



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:26 PM UTC

PDB ID : 1AYX / pdb_00001ayx
Title : CRYSTAL STRUCTURE OF GLUCOAMYLASE FROM SACCHAROMY-
COPSIS FIBULIGERA AT 1.7 ANGSTROMS
Authors : Sevcik, J.; Hostinova, E.; Gasperik, J.; Solovicova, A.; Wilson, K.S.; Dauter,
Z.
Deposited on : 1997-11-12
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

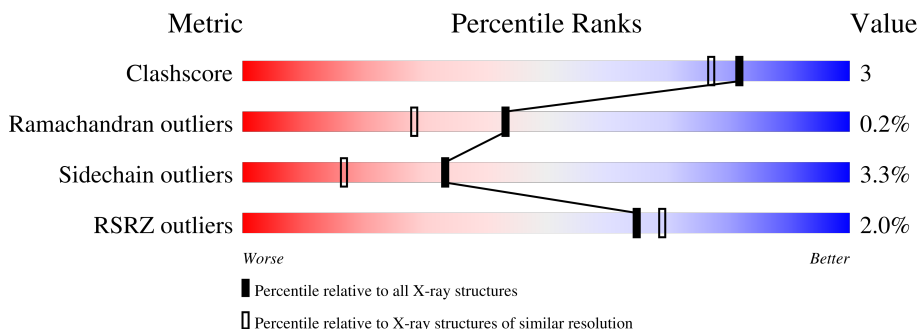
1 Overall quality at a glance

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	492	2% 70% 28% ..

2 Entry composition [i](#)

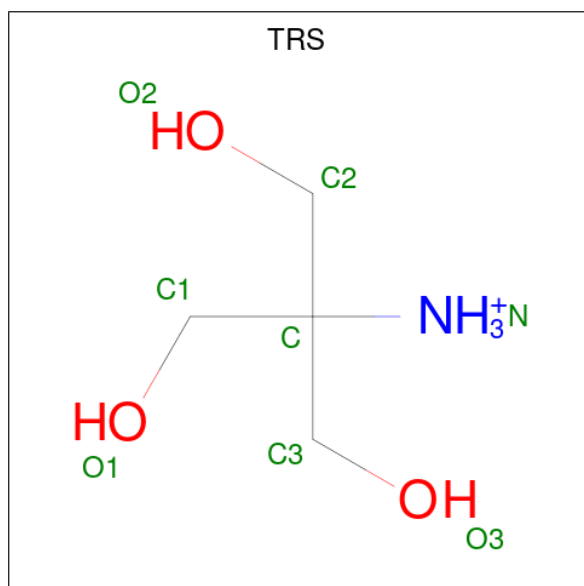
There are 3 unique types of molecules in this entry. The entry contains 4279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOAMYLASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	492	3870	2438	624	808	0	0	0

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	401	Total	O	0	0
			401	401		

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: GLUCOAMYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.14Å 87.79Å 99.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 30.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-1.70) 99.4 (30.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.181 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4279	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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: TRS

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	1.38	11/3960 (0.3%)	2.20	162/5398 (3.0%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	TYR	C-N	6.13	1.42	1.34
1	A	447	HIS	CG-ND1	5.93	1.44	1.38
1	A	251	SER	CA-CB	5.80	1.62	1.53
1	A	408	ASN	CA-C	-5.60	1.46	1.52
1	A	139	TRP	N-CA	5.33	1.52	1.46
1	A	375	LYS	C-O	5.32	1.30	1.24
1	A	94	ALA	C-N	-5.28	1.27	1.33
1	A	230	ALA	C-N	-5.27	1.27	1.33
1	A	460	ARG	CD-NE	-5.17	1.39	1.46
1	A	405	SER	C-O	5.08	1.30	1.24
1	A	105	LEU	C-O	5.05	1.30	1.24

