



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 10:21 PM EDT

PDB ID : 1GOG / pdb_00001gog
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 : 1.90 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

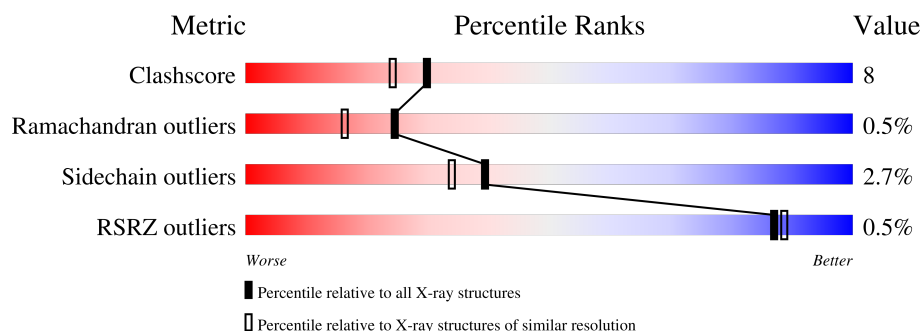
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 4 unique types of molecules in this entry. The entry contains 5142 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		

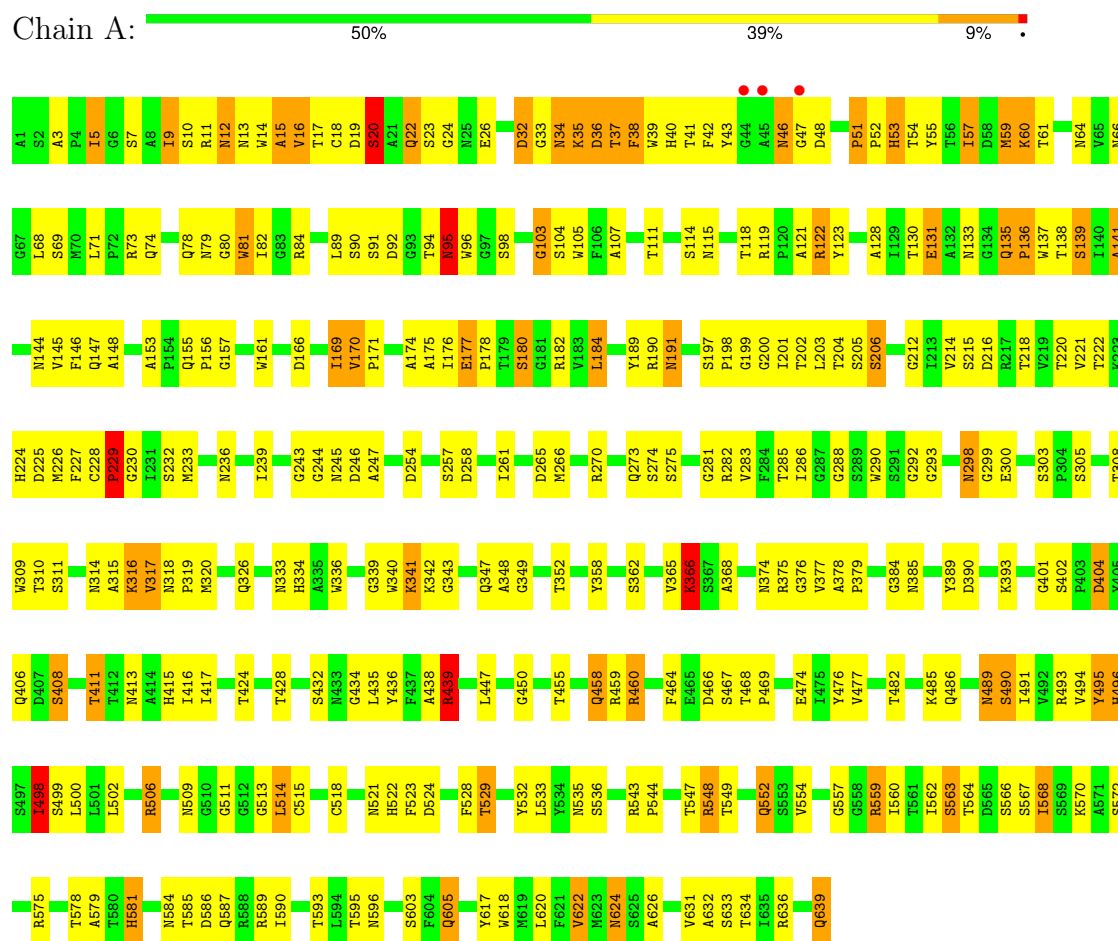
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	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



