Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:28 PM GMT

PDB ID	:	1AYX
Title	:	CRYSTAL STRUCTURE OF GLUCOAMYLASE FROM SACCHAROMYCOPSIS 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

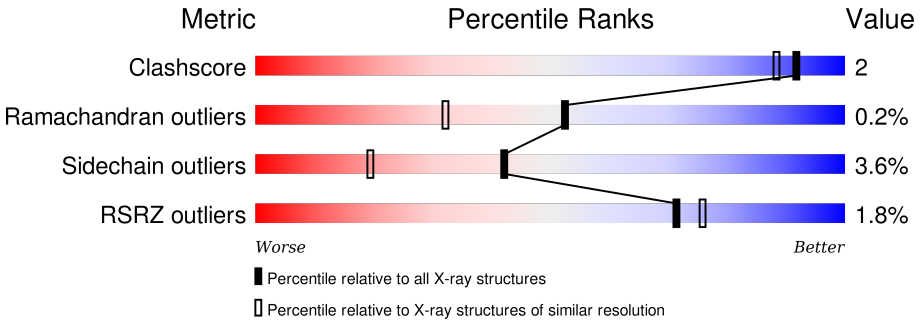
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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% 78% 20%

2 Entry composition

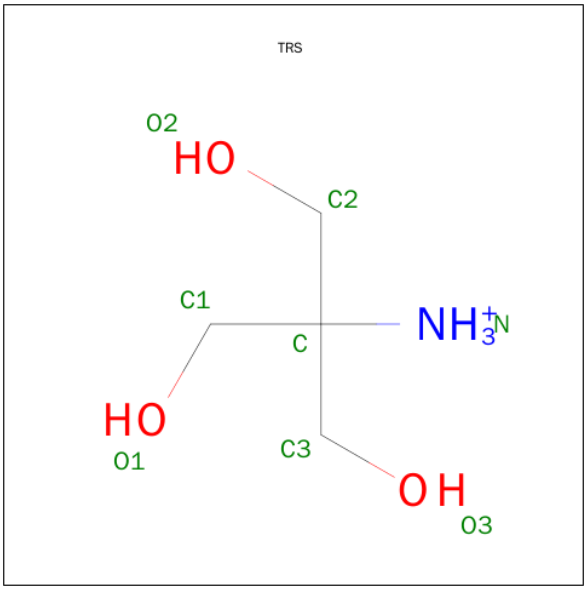
There are 3 unique types of molecules in this entry. The entry contains 4279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	492	Total	C	N	O	0	0	0
			3870	2438	624	808			

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 3 is water.

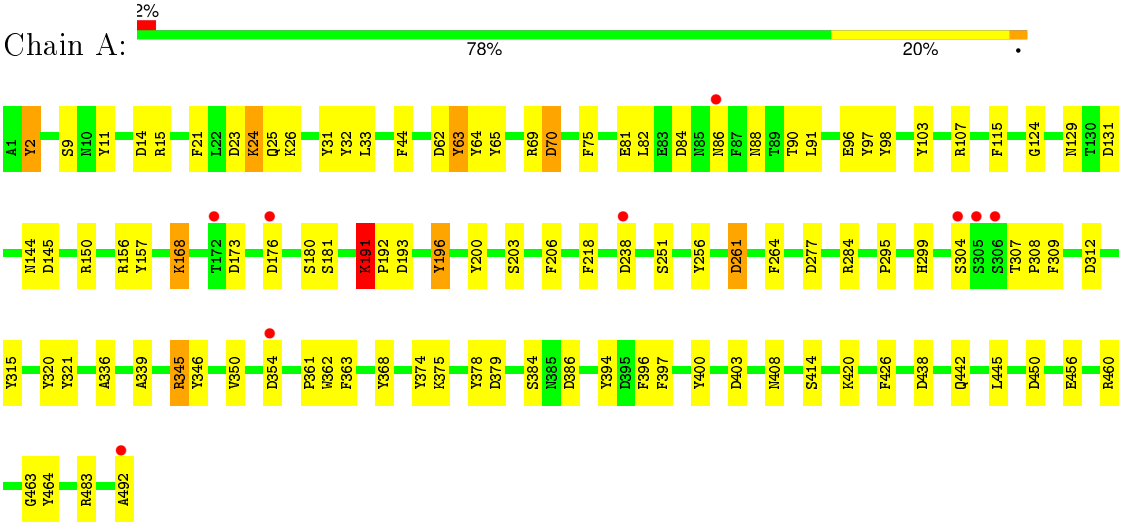
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	401	Total	O	0	0
			401	401		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A:



4 Data and refinement statistics (i)

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 29.07 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-1.70) 99.4 (29.07-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.181 0.145 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 56652 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.07	2/3960 (0.1%)	1.99	124/5398 (2.3%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	SER	CA-CB	6.37	1.62	1.52
1	A	315	TYR	CB-CG	5.31	1.59	1.51