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	ARG	CD-NE-CZ	16.17	147.04	124.40
1	A	294	GLY	O-C-N	14.81	126.40	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	NE-CZ-NH2	-13.79	106.79	119.20
1	A	460	ARG	NE-CZ-NH1	12.76	134.26	121.50
1	A	384	SER	CA-C-O	10.49	133.77	121.28
1	A	25	GLN	CB-CG-CD	9.46	128.68	112.60
1	A	463	GLY	CA-C-O	9.45	129.51	119.02
1	A	384	SER	O-C-N	-9.08	110.24	122.41
1	A	191	LYS	CA-CB-CG	-8.89	96.31	114.10
1	A	181	SER	O-C-N	8.51	132.20	123.26
1	A	90	THR	O-C-N	8.43	131.05	122.12
1	A	191	LYS	CB-CG-CD	-8.31	92.17	111.30
1	A	408	ASN	OD1-CG-ND2	8.19	130.78	122.60
1	A	223	GLN	OE1-CD-NE2	8.18	130.78	122.60
1	A	203	SER	CA-C-O	-7.97	112.14	121.46
1	A	150	ARG	NE-CZ-NH1	7.85	129.35	121.50
1	A	172	THR	N-CA-C	7.84	119.82	111.28
1	A	408	ASN	O-C-N	-7.83	113.26	123.28
1	A	327	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	A	134	ALA	CA-C-O	7.76	129.73	121.19
1	A	243	ALA	CA-C-O	7.74	129.18	120.90
1	A	25	GLN	O-C-N	-7.68	112.82	122.27
1	A	48	VAL	CA-C-N	7.62	128.09	119.93
1	A	48	VAL	C-N-CA	7.62	128.09	119.93
1	A	327	ASN	CB-CG-ND2	7.61	127.81	116.40
1	A	36	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	A	71	SER	CA-C-O	7.51	128.38	120.42
1	A	191	LYS	N-CA-CB	-7.50	98.80	110.43
1	A	129	ASN	O-C-N	-7.49	114.25	122.79
1	A	103	TYR	O-C-N	-7.35	114.45	122.09
1	A	149	LEU	CA-C-O	-7.34	112.64	120.42
1	A	25	GLN	CG-CD-NE2	7.28	127.32	116.40
1	A	442	GLN	O-C-N	-7.26	113.34	122.27
1	A	25	GLN	CA-C-O	7.16	128.21	119.97
1	A	3	PRO	CA-C-N	7.15	132.65	120.72
1	A	3	PRO	C-N-CA	7.15	132.65	120.72
1	A	463	GLY	O-C-N	-6.99	113.51	122.39
1	A	390	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	A	146	GLY	O-C-N	-6.97	114.80	121.77
1	A	212	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	A	269	VAL	CA-C-N	6.92	132.19	122.36
1	A	269	VAL	C-N-CA	6.92	132.19	122.36
1	A	191	LYS	CG-CD-CE	-6.86	95.52	111.30
1	A	308	PRO	O-C-N	6.84	131.25	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ASP	CA-CB-CG	6.75	119.35	112.60
1	A	100	ASN	OD1-CG-ND2	6.75	129.34	122.60
1	A	107	ARG	NE-CZ-NH1	-6.75	114.75	121.50
1	A	315	TYR	CD1-CG-CD2	6.72	128.18	118.10
1	A	212	ASN	CA-C-O	6.68	128.93	121.11
1	A	310	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	384	SER	N-CA-CB	-6.68	102.05	112.13
1	A	82	LEU	CA-C-N	6.67	129.76	120.29
1	A	82	LEU	C-N-CA	6.67	129.76	120.29
1	A	271	HIS	CA-CB-CG	6.64	120.44	113.80
1	A	361	PRO	N-CA-CB	6.63	109.63	103.39
1	A	75	PHE	CA-CB-CG	-6.63	107.17	113.80
1	A	202	ASP	CA-C-N	6.63	133.94	122.81
1	A	202	ASP	C-N-CA	6.63	133.94	122.81
1	A	63	TYR	CA-C-O	6.62	127.76	119.95
1	A	191	LYS	O-C-N	6.60	126.92	120.71
1	A	398	ASN	OD1-CG-ND2	6.60	129.20	122.60
1	A	334	ASN	OD1-CG-ND2	6.56	129.16	122.60
1	A	15	ARG	O-C-N	6.56	130.85	122.39
1	A	184	ASP	O-C-N	6.50	129.01	122.12
1	A	134	ALA	O-C-N	-6.49	114.89	122.87
1	A	96	GLU	O-C-N	-6.44	114.35	122.27
1	A	42	GLY	O-C-N	-6.40	116.80	122.88
1	A	94	ALA	CA-C-O	-6.37	113.79	120.55
1	A	272	ILE	CA-C-O	6.36	128.67	121.11
1	A	379	ASP	CA-C-O	-6.35	113.82	120.55
1	A	452	GLY	CA-C-O	-6.30	112.02	119.02
1	A	32	TYR	O-C-N	6.29	130.00	122.27
1	A	233	ILE	CA-C-O	6.28	127.82	121.17
1	A	203	SER	O-C-N	6.27	131.52	123.11
1	A	38	ALA	O-C-N	-6.27	115.71	123.04
1	A	247	SER	CA-C-O	6.27	127.40	120.82
1	A	234	ALA	CA-C-O	-6.25	113.92	120.55
1	A	107	ARG	CD-NE-CZ	6.25	133.15	124.40
1	A	13	VAL	O-C-N	6.24	129.41	122.61
1	A	64	TYR	CA-C-N	6.18	132.25	122.36
1	A	64	TYR	C-N-CA	6.18	132.25	122.36