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 – 1.90 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 83.0 (10.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.90Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.170 , (Not available) 0.142 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.0	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	5142	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 6.65% 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, 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	1.45	15/4959 (0.3%)	2.53	383/6765 (5.7%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	581	HIS	CE1-NE2	-7.09	1.25	1.32
1	A	590	ILE	N-CA	7.06	1.52	1.46
1	A	115	ASN	N-CA	6.46	1.53	1.46
1	A	347	GLN	N-CA	6.26	1.53	1.46
1	A	216	ASP	N-CA	5.61	1.52	1.45
1	A	300	GLU	N-CA	5.49	1.52	1.45
1	A	624	ASN	N-CA	5.49	1.52	1.45
1	A	5	ILE	CA-CB	5.47	1.61	1.54
1	A	170	VAL	N-CA	5.27	1.50	1.46
1	A	376	GLY	N-CA	5.18	1.51	1.45
1	A	146	PHE	N-CA	5.14	1.52	1.45
1	A	415	HIS	CA-CB	5.12	1.63	1.54
1	A	33	GLY	N-CA	5.06	1.52	1.45
1	A	202	THR	CA-CB	5.04	1.62	1.53
1	A	460	ARG	N-CA	5.01	1.52	1.46

All (383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ARG	CD-NE-CZ	14.87	145.22	124.40
1	A	566	SER	O-C-N	11.88	136.13	123.42
1	A	114	SER	N-CA-CB	11.16	127.80	110.84
1	A	265	ASP	CA-CB-CG	10.89	123.49	112.60
1	A	66	ASN	CA-CB-CG	10.86	123.46	112.60
1	A	631	VAL	N-CA-C	-10.84	98.24	110.05
1	A	486	GLN	OE1-CD-NE2	-10.73	111.87	122.60
1	A	216	ASP	CB-CA-C	10.64	130.30	109.33
1	A	84	ARG	NE-CZ-NH2	-10.08	110.13	119.20
1	A	333	ASN	O-C-N	9.62	133.71	122.94
1	A	247	ALA	CA-C-O	-9.47	109.59	120.20
1	A	141	ALA	CA-C-O	9.37	130.55	120.90
1	A	460	ARG	NH1-CZ-NH2	9.36	131.47	119.30
1	A	146	PHE	CA-CB-CG	-8.97	104.83	113.80
1	A	384	GLY	N-CA-C	-8.83	99.01	112.51
1	A	38	PHE	CA-CB-CG	8.71	122.51	113.80
1	A	98	SER	N-CA-CB	-8.64	99.57	110.03
1	A	36	ASP	O-C-N	8.37	133.92	122.46
1	A	64	ASN	OD1-CG-ND2	8.35	130.95	122.60
1	A	617	TYR	O-C-N	8.26	132.74	123.16
1	A	200	GLY	CA-C-O	8.25	128.30	119.06
1	A	118	THR	O-C-N	8.16	133.07	122.95
1	A	521	ASN	CA-CB-CG	-8.15	104.45	112.60
1	A	3	ALA	O-C-N	8.14	129.12	121.71
1	A	176	ILE	CA-C-O	-8.14	111.51	120.71
1	A	605	GLN	OE1-CD-NE2	8.14	130.74	122.60
1	A	274	SER	CA-C-O	-8.00	111.89	121.66
1	A	73	ARG	NE-CZ-NH1	7.99	129.49	121.50
1	A	144	ASN	OD1-CG-ND2	7.98	130.58	122.60
1	A	286	ILE	O-C-N	7.94	129.88	122.97
1	A	564	THR	CA-CB-OG1	-7.94	97.69	109.60
1	A	57	ILE	O-C-N	7.93	131.75	123.18
1	A	557	GLY	CA-C-N	7.92	129.48	120.53
1	A	557	GLY	C-N-CA	7.92	129.48	120.53
1	A	24	GLY	N-CA-C	-7.89	105.30	114.69
1	A	215	SER	CA-CB-OG	7.88	126.86	111.10
1	A	408	SER	N-CA-CB	-7.80	97.03	111.53
1	A	261	ILE	CA-C-O	7.79	124.34	119.51
1	A	460	ARG	NE-CZ-NH2	-7.71	112.26	119.20
1	A	81	TRP	CA-C-O	-7.70	112.14	120.92
1	A	138	THR	CA-CB-OG1	-7.70	98.05	109.60