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	460	ARG	NE-CZ-NH1	27.93	134.26	120.30
1	A	460	ARG	NE-CZ-NH2	-27.03	106.79	120.30
1	A	150	ARG	NE-CZ-NH1	18.10	129.35	120.30
1	A	483	ARG	CD-NE-CZ	16.74	147.04	123.60
1	A	379	ASP	CB-CG-OD1	13.93	130.83	118.30
1	A	193	ASP	CB-CG-OD1	11.39	128.55	118.30
1	A	69	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	A	107	ARG	NE-CZ-NH1	-11.09	114.75	120.30
1	A	379	ASP	CB-CG-OD2	-10.19	109.13	118.30
1	A	150	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	A	173	ASP	CB-CG-OD1	9.91	127.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	97	TYR	CB-CG-CD1	-9.54	115.27	121.00
1	A	378	TYR	CB-CG-CD1	-9.52	115.29	121.00
1	A	315	TYR	CD1-CG-CD2	9.34	128.18	117.90
1	A	400	TYR	CB-CG-CD1	-9.29	115.43	121.00
1	A	75	PHE	CB-CG-CD1	-9.12	114.41	120.80
1	A	321	TYR	CB-CG-CD2	-9.03	115.58	121.00
1	A	386	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	A	315	TYR	CB-CG-CD1	-8.85	115.69	121.00
1	A	394	TYR	CB-CG-CD1	8.80	126.28	121.00
1	A	97	TYR	CG-CD1-CE1	-8.52	114.49	121.30
1	A	309	PHE	CB-CG-CD1	8.47	126.73	120.80
1	A	284	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	315	TYR	CG-CD2-CE2	-8.19	114.75	121.30
1	A	145	ASP	CB-CG-OD1	8.17	125.65	118.30
1	A	31	TYR	CB-CG-CD2	-8.14	116.11	121.00
1	A	315	TYR	CB-CG-CD2	-8.11	116.13	121.00
1	A	394	TYR	CB-CG-CD2	-8.06	116.16	121.00
1	A	345	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	384	SER	O-C-N	-7.79	110.24	122.70
1	A	191	LYS	CA-CB-CG	-7.77	96.31	113.40
1	A	98	TYR	CB-CG-CD2	-7.72	116.37	121.00
1	A	309	PHE	CG-CD1-CE1	7.70	129.27	120.80
1	A	44	PHE	CB-CG-CD1	7.68	126.18	120.80
1	A	70	ASP	CB-CG-OD1	7.67	125.21	118.30
1	A	315	TYR	CG-CD1-CE1	-7.61	115.21	121.30
1	A	396	PHE	CB-CG-CD2	7.52	126.06	120.80
1	A	15	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	A	191	LYS	CB-CG-CD	-7.47	92.17	111.60
1	A	84	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	426	PHE	CB-CG-CD2	-7.09	115.84	120.80
1	A	277	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	309	PHE	CD1-CE1-CZ	-7.05	111.64	120.10
1	A	173	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	378	TYR	CD1-CG-CD2	6.84	125.43	117.90
1	A	107	ARG	CD-NE-CZ	6.82	133.15	123.60
1	A	284	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	63	TYR	CB-CG-CD1	6.78	125.07	121.00
1	A	103	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	A	97	TYR	CD1-CG-CD2	6.67	125.24	117.90
1	A	75	PHE	CB-CG-CD2	6.62	125.43	120.80
1	A	363	PHE	CB-CG-CD2	-6.61	116.17	120.80
1	A	25	GLN	CB-CG-CD	6.57	128.68	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	191	LYS	N-CA-CB	-6.56	98.80	110.60
1	A	62	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	384	SER	CA-C-O	6.51	133.77	120.10
1	A	397	PHE	CB-CG-CD1	-6.47	116.27	120.80
1	A	309	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	A	374	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	64	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	A	157	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	A	261	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	A	98	TYR	CG-CD1-CE1	-6.20	116.34	121.30
1	A	464	TYR	CB-CG-CD1	-6.19	117.28	121.00
1	A	25	GLN	O-C-N	-6.18	112.82	122.70
1	A	438	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	11	TYR	CB-CG-CD1	6.07	124.64	121.00
1	A	456	GLU	OE1-CD-OE2	6.06	130.57	123.30
1	A	2	TYR	CD1-CE1-CZ	-6.05	114.36	119.80
1	A	131	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	115	PHE	CB-CG-CD2	6.03	125.02	120.80
1	A	397	PHE	CD1-CG-CD2	5.98	126.07	118.30
1	A	181	SER	O-C-N	5.94	132.20	122.70
1	A	408	ASN	O-C-N	-5.90	113.26	122.70
1	A	14	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	98	TYR	CD1-CG-CD2	5.90	124.39	117.90
1	A	442	GLN	O-C-N	-5.85	113.34	122.70
1	A	345	ARG	NH1-CZ-NH2	5.81	125.79	119.40
1	A	206	PHE	CB-CG-CD1	-5.81	116.74	120.80
1	A	312	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	463	GLY	O-C-N	-5.74	113.51	122.70
1	A	31	TYR	CB-CG-CD1	5.65	124.39	121.00
1	A	384	SER	N-CA-CB	-5.64	102.05	110.50
1	A	9	SER	N-CA-CB	-5.60	102.10	110.50
1	A	156	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	378	TYR	CG-CD2-CE2	-5.58	116.84	121.30
1	A	261	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	81	GLU	CA-CB-CG	5.56	125.64	113.40
1	A	339	ALA	CB-CA-C	5.51	118.37	110.10
1	A	203	SER	O-C-N	5.51	131.52	122.70
1	A	65	TYR	CG-CD1-CE1	-5.51	116.89	121.30
1	A	256	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	464	TYR	CD1-CG-CD2	5.47	123.92	117.90
1	A	191	LYS	CG-CD-CE	-5.46	95.52	111.90
1	A	320	TYR	CG-CD2-CE2	-5.45	116.94	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	346	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	277	ASP	OD1-CG-OD2	-5.38	113.09	123.30
1	A	32	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	308	PRO	O-C-N	5.34	131.25	122.70
1	A	368	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	98	TYR	CZ-CE2-CD2	-5.30	115.03	119.80
1	A	397	PHE	CG-CD1-CE1	-5.30	114.97	120.80
1	A	129	ASN	O-C-N	-5.28	114.25	122.70
1	A	361	PRO	N-CA-CB	5.27	109.63	103.30
1	A	103	TYR	CG-CD1-CE1	-5.26	117.09	121.30
1	A	320	TYR	CZ-CE2-CD2	5.26	124.53	119.80
1	A	321	TYR	CG-CD1-CE1	-5.25	117.10	121.30
1	A	394	TYR	CD1-CE1-CZ	-5.24	115.08	119.80
1	A	264	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	A	450	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	90	THR	O-C-N	5.22	131.05	122.70
1	A	96	GLU	O-C-N	-5.22	114.35	122.70
1	A	124	GLY	O-C-N	-5.20	114.39	122.70
1	A	103	TYR	O-C-N	-5.16	114.45	122.70
1	A	284	ARG	CD-NE-CZ	-5.14	116.40	123.60
1	A	196	TYR	CG-CD1-CE1	5.12	125.40	121.30
1	A	15	ARG	O-C-N	5.09	130.85	122.70
1	A	218	PHE	CB-CG-CD1	5.09	124.36	120.80
1	A	256	TYR	CB-CG-CD1	5.06	124.04	121.00
1	A	11	TYR	CZ-CE2-CD2	5.05	124.35	119.80
1	A	107	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	A	350	VAL	CG1-CB-CG2	5.04	118.96	110.90
1	A	65	TYR	CZ-CE2-CD2	-5.04	115.27	119.80

