39	0.68
1:A:22:GLN:NE2	1:A:43:TYR:O	2.27	0.67
1:A:22:GLN:HG3	1:A:42:PHE:HA	1.79	0.65
1:A:298:ASN:ND2	1:A:317:VAL:H	1.94	0.65
1:A:448:PRO:HA	1:A:574:ILE:HD11	1.83	0.61
1:A:59:MET:O	1:A:60:LYS:HB2	2.02	0.59
1:A:340:TRP:CG	1:A:341:LYS:H	2.21	0.58
1:A:35:LYS:HE2	1:A:74:GLN:HG3	1.86	0.57
1:A:22:GLN:NE2	1:A:43:TYR:H	2.05	0.55
1:A:171:PRO:HD2	1:A:511:GLY:HA2	1.91	0.53
1:A:78:GLN:HG2	1:A:81:TRP:CH2	2.46	0.51
1:A:529:THR:HG23	1:A:533:LEU:HD12	1.92	0.51
1:A:506:ARG:HD3	5:A:820:HOH:O	2.11	0.50
1:A:554:VAL:HG11	1:A:560:ILE:HD11	1.94	0.50
1:A:228:CYS:N	1:A:229:PRO:HD3	2.27	0.49
1:A:13:ASN:O	1:A:60:LYS:HG3	2.12	0.49
1:A:135:GLN:HB3	1:A:136:PRO:CD	2.42	0.49
1:A:404:ASP:HB2	1:A:408:SER:HB2	1.96	0.48
1:A:95:ASN:HD22	1:A:95:ASN:N	2.12	0.47
1:A:560:ILE:O	1:A:603:SER:HA	2.15	0.47
1:A:39:TRP:O	1:A:139:SER:HA	2.14	0.46
1:A:439:ARG:NH2	1:A:474:GLU:HG3	2.30	0.46
1:A:398:THR:O	1:A:414:ALA:HA	2.16	0.46
1:A:174:ALA:HA	1:A:184:LEU:O	2.16	0.46
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.52	0.45
1:A:573:LEU:HG	1:A:592:LEU:HD11	1.98	0.45
1:A:135:GLN:HB3	1:A:136:PRO:HD2	1.98	0.45
1:A:103:GLY:HA3	1:A:166:ASP:O	2.17	0.45
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.99	0.44
1:A:189:TYR:CD1	1:A:197:SER:HB2	2.51	0.44
1:A:11:ARG:HG2	1:A:14:TRP:CZ3	2.51	0.44
1:A:30:ALA:O	1:A:142:GLU:HA	2.18	0.44
1:A:59:MET:C	1:A:61:THR:H	2.26	0.44
1:A:146:PHE:N	1:A:146:PHE:CD1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PHE:O	1:A:244:GLY:HA3	2.18	0.44
1:A:248:LYS:HE3	1:A:266:MET:O	2.17	0.43
1:A:460:ARG:HH11	1:A:460:ARG:HD2	1.57	0.43
1:A:205:SER:HA	1:A:215:SER:O	2.18	0.43
1:A:298:ASN:HD22	1:A:317:VAL:N	2.11	0.43
1:A:253:TYR:CE2	1:A:255:SER:HA	2.54	0.42
1:A:11:ARG:HG2	1:A:14:TRP:CH2	2.55	0.42
1:A:467:SER:C	1:A:469:PRO:HD3	2.45	0.41
1:A:9:ILE:HD12	1:A:145:VAL:HG12	2.01	0.41
1:A:131:GLU:HG3	1:A:137:TRP:O	2.21	0.41
1:A:21:ALA:HA	1:A:40:HIS:O	2.21	0.41
1:A:194:PHE:CD1	1:A:194:PHE:C	2.98	0.41
1:A:549:THR:HG22	1:A:562:ILE:HG22	2.02	0.41
1:A:51:PRO:HA	1:A:52:PRO:C	2.46	0.40
1:A:444:SER:HA	1:A:453:PHE:O	2.21	0.40
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.57	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	637/639 (100%)	609 (96%)	26 (4%)	2 (0%)	36 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	LEU
1	A	494	VAL

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%)	512 (97%)	14 (3%)	39	23

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	20	SER
1	A	46	ASN
1	A	68	LEU
1	A	84	ARG
1	A	95	ASN
1	A	165	ILE
1	A	215	SER
1	A	229	PRO
1	A	248	LYS
1	A	439	ARG
1	A	536	SER
1	A	563	SER
1	A	639	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	22	GLN
1	A	25	ASN
1	A	46	ASN
1	A	63	GLN
1	A	78	GLN
1	A	95	ASN
1	A	267	GLN
1	A	298	ASN
1	A	355	ASN
1	A	372	GLN

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Mol	Chain	Res	Type
1	A	413	ASN
1	A	537	ASN
1	A	600	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACY	A	701	-	3,3,3	1.46	0	3,3,3	1.26	0
4	ACY	A	703	2	3,3,3	1.08	0	3,3,3	1.99	2 (66%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	ACY	OXT-C-O	2.67	131.95	122.03
4	A	703	ACY	O-C-CH3	-2.15	113.72	122.53

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

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%)	-0.72	2 (0%) 90 91	6, 18, 57, 98	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLY	2.4
1	A	45	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(Å ²)	Q<0.9
3	NA	A	702	1/1	0.91	0.05	22,22,22,22	0
4	ACY	A	703	4/4	0.95	0.10	18,28,39,40	0
4	ACY	A	701	4/4	0.99	0.02	9,11,13,14	0
2	CU	A	700	1/1	0.99	0.04	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.