1	A	273	GLN	OE1-CD-NE2	-7.67	114.94	122.60
1	A	300	GLU	CB-CG-CD	-7.60	99.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	GLU	CB-CG-CD	7.59	125.50	112.60
1	A	178	PRO	O-C-N	7.58	131.33	122.23
1	A	201	ILE	O-C-N	7.57	131.88	123.09
1	A	498	ILE	O-C-N	7.57	131.07	122.82
1	A	216	ASP	CA-CB-CG	7.54	120.14	112.60
1	A	107	ALA	CA-C-O	-7.54	113.29	122.41
1	A	543	ARG	NE-CZ-NH2	-7.52	112.43	119.20
1	A	95	ASN	O-C-N	7.50	131.98	123.05
1	A	169	ILE	CA-C-N	-7.49	117.19	122.59
1	A	169	ILE	C-N-CA	-7.49	117.19	122.59
1	A	104	SER	CA-C-O	-7.46	112.38	121.11
1	A	377	VAL	CA-C-O	-7.45	112.24	121.11
1	A	170	VAL	CA-C-O	-7.43	114.77	119.15
1	A	229	PRO	N-CA-CB	-7.43	95.45	103.25
1	A	524	ASP	CA-CB-CG	7.43	120.03	112.60
1	A	639	GLN	OE1-CD-NE2	7.43	130.03	122.60
1	A	506	ARG	CD-NE-CZ	7.34	134.68	124.40
1	A	82	ILE	CA-C-O	-7.32	112.10	120.74
1	A	190	ARG	NE-CZ-NH2	-7.32	112.61	119.20
1	A	375	ARG	CA-C-O	-7.31	110.44	119.28
1	A	205	SER	O-C-N	-7.30	114.87	123.41
1	A	33	GLY	N-CA-C	-7.29	104.99	115.27
1	A	51	PRO	CB-CA-C	7.27	119.79	110.92
1	A	352	THR	O-C-N	7.24	129.80	122.12
1	A	424	THR	CA-CB-OG1	-7.21	98.79	109.60
1	A	69	SER	CA-C-O	7.19	129.23	121.11
1	A	460	ARG	CA-CB-CG	-7.07	99.96	114.10
1	A	316	LYS	O-C-N	7.06	131.30	123.04
1	A	495	TYR	N-CA-CB	-7.04	98.50	109.69
1	A	436	TYR	N-CA-C	-7.01	103.72	111.36
1	A	236	ASN	OD1-CG-ND2	7.00	129.60	122.60
1	A	82	ILE	O-C-N	6.99	130.66	122.83
1	A	389	TYR	CA-C-O	-6.98	110.87	119.18
1	A	524	ASP	N-CA-CB	-6.97	100.10	110.97
1	A	38	PHE	N-CA-C	6.94	119.99	109.23
1	A	493	ARG	NE-CZ-NH2	-6.93	112.97	119.20
1	A	634	THR	CA-CB-OG1	-6.91	99.23	109.60
1	A	243	GLY	CA-C-N	-6.89	114.84	121.31
1	A	243	GLY	C-N-CA	-6.89	114.84	121.31
1	A	593	THR	CB-CA-C	6.88	121.10	109.75
1	A	104	SER	O-C-N	6.87	131.69	123.24
1	A	48	ASP	O-C-N	6.87	127.67	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	GLY	CA-C-O	-6.83	108.69	120.57
1	A	595	THR	CA-CB-OG1	-6.82	99.37	109.60
1	A	490	SER	N-CA-CB	-6.82	100.64	110.80
1	A	587	GLN	OE1-CD-NE2	6.80	129.40	122.60
1	A	46	ASN	N-CA-C	-6.78	104.91	113.72
1	A	20	SER	CB-CA-C	-6.75	95.93	110.45
1	A	141	ALA	O-C-N	-6.75	114.74	122.03
1	A	273	GLN	CG-CD-NE2	6.75	126.52	116.40
1	A	589	ARG	CA-C-N	-6.74	113.78	123.28
1	A	589	ARG	C-N-CA	-6.74	113.78	123.28
1	A	20	SER	N-CA-CB	6.72	122.89	111.66
1	A	7	SER	CA-C-O	6.72	127.83	120.71
1	A	432	SER	N-CA-CB	-6.72	99.14	110.49
1	A	54	THR	N-CA-CB	-6.69	99.16	111.13
1	A	636	ARG	CA-C-N	6.68	131.80	123.12
1	A	636	ARG	C-N-CA	6.68	131.80	123.12
1	A	226	MET	N-CA-C	6.67	120.88	113.21
1	A	310	THR	O-C-N	6.67	131.11	123.31
1	A	224	HIS	N-CA-CB	-6.66	99.62	110.81
1	A	341	LYS	CA-C-O	6.63	128.78	121.56
1	A	513	GLY	O-C-N	6.63	131.31	122.70
1	A	221	VAL	O-C-N	6.61	128.55	121.87
1	A	288	GLY	O-C-N	6.56	131.22	122.70
1	A	404	ASP	CA-CB-CG	-6.55	106.05	112.60
1	A	529	THR	CA-C-O	6.55	125.61	119.59
1	A	122	ARG	N-CA-C	-6.52	105.86	113.88