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 (i)

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	16	0
2	A	8	0	12	1	0
3	A	401	0	0	4	0
All	All	4279	0	3621	16	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 2.

All (16) 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: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: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%)	52 32

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%)	407 (96%)	15 (4%)	42 19

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	23	ASP
1	A	24	LYS
1	A	26	LYS
1	A	33	LEU
1	A	70	ASP
1	A	86	ASN
1	A	168	LYS
1	A	176	ASP
1	A	180	SER
1	A	191	LYS
1	A	238	ASP
1	A	304	SER
1	A	414	SER
1	A	420	LYS

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

Mol	Chain	Res	Type
1	A	104	ASN
1	A	144	ASN
1	A	285	GLN
1	A	299	HIS
1	A	385	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	0.58	0	9,9,9	2.16	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	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	493	TRS	C1-C-N	-3.58	101.56	108.09
2	A	493	TRS	O1-C1-C	-3.23	104.65	111.18
2	A	493	TRS	C3-C-C2	2.41	116.01	110.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	493	TRS	1	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.24	9 (1%) 71 76	7, 16, 34, 59	5 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	ALA	13.7
1	A	86	ASN	6.2
1	A	306	SER	3.7
1	A	304	SER	3.6
1	A	354	ASP	2.7
1	A	176	ASP	2.7
1	A	305	SER	2.4
1	A	238	ASP	2.1
1	A	172	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	TRS	A	493	8/8	0.94	0.12	1.34	14,19,24,32	0

6.5 Other polymers (i)

There are no such residues in this entry.