1	A	227	LEU	CA-C-N	6.16	128.45	120.44
1	A	227	LEU	C-N-CA	6.16	128.45	120.44
1	A	181	SER	CA-C-O	-6.16	114.86	121.38
1	A	250	ALA	O-C-N	-6.16	115.60	122.12
1	A	269	VAL	O-C-N	-6.12	116.07	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	198	ILE	CA-C-O	-6.11	114.60	120.95
1	A	173	ASP	CA-C-O	6.05	127.96	120.15
1	A	17	ASP	CA-CB-CG	-6.04	106.56	112.60
1	A	201	TRP	O-C-N	6.01	129.00	122.15
1	A	238	ASP	CA-CB-CG	-6.00	106.60	112.60
1	A	38	ALA	CA-C-O	6.00	127.53	120.69
1	A	469	TYR	CA-C-N	5.99	130.87	122.36
1	A	469	TYR	C-N-CA	5.99	130.87	122.36
1	A	10	ASN	CA-C-O	5.97	128.46	121.54
1	A	303	GLU	CB-CG-CD	5.97	122.75	112.60
1	A	457	GLN	OE1-CD-NE2	5.95	128.55	122.60
1	A	118	GLU	O-C-N	5.95	130.27	122.89
1	A	24	LYS	CA-C-O	5.94	126.72	120.42
1	A	39	TYR	N-CA-CB	5.91	118.99	110.77
1	A	100	ASN	CA-C-O	5.91	126.81	120.55
1	A	145	ASP	O-C-N	5.85	130.17	122.33
1	A	450	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	402	VAL	CA-C-O	-5.80	116.09	120.96
1	A	115	PHE	O-C-N	5.78	129.38	122.27
1	A	64	TYR	O-C-N	-5.78	115.49	122.71
1	A	81	GLU	CA-CB-CG	5.77	125.64	114.10
1	A	194	LEU	CA-C-O	-5.76	113.35	119.97
1	A	18	LEU	O-C-N	-5.75	116.02	122.12
1	A	314	GLU	N-CA-C	5.75	117.55	111.28
1	A	489	LYS	CB-CG-CD	5.74	124.49	111.30
1	A	466	THR	O-C-N	-5.73	117.24	123.26
1	A	35	GLN	CA-C-O	5.72	126.41	119.49
1	A	284	ARG	CD-NE-CZ	-5.71	116.40	124.40
1	A	272	ILE	O-C-N	-5.71	115.98	122.72
1	A	446	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	88	ASN	CA-CB-CG	5.64	118.24	112.60
1	A	469	TYR	O-C-N	-5.63	116.37	123.01
1	A	288	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	33	LEU	O-C-N	5.55	128.09	122.09
1	A	67	TRP	O-C-N	-5.55	116.17	123.16
1	A	84	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	442	GLN	CA-C-O	5.54	126.34	119.97
1	A	49	PRO	N-CA-CB	5.53	108.16	103.19
1	A	9	SER	N-CA-C	5.49	118.29	110.10
1	A	396	PHE	O-C-N	-5.49	116.42	122.07
1	A	127	LYS	O-C-N	5.48	129.50	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	428	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	245	THR	CA-CB-OG1	-5.43	101.45	109.60
1	A	215	ARG	CA-C-N	-5.41	113.24	122.33
1	A	215	ARG	C-N-CA	-5.41	113.24	122.33
1	A	246	LEU	CA-C-N	5.41	127.47	120.44
1	A	246	LEU	C-N-CA	5.41	127.47	120.44
1	A	379	ASP	CB-CG-OD1	5.41	130.83	118.40
1	A	269	VAL	CA-C-O	5.38	124.07	118.96
1	A	194	LEU	O-C-N	5.35	128.85	122.27
1	A	230	ALA	CA-C-O	-5.34	112.10	119.05
1	A	449	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	366	THR	CA-C-O	-5.33	114.77	120.42
1	A	58	THR	O-C-N	-5.32	115.69	122.34
1	A	124	GLY	O-C-N	-5.28	114.39	122.26
1	A	371	GLN	OE1-CD-NE2	5.28	127.88	122.60
1	A	90	THR	CA-C-O	-5.28	114.96	120.55
1	A	240	GLY	N-CA-C	5.26	119.04	112.73
1	A	25	GLN	CB-CA-C	-5.22	100.65	110.67
1	A	23	ASP	N-CA-CB	-5.19	102.54	110.07
1	A	245	THR	CA-C-N	-5.18	113.33	120.28
1	A	245	THR	C-N-CA	-5.18	113.33	120.28
1	A	220	SER	N-CA-C	5.18	117.67	111.71
1	A	393	ASN	OD1-CG-ND2	5.18	127.78	122.60
1	A	488	VAL	CA-C-O	-5.17	115.17	120.71
1	A	75	PHE	O-C-N	-5.17	115.51	122.43
1	A	397	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	32	TYR	CA-C-O	-5.12	114.08	119.97
1	A	335	SER	CA-C-O	-5.07	113.36	119.49
1	A	206	PHE	CA-C-O	5.06	127.29	121.47
1	A	408	ASN	CA-C-O	5.04	126.35	120.20
1	A	100	ASN	O-C-N	-5.04	116.78	122.12
1	A	309	PHE	CG-CD1-CE1	5.04	129.27	120.70
1	A	69	ARG	NE-CZ-NH2	-5.02	114.68	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	LYS	Mainchain
1	A	200	TYR	Mainchain