1	A	309	TRP	CA-C-O	-6.51	113.28	120.38
1	A	368	ALA	N-CA-C	-6.51	103.94	112.41
1	A	310	THR	CA-CB-OG1	-6.50	99.85	109.60
1	A	411	THR	OG1-CB-CG2	-6.50	96.30	109.30
1	A	320	MET	CA-C-O	-6.50	111.75	119.35
1	A	190	ARG	NE-CZ-NH1	6.49	127.98	121.50
1	A	212	GLY	N-CA-C	-6.49	106.73	115.36
1	A	390	ASP	CB-CA-C	6.48	120.76	111.82
1	A	339	GLY	N-CA-C	-6.47	102.74	111.54
1	A	385	ASN	OD1-CG-ND2	6.47	129.07	122.60
1	A	107	ALA	O-C-N	6.46	130.91	122.38
1	A	365	VAL	N-CA-C	-6.45	99.84	108.35
1	A	568	ILE	CB-CA-C	6.44	120.60	110.81
1	A	18	CYS	O-C-N	6.44	131.52	123.15
1	A	634	THR	OG1-CB-CG2	6.44	122.17	109.30
1	A	455	THR	N-CA-CB	-6.43	100.91	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	ARG	NH1-CZ-NH2	6.43	127.67	119.30
1	A	333	ASN	CB-CG-ND2	6.43	126.05	116.40
1	A	417	ILE	O-C-N	6.43	129.70	123.14
1	A	32	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	180	SER	CA-C-O	-6.43	112.07	119.14
1	A	55	TYR	CA-C-O	-6.42	113.43	120.24
1	A	435	LEU	O-C-N	6.40	130.09	122.79
1	A	136	PRO	CB-CA-C	-6.39	101.01	111.56
1	A	459	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	A	199	GLY	CA-C-O	-6.37	109.48	120.57
1	A	184	LEU	CA-C-O	6.35	127.15	120.36
1	A	119	ARG	CD-NE-CZ	6.34	133.28	124.40
1	A	221	VAL	CA-C-O	-6.34	113.78	120.57
1	A	417	ILE	CA-C-N	-6.34	114.06	123.00
1	A	417	ILE	C-N-CA	-6.34	114.06	123.00
1	A	447	LEU	CA-C-N	6.33	126.53	119.32
1	A	447	LEU	C-N-CA	6.33	126.53	119.32
1	A	458	GLN	CA-C-O	6.31	128.53	121.40
1	A	406	GLN	OE1-CD-NE2	-6.30	116.30	122.60
1	A	135	GLN	O-C-N	6.29	126.97	120.99
1	A	549	THR	N-CA-CB	6.28	120.63	110.77
1	A	589	ARG	O-C-N	6.28	130.93	123.27
1	A	366	LYS	CA-C-N	6.27	129.77	120.87
1	A	366	LYS	C-N-CA	6.27	129.77	120.87
1	A	273	GLN	CB-CG-CD	6.27	123.25	112.60
1	A	496	HIS	CA-CB-CG	-6.26	107.53	113.80
1	A	47	GLY	N-CA-C	-6.23	103.59	112.81
1	A	205	SER	CA-C-N	6.21	132.26	122.94
1	A	205	SER	C-N-CA	6.21	132.26	122.94
1	A	311	SER	CA-C-O	-6.20	114.22	121.16
1	A	115	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	A	438	ALA	CA-C-O	6.19	128.00	121.19
1	A	622	VAL	CA-C-O	-6.18	113.17	121.32
1	A	233	MET	N-CA-C	-6.18	98.66	108.73
1	A	10	SER	N-CA-CB	6.17	119.20	109.71
1	A	352	THR	CA-C-O	-6.16	114.02	120.55
1	A	498	ILE	CA-C-O	-6.16	115.29	121.45
1	A	586	ASP	CA-C-O	-6.15	112.50	120.00
1	A	570	LYS	N-CA-CB	-6.14	101.00	111.69
1	A	178	PRO	CA-C-O	-6.14	110.28	119.86
1	A	559	ARG	CD-NE-CZ	-6.14	115.81	124.40
1	A	326	GLN	CA-CB-CG	6.13	126.36	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	GLN	CG-CD-NE2	-6.12	107.22	116.40
1	A	413	ASN	CA-CB-CG	6.11	118.71	112.60
1	A	482	THR	O-C-N	6.10	130.71	123.33
1	A	200	GLY	N-CA-C	6.09	123.73	115.32
1	A	518	CYS	CA-C-N	-6.08	113.11	122.60
1	A	518	CYS	C-N-CA	-6.08	113.11	122.60
1	A	447	LEU	CD1-CG-CD2	-6.08	97.43	110.80
1	A	348	ALA	CA-C-O	-6.06	111.35	119.11
1	A	506	ARG	O-C-N	-6.06	115.59	122.68
