



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5A2A / pdb_00005a2a
Title : Crystal Structure of Anoxybacillus Alpha-amylase Provides Insights into a New Glycosyl Hydrolase Subclass
Authors : Ng, C.L.; Chai, K.P.; Othman, N.F.; Teh, A.H.; Ho, K.L.; Chan, K.G.; Goh, K.M.
Deposited on : 2015-05-16
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
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

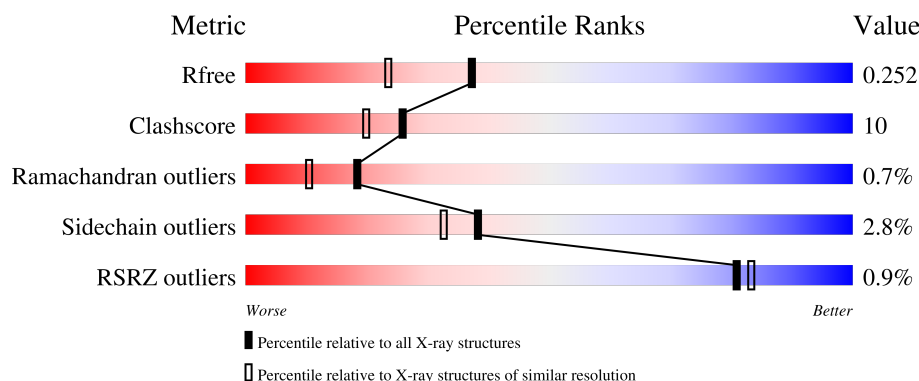
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	180053	7789 (1.90-1.90)
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	454	 74% 25% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	1479	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4193 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 APO FORM OF ANOXYBACILLUS ALPHA-AMYLASES.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	452	3776	2443	628	699	6	0	2	0

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		

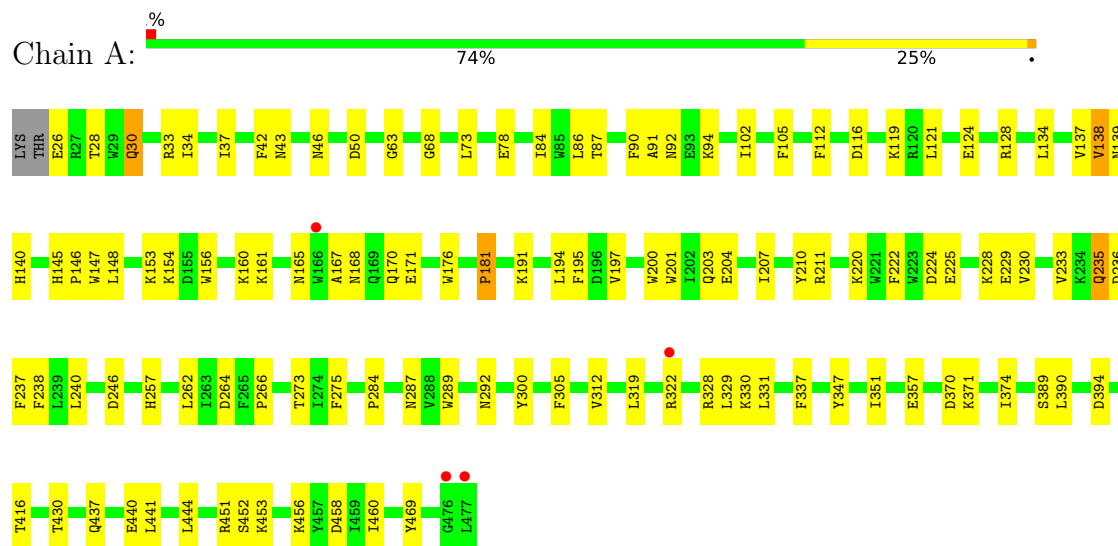
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	405	Total 405	O 405	0	0

3 Residue-property plots [i](#)

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: APO FORM OF ANOXYBACILLUS ALPHA-AMYLASES