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	3870	0	3609	19	0
2	A	8	0	12	2	0
3	A	401	0	0	4	0
All	All	4279	0	3621	19	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 3.

All (19) 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:403:ASP:HB2	3:A:699:HOH:O	2.01	0.61
1:A:82:LEU:HD13	1:A:91:LEU:HB2	1.83	0.60
1:A:295:PRO:O	1:A:299:HIS:HD2	1.88	0.55
1:A:261:ASP:HB2	3:A:742:HOH:O	2.06	0.55
1:A:191:LYS:CB	1:A:192:PRO:HD3	2.38	0.53
1:A:299:HIS:O	1:A:375:LYS:HE3	2.09	0.53
1:A:299:HIS:HE1	1:A:307:THR:O	1.94	0.51
1:A:88:ASN:ND2	1:A:91:LEU:HG	2.25	0.51
1:A:336:ALA:HB3	3:A:874:HOH:O	2.12	0.49
1:A:492:ALA:HB2	3:A:783:HOH:O	2.13	0.47
1:A:26:LYS:HZ3	1:A:26:LYS:HB2	1.80	0.45
1:A:24:LYS:HD2	1:A:24:LYS:HA	1.68	0.45
1:A:63:TYR:CE2	2:A:493:TRS:N	2.84	0.45
1:A:21:PHE:CG	1:A:445:LEU:HD13	2.53	0.43
1:A:352:ASN:OD1	1:A:352:ASN:C	2.62	0.43
1:A:63:TYR:HE2	2:A:493:TRS:HN1	1.67	0.41
1:A:345:ARG:HD3	1:A:362:TRP:CZ2	2.56	0.41
1:A:82:LEU:HD13	1:A:91:LEU:CB	2.50	0.41
1:A:144:ASN:ND2	1:A:196:TYR:OH	2.54	0.41

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	490/492 (100%)	475 (97%)	14 (3%)	1 (0%)	43 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASP

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	422/422 (100%)	408 (97%)	14 (3%)	33 17

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

Mol	Chain	Res	Type
1	A	23	ASP
1	A	24	LYS
1	A	86	ASN
1	A	88	ASN
1	A	168	LYS
1	A	176	ASP
1	A	180	SER
1	A	191	LYS
1	A	233	ILE
1	A	238	ASP

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Mol	Chain	Res	Type
1	A	253	LEU
1	A	304	SER
1	A	414	SER
1	A	420	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	144	ASN
1	A	299	HIS
1	A	385	ASN
1	A	449	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](#)

1 ligand is modelled in this entry.

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
2	TRS	A	493	-	7,7,7	0.37	0	9,9,9	1.61	3 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	A	493	-	-	0/9/9/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	493	TRS	C1-C-N	-2.59	101.56	108.17
2	A	493	TRS	O1-C1-C	-2.23	104.65	110.88
2	A	493	TRS	C3-C-C2	2.01	116.01	110.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	493	TRS	2	0

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	492/492 (100%)	-0.25	10 (2%) 65 69	7, 16, 34, 59	5 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	ALA	9.0
1	A	86	ASN	4.4
1	A	306	SER	2.6
1	A	305	SER	2.5
1	A	172	THR	2.5
1	A	82	LEU	2.4
1	A	176	ASP	2.3
1	A	354	ASP	2.3
1	A	336	ALA	2.1
1	A	304	SER	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($\text{\AA}^2$)	Q<0.9
2	TRS	A	493	8/8	0.93	0.08	14,19,24,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.