1	A	290	TRP	CA-C-O	6.06	126.97	120.55
1	A	536	SER	N-CA-C	6.06	118.66	111.33
1	A	450	GLY	O-C-N	6.05	130.34	122.42
1	A	459	ARG	CA-C-O	-6.04	111.81	119.31
1	A	104	SER	CA-CB-OG	-6.04	99.03	111.10
1	A	566	SER	CA-C-O	-6.03	114.78	121.23
1	A	22	GLN	CA-CB-CG	-6.03	102.04	114.10
1	A	390	ASP	OD1-CG-OD2	6.03	137.37	122.90
1	A	254	ASP	CA-C-O	-6.03	114.27	120.54
1	A	81	TRP	O-C-N	6.00	130.38	122.95
1	A	385	ASN	CB-CG-OD1	-5.99	108.81	120.80
1	A	544	PRO	N-CA-C	-5.99	101.68	111.21
1	A	89	LEU	O-C-N	5.99	130.61	123.24
1	A	311	SER	N-CA-CB	-5.99	101.17	109.97
1	A	80	GLY	CA-C-O	-5.96	112.39	119.01
1	A	366	LYS	N-CA-CB	-5.96	100.22	111.00
1	A	286	ILE	CA-C-O	-5.96	115.96	120.96
1	A	258	ASP	CA-C-N	-5.94	112.59	122.21
1	A	258	ASP	C-N-CA	-5.94	112.59	122.21
1	A	622	VAL	CA-C-N	5.93	131.84	122.94
1	A	622	VAL	C-N-CA	5.93	131.84	122.94
1	A	169	ILE	O-C-N	5.93	129.52	123.00
1	A	245	ASN	CA-C-O	-5.93	113.40	120.10
1	A	584	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	366	LYS	O-C-N	-5.92	116.05	123.27
1	A	15	ALA	CA-C-O	-5.92	113.97	120.24
1	A	26	GLU	CA-CB-CG	5.92	125.93	114.10
1	A	333	ASN	CA-C-O	-5.91	114.75	121.72
1	A	535	ASN	N-CA-C	-5.90	101.26	110.17
1	A	275	SER	N-CA-C	-5.89	100.19	109.50
1	A	122	ARG	NH1-CZ-NH2	-5.89	111.65	119.30
1	A	111	THR	CA-CB-OG1	-5.89	100.77	109.60
1	A	552	GLN	CB-CG-CD	5.88	122.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	GLU	CB-CG-CD	5.88	122.60	112.60
1	A	428	THR	OG1-CB-CG2	-5.88	97.54	109.30
1	A	375	ARG	CA-C-N	-5.87	113.18	122.92
1	A	375	ARG	C-N-CA	-5.87	113.18	122.92
1	A	581	HIS	CA-CB-CG	-5.87	107.94	113.80
1	A	523	PHE	CA-C-N	-5.86	112.01	122.32
1	A	523	PHE	C-N-CA	-5.86	112.01	122.32
1	A	270	ARG	CB-CA-C	-5.85	97.87	110.45
1	A	64	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	490	SER	O-C-N	5.84	129.09	122.20
1	A	572	SER	N-CA-CB	-5.83	101.92	111.66
1	A	18	CYS	CA-C-O	-5.83	114.62	121.44
1	A	292	GLY	CA-C-O	-5.83	112.02	119.13
1	A	147	GLN	O-C-N	5.82	130.39	123.24
1	A	191	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	59	MET	CA-C-O	-5.79	111.54	119.12
1	A	315	ALA	N-CA-C	-5.78	96.36	107.57
1	A	490	SER	CA-CB-OG	-5.76	99.58	111.10
1	A	489	ASN	CA-CB-CG	-5.75	106.85	112.60
1	A	639	GLN	N-CA-CB	5.75	120.28	110.50
1	A	352	THR	CA-CB-OG1	-5.74	100.98	109.60
1	A	485	LYS	O-C-N	-5.74	116.09	122.86
1	A	491	ILE	O-C-N	5.73	129.19	123.18
1	A	579	ALA	O-C-N	5.72	130.10	123.41
1	A	290	TRP	O-C-N	-5.72	116.06	122.12
1	A	299	GLY	O-C-N	5.72	131.16	122.69
1	A	16	VAL	CA-C-N	5.71	131.99	122.73
1	A	16	VAL	C-N-CA	5.71	131.99	122.73
1	A	460	ARG	CB-CA-C	5.70	120.02	109.70
1	A	40	HIS	CA-CB-CG	5.70	119.50	113.80
1	A	310	THR	CA-C-O	-5.69	114.00	120.32
1	A	92	ASP	N-CA-C	5.68	121.09	114.04
1	A	175	ALA	CA-C-O	-5.68	115.19	121.33
1	A	133	ASN	OD1-CG-ND2	5.68	128.28	122.60
1	A	103	GLY	O-C-N	5.67	130.07	122.70
1	A	477	VAL	O-C-N	5.63	127.52	121.10