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.43Å 63.44Å 122.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.90 19.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (19.99-1.90) 93.4 (19.99-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.177 , 0.236 0.191 , 0.252	Depositor DCC
R_{free} test set	1847 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
Reported twinning fraction	0.875 for H, K, L 0.125 for K, H, -L	Depositor
Outliers	0 of 36199 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4193	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CA

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	15/3887 (0.4%)	1.40	21/5267 (0.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	LEU	C-O	-7.82	1.15	1.24
1	A	240	LEU	CA-C	-7.39	1.43	1.52
1	A	284	PRO	CA-CB	7.03	1.63	1.53
1	A	73	LEU	C-O	-6.53	1.16	1.24
1	A	112	PHE	N-CA	6.10	1.54	1.46
1	A	347	TYR	N-CA	5.78	1.53	1.46
1	A	390	LEU	N-CA	5.71	1.53	1.46
1	A	28	THR	N-CA	5.58	1.53	1.45
1	A	460	ILE	C-O	-5.53	1.18	1.24
1	A	238	PHE	CA-C	5.33	1.59	1.52
1	A	30	GLN	N-CA	5.27	1.52	1.46
1	A	292	ASN	N-CA	-5.23	1.40	1.46
1	A	329	LEU	CA-C	5.17	1.59	1.52
1	A	319	LEU	N-CA	5.14	1.52	1.46
1	A	262	LEU	CA-C	-5.02	1.46	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ASN	CA-C-N	-10.50	108.95	119.87
1	A	46	ASN	C-N-CA	-10.50	108.95	119.87
1	A	87	THR	CA-C-N	-8.60	111.16	119.85
1	A	87	THR	C-N-CA	-8.60	111.16	119.85
1	A	240	LEU	CA-C-N	-7.26	115.31	122.36
1	A	240	LEU	C-N-CA	-7.26	115.31	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ILE	N-CA-C	6.95	119.00	111.77
1	A	374	ILE	N-CA-C	-6.46	104.46	110.53
1	A	452	SER	N-CA-C	-6.35	100.64	110.10
1	A	230	VAL	N-CA-C	6.19	116.98	110.72
1	A	34	ILE	N-CA-C	6.15	116.97	107.99
1	A	238	PHE	N-CA-C	5.95	119.22	109.76
1	A	394	ASP	N-CA-C	-5.67	103.16	110.19
1	A	167	ALA	N-CA-C	-5.49	106.63	113.38
1	A	63	GLY	CA-C-N	-5.29	115.07	120.10
1	A	63	GLY	C-N-CA	-5.29	115.07	120.10
1	A	138	VAL	CB-CA-C	-5.25	105.51	110.65
1	A	289	TRP	N-CA-C	5.15	117.30	111.02
1	A	287	ASN	N-CA-C	5.09	117.56	111.71
1	A	444	LEU	N-CA-C	-5.07	107.10	113.28
1	A	229	GLU	N-CA-C	5.05	116.60	111.14

There are no chirality outliers.

There are no planarity outliers.