1	A	336	TRP	CA-C-O	-5.63	115.90	122.37
1	A	535	ASN	CA-C-N	5.62	128.08	120.38
1	A	535	ASN	C-N-CA	5.62	128.08	120.38
1	A	115	ASN	CA-C-O	-5.61	114.76	120.71
1	A	233	MET	CA-C-O	-5.61	114.36	120.36
1	A	305	SER	CB-CA-C	5.61	120.21	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	A	270	ARG	N-CA-CB	-5.58	102.33	111.66
1	A	416	ILE	CA-C-O	-5.57	114.57	120.53
1	A	578	THR	CA-C-N	-5.57	112.14	121.94
1	A	578	THR	C-N-CA	-5.57	112.14	121.94
1	A	57	ILE	CA-CB-CG2	5.57	119.97	110.50
1	A	222	THR	CA-C-O	-5.56	112.85	119.35
1	A	343	GLY	O-C-N	5.56	129.35	122.41
1	A	261	ILE	CB-CG1-CD1	-5.55	102.14	113.80
1	A	548	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	A	318	ASN	CA-CB-CG	-5.55	107.05	112.60
1	A	585	THR	CA-C-O	5.54	125.99	119.28
1	A	314	ASN	CB-CG-ND2	5.53	124.69	116.40
1	A	460	ARG	CD-NE-CZ	-5.52	116.67	124.40
1	A	55	TYR	O-C-N	5.52	129.73	123.27
1	A	182	ARG	N-CA-CB	-5.51	102.07	110.45
1	A	205	SER	CB-CA-C	5.51	120.59	109.68
1	A	434	GLY	CA-C-O	-5.50	116.18	122.78
1	A	633	SER	N-CA-CB	5.49	119.53	110.69
1	A	563	SER	N-CA-C	-5.49	100.94	109.72
1	A	128	ALA	CA-C-O	-5.49	114.71	120.58
1	A	257	SER	CA-CB-OG	5.49	122.07	111.10
1	A	258	ASP	N-CA-CB	5.47	119.80	111.70
1	A	293	GLY	O-C-N	5.47	128.56	122.87
1	A	509	ASN	CA-C-N	-5.47	111.31	121.15
1	A	509	ASN	C-N-CA	-5.47	111.31	121.15
1	A	220	THR	CA-C-O	5.46	124.78	118.55
1	A	417	ILE	CA-CB-CG1	-5.46	101.11	110.40
1	A	130	THR	N-CA-CB	5.46	120.47	111.62
1	A	316	LYS	N-CA-CB	-5.46	101.48	109.95
1	A	581	HIS	CB-CA-C	-5.44	103.86	111.80
1	A	239	ILE	CA-CB-CG1	-5.44	101.16	110.40
1	A	581	HIS	CE1-NE2-CD2	5.44	114.44	109.00
1	A	578	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	128	ALA	N-CA-C	-5.42	99.69	108.41
1	A	581	HIS	N-CA-C	5.41	118.90	111.54
1	A	34	ASN	O-C-N	5.40	130.25	123.12
1	A	169	ILE	CA-C-O	-5.40	116.16	121.67
1	A	266	MET	N-CA-C	-5.40	103.41	110.53
1	A	19	ASP	CA-C-N	5.39	131.07	121.75
1	A	19	ASP	C-N-CA	5.39	131.07	121.75
1	A	122	ARG	CD-NE-CZ	5.37	131.91	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	PRO	N-CA-CB	5.36	108.45	103.41
1	A	261	ILE	N-CA-CB	-5.35	106.70	112.37
1	A	496	HIS	CE1-NE2-CD2	5.35	114.35	109.00
1	A	300	GLU	N-CA-CB	5.35	120.59	111.66
1	A	246	ASP	O-C-N	5.34	129.25	122.84
1	A	281	GLY	CA-C-O	-5.34	113.72	119.27
1	A	89	LEU	CA-C-O	-5.34	114.87	121.11
1	A	362	SER	O-C-N	5.33	129.19	122.37
1	A	53	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	64	ASN	CA-C-N	5.32	128.31	120.91
1	A	64	ASN	C-N-CA	5.32	128.31	120.91
1	A	283	VAL	CA-CB-CG2	5.32	119.45	110.40
1	A	203	LEU	O-C-N	5.32	129.25	123.13
1	A	585	THR	CA-CB-OG1	-5.32	101.62	109.60
1	A	596	ASN	O-C-N	5.30	129.29	122.93
1	A	299	GLY	CA-C-N	-5.29	112.60	121.75
1	A	299	GLY	C-N-CA	-5.29	112.60	121.75
1	A	222	THR	O-C-N	5.29	128.95	122.34
1	A	282	ARG	CA-CB-CG	-5.29	103.52	114.10
1	A	216	ASP	CA-C-O	5.28	127.08	121.11
1	A	118	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	233	MET	CA-CB-CG	-5.28	103.54	114.10
1	A	3	ALA	N-CA-CB	-5.27	105.57	111.10
1	A	84	ARG	NH1-CZ-NH2	5.26	126.14	119.30
1	A	349	GLY	N-CA-C	-5.26	101.60	112.34
1	A	184	LEU	O-C-N	-5.26	117.22	123.22
1	A	567	SER	CA-C-N	-5.26	116.31	123.10
1	A	567	SER	C-N-CA	-5.26	116.31	123.10
1	A	566	SER	CA-CB-OG	5.26	121.62	111.10
1	A	389	TYR	O-C-N	5.26	129.88	122.41
1	A	131	GLU	N-CA-C	-5.25	101.14	109.59
1	A	153	ALA	O-C-N	5.24	126.70	121.30
1	A	136	PRO	N-CA-C	5.24	123.26	112.47
1	A	40	HIS	CB-CG-ND1	5.23	130.55	122.70
1	A	292	GLY	O-C-N	5.23	128.95	122.41
1	A	544	PRO	O-C-N	5.23	129.50	123.01
1	A	460	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	A	342	LYS	CA-C-O	-5.22	115.78	121.84
1	A	204	THR	OG1-CB-CG2	5.22	119.73	109.30
1	A	490	SER	CA-C-O	-5.21	113.03	119.18
1	A	298	ASN	CA-CB-CG	-5.20	107.40	112.60
1	A	37	THR	CA-CB-OG1	-5.19	101.81	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	THR	CA-CB-OG1	-5.18	101.82	109.60
1	A	35	LYS	CA-CB-CG	5.18	124.46	114.10
1	A	157	GLY	CA-C-O	-5.17	113.28	119.02
1	A	9	ILE	CB-CG1-CD1	-5.17	102.94	113.80
1	A	282	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	A	303	SER	CA-CB-OG	-5.16	100.79	111.10
1	A	317	VAL	O-C-N	-5.16	115.01	122.12
1	A	230	GLY	N-CA-C	-5.14	102.53	111.62
1	A	198	PRO	N-CA-C	-5.13	107.94	114.35
1	A	73	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	A	225	ASP	N-CA-C	-5.13	98.96	107.99
1	A	567	SER	O-C-N	5.13	129.15	122.89
1	A	218	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	60	LYS	CB-CA-C	-5.12	100.24	110.42
1	A	206	SER	CB-CA-C	-5.12	99.60	109.37
1	A	502	LEU	CA-C-O	5.11	125.20	120.60
1	A	308	THR	CA-CB-OG1	-5.11	101.93	109.60
1	A	216	ASP	O-C-N	-5.11	116.55	123.19
1	A	342	LYS	N-CA-C	5.10	118.43	111.39
1	A	500	LEU	O-C-N	5.10	129.18	123.27
1	A	523	PHE	O-C-N	5.10	129.52	122.08
1	A	402	SER	CA-C-N	5.09	124.87	119.28
1	A	402	SER	C-N-CA	5.09	124.87	119.28
1	A	232	SER	CA-C-O	-5.08	115.17	121.06
1	A	374	ASN	N-CA-C	-5.08	106.91	113.01
1	A	476	TYR	CB-CA-C	-5.08	101.37	109.75
1	A	547	THR	CB-CA-C	5.08	119.87	109.67
1	A	198	PRO	CA-C-N	5.07	131.35	121.41
1	A	198	PRO	C-N-CA	5.07	131.35	121.41
1	A	378	ALA	N-CA-CB	-5.07	102.99	110.14
1	A	243	GLY	N-CA-C	5.07	121.02	111.80
1	A	460	ARG	N-CA-C	-5.06	100.20	108.76
1	A	148	ALA	N-CA-C	-5.06	103.72	110.55
1	A	79	ASN	CA-C-N	-5.06	113.95	122.25
1	A	79	ASN	C-N-CA	-5.06	113.95	122.25
1	A	617	TYR	CA-C-O	-5.04	115.12	120.92
1	A	384	GLY	CA-C-O	5.04	129.98	122.62
1	A	417	ILE	CA-C-O	-5.04	114.98	120.72
1	A	121	ALA	O-C-N	5.03	129.11	123.48
1	A	499	SER	N-CA-CB	5.03	120.12	111.13
1	A	20	SER	CA-C-O	-5.02	115.91	121.33
1	A	447	LEU	O-C-N	5.02	127.86	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	TRP	CA-C-O	-5.02	115.49	121.16
1	A	285	THR	CA-CB-OG1	-5.01	102.09	109.60
1	A	521	ASN	N-CA-CB	5.00	117.62	110.06
1	A	528	PHE	N-CA-CB	5.00	118.42	110.57

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	439	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	4830	0	4603	80	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	310	0	0	5	0
All	All	5142	0	4603	80	1

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 8.

All (80) 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	1.15	1.11
1:A:22:GLN:HG3	1:A:42:PHE:HA	1.43	1.00
1:A:298:ASN:HD22	1:A:317:VAL:H	1.21	0.89
1:A:22:GLN:NE2	1:A:46:ASN:HB2	1.92	0.82
1:A:35:LYS:HE3	1:A:71:LEU:HD21	1.64	0.80
1:A:298:ASN:ND2	1:A:317:VAL:H	1.83	0.74
1:A:170:VAL:HB	1:A:514:LEU:HD13	1.79	0.65
1:A:32:ASP:OD2	1:A:37:THR:OG1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:SER:OG	4:A:999:HOH:O	2.17	0.60
1:A:298:ASN:HD22	1:A:317:VAL:N	1.97	0.58
1:A:171:PRO:HD2	1:A:511:GLY:HA2	1.85	0.58
1:A:522:HIS:HD2	4:A:822:HOH:O	1.86	0.58
1:A:379:PRO:HD2	4:A:770:HOH:O	2.04	0.57
1:A:466:ASP:OD2	1:A:522:HIS:HE1	1.87	0.57
1:A:340:TRP:CG	1:A:341:LYS:H	2.23	0.57
1:A:529:THR:HG23	1:A:533:LEU:HD12	1.88	0.55
1:A:174:ALA:HB3	1:A:498:ILE:HD13	1.89	0.55
1:A:174:ALA:HA	1:A:184:LEU:O	2.07	0.55
1:A:35:LYS:HE2	1:A:74:GLN:HG3	1.90	0.55
1:A:95:ASN:HD22	1:A:95:ASN:N	2.06	0.54
1:A:174:ALA:CB	1:A:498:ILE:HD13	2.38	0.53
1:A:78:GLN:HG2	1:A:81:TRP:CH2	2.44	0.53
1:A:59:MET:C	1:A:61:THR:H	2.16	0.53
1:A:135:GLN:HB3	1:A:136:PRO:CD	2.38	0.52
1:A:15:ALA:HB2	1:A:60:LYS:NZ	2.24	0.52
1:A:22:GLN:NE2	1:A:43:TYR:O	2.42	0.52
1:A:506:ARG:HD3	4:A:821:HOH:O	2.10	0.52
1:A:554:VAL:HG11	1:A:560:ILE:HD11	1.92	0.52
1:A:358:TYR:HE2	1:A:366:LYS:HB2	1.75	0.52
1:A:228:CYS:N	1:A:229:PRO:HD3	2.25	0.51
1:A:5:ILE:HD12	1:A:490:SER:HB3	1.92	0.51
1:A:404:ASP:HB2	1:A:408:SER:HB2	1.93	0.51
1:A:439:ARG:NH2	1:A:474:GLU:HG3	2.25	0.51
1:A:495:TYR:O	1:A:496:HIS:HB2	2.11	0.51
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.47	0.50
1:A:131:GLU:HG3	1:A:137:TRP:O	2.12	0.50
1:A:401:GLY:O	1:A:411:THR:HG22	2.12	0.50
1:A:298:ASN:ND2	1:A:316:LYS:HA	2.27	0.49
1:A:11:ARG:HG2	1:A:14:TRP:CH2	2.47	0.49
1:A:13:ASN:HB3	1:A:60:LYS:HG3	1.95	0.48
1:A:103:GLY:HA3	1:A:166:ASP:O	2.14	0.47
1:A:227:PHE:O	1:A:244:GLY:HA3	2.15	0.47
1:A:458:GLN:HA	1:A:468:THR:O	2.15	0.47
1:A:135:GLN:HB3	1:A:136:PRO:HD2	1.96	0.47
1:A:9:ILE:HD12	1:A:145:VAL:HG12	1.98	0.46
1:A:22:GLN:HE21	1:A:46:ASN:CB	2.06	0.46
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.98	0.46
1:A:122:ARG:HD3	1:A:123:TYR:CE1	2.50	0.46
1:A:177:GLU:HB2	1:A:180:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PRO:HA	1:A:52:PRO:C	2.42	0.45
1:A:95:ASN:N	1:A:95:ASN:ND2	2.64	0.45
1:A:189:TYR:CD1	1:A:197:SER:HB2	2.51	0.44
1:A:559:ARG:HG3	1:A:605:GLN:HG3	2.00	0.44
1:A:568:ILE:HD13	1:A:622:VAL:HB	1.99	0.44
1:A:552:GLN:HG3	4:A:978:HOH:O	2.17	0.44
1:A:560:ILE:O	1:A:603:SER:HA	2.18	0.43
1:A:334:HIS:CE1	1:A:581:HIS:HB3	2.53	0.43
1:A:16:VAL:HG12	1:A:57:ILE:HG12	2.01	0.43
1:A:170:VAL:HB	1:A:514:LEU:CD1	2.47	0.43
1:A:575:ARG:HD2	1:A:618:TRP:CZ2	2.54	0.43
1:A:35:LYS:HE3	1:A:35:LYS:HB2	1.93	0.42
1:A:467:SER:C	1:A:469:PRO:HD3	2.44	0.42
1:A:41:THR:HG21	1:A:53:HIS:CG	2.55	0.42
1:A:51:PRO:HD3	1:A:136:PRO:HA	2.01	0.41
1:A:61:THR:O	1:A:122:ARG:HA	2.20	0.41
1:A:460:ARG:HH11	1:A:460:ARG:HD2	1.56	0.41
1:A:60:LYS:HA	1:A:122:ARG:HH21	1.85	0.41
1:A:548:ARG:O	1:A:562:ILE:HA	2.20	0.41
1:A:155:GLN:HA	1:A:156:PRO:HD3	1.83	0.41
1:A:34:ASN:OD1	1:A:36:ASP:HB2	2.21	0.41
1:A:38:PHE:HB3	1:A:141:ALA:HA	2.02	0.41
1:A:620:LEU:O	1:A:632:ALA:HA	2.21	0.41
1:A:206:SER:O	1:A:214:VAL:HA	2.21	0.40
1:A:393:LYS:HA	1:A:393:LYS:HD2	1.95	0.40
1:A:624:ASN:OD1	1:A:626:ALA:HB3	2.21	0.40
1:A:94:THR:HB	1:A:95:ASN:HD22	1.86	0.40
1:A:464:PHE:CD1	1:A:515:CYS:HB3	2.56	0.40
1:A:559:ARG:HE	1:A:605:GLN:HG3	1.87	0.40
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.56	0.40
1:A:39:TRP:O	1:A:139:SER:HA	2.22	0.40

All (1) 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

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%)	610 (96%)	24 (4%)	3 (0%)	24 16

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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 34

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

Mol	Chain	Res	Type
1	A	17	THR
1	A	20	SER
1	A	23	SER
1	A	68	LEU
1	A	91	SER
1	A	95	ASN
1	A	139	SER
1	A	229	PRO

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Mol	Chain	Res	Type
1	A	366	LYS
1	A	439	ARG
1	A	498	ILE
1	A	532	TYR
1	A	563	SER
1	A	639	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	25	ASN
1	A	46	ASN
1	A	78	GLN
1	A	95	ASN
1	A	144	ASN
1	A	267	GLN
1	A	298	ASN
1	A	355	ASN
1	A	522	HIS
1	A	537	ASN
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 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	639/639 (100%)	-0.77	3 (0%) 87 89	6, 18, 56, 98	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLY	2.5
1	A	45	ALA	2.5
1	A	44	GLY	2.4

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	0.97	0.03	15,15,15,15	0
2	CU	A	700	1/1	1.00	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.