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	3776	0	3661	68	3
2	A	8	0	6	3	0
3	A	4	0	0	0	0
4	A	405	0	0	22	4
All	All	4193	0	3667	71	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (71) 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:116:ASP:HB3	4:A:2125:HOH:O	1.39	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1479:ACT:H3	4:A:2403:HOH:O	1.68	0.93
1:A:138:VAL:HG13	1:A:194:LEU:HD13	1.54	0.89
1:A:331:LEU:HG	4:A:2311:HOH:O	1.73	0.88
1:A:224:ASP:OD2	4:A:2220:HOH:O	1.92	0.87
1:A:102:ILE:CD1	4:A:2152:HOH:O	2.24	0.84
1:A:273:THR:HG22	4:A:2252:HOH:O	1.77	0.84
1:A:116:ASP:OD2	4:A:2122:HOH:O	1.95	0.82
1:A:257:HIS:HE1	4:A:2238:HOH:O	1.62	0.82
1:A:137:VAL:HB	4:A:2152:HOH:O	1.81	0.81
2:A:1479:ACT:CH3	4:A:2403:HOH:O	2.27	0.75
1:A:440:GLU:OE1	1:A:451:ARG:NH1	2.20	0.74
1:A:139:ASN:HD22	1:A:140:HIS:HD2	1.45	0.64
1:A:225:GLU:HG2	4:A:2103:HOH:O	1.97	0.64
1:A:30:GLN:HG2	1:A:300:TYR:HB3	1.79	0.64
1:A:138:VAL:O	1:A:138:VAL:HG12	1.98	0.63
1:A:43:ASN:O	1:A:68:GLY:HA3	2.02	0.59
1:A:191:LYS:HG2	1:A:195:PHE:CE2	2.38	0.58
1:A:430:THR:HG21	1:A:456:LYS:HE3	1.87	0.55
1:A:105:PHE:HB3	1:A:197:VAL:HG21	1.89	0.55
1:A:264:ASP:OD1	1:A:266:PRO:HD2	2.07	0.54
1:A:91:ALA:HB2	4:A:2115:HOH:O	2.07	0.54
1:A:168:ASN:HB3	1:A:171:GLU:HB3	1.89	0.53
1:A:200:TRP:CZ2	1:A:204:GLU:HG3	2.44	0.53
1:A:78:GLU:HG3	4:A:2072:HOH:O	2.10	0.52
1:A:200:TRP:CE2	1:A:204:GLU:HG3	2.45	0.52
1:A:124:GLU:OE1	1:A:128:ARG:NH2	2.43	0.51
1:A:458:ASP:CG	4:A:2391:HOH:O	2.53	0.51
1:A:37:ILE:HG23	1:A:42:PHE:HB2	1.93	0.51
1:A:121:LEU:O	1:A:121:LEU:HD23	2.11	0.50
1:A:145:HIS:CE1	1:A:147:TRP:CD2	3.00	0.50
1:A:102:ILE:HD11	4:A:2152:HOH:O	2.03	0.49
1:A:441:LEU:HB3	1:A:469:TYR:CD2	2.48	0.48
1:A:119:LYS:HE2	1:A:204:GLU:O	2.13	0.48
1:A:441:LEU:HB3	1:A:469:TYR:HB3	1.96	0.48
1:A:138:VAL:O	1:A:138:VAL:CG1	2.59	0.48
1:A:371:LYS:HG3	4:A:2334:HOH:O	2.14	0.48
1:A:257:HIS:CE1	4:A:2238:HOH:O	2.49	0.47
1:A:331:LEU:CD2	4:A:2311:HOH:O	2.63	0.47
1:A:224:ASP:OD2	1:A:257:HIS:HD2	1.97	0.47
2:A:1478:ACT:H2	4:A:2299:HOH:O	2.15	0.47
1:A:160:LYS:HD2	1:A:176:TRP:CZ3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:N	1:A:171:GLU:OE2	2.46	0.47
1:A:211:ARG:HD3	1:A:211:ARG:C	2.39	0.47
1:A:220:LYS:HB3	1:A:257:HIS:CD2	2.49	0.47
1:A:30:GLN:HG2	1:A:300:TYR:CB	2.45	0.46
1:A:330:LYS:HB2	4:A:2311:HOH:O	2.15	0.46
1:A:430:THR:HG21	1:A:456:LYS:CE	2.45	0.46
1:A:139:ASN:HB3	1:A:140:HIS:CD2	2.50	0.46
1:A:305:PHE:CD1	1:A:305:PHE:N	2.84	0.46
1:A:124:GLU:HB3	1:A:128:ARG:HH21	1.81	0.45
1:A:235:GLN:HE21	1:A:235:GLN:N	2.14	0.45
1:A:236:ASP:O	1:A:237:PHE:C	2.60	0.45
1:A:275:PHE:O	1:A:328:ARG:HD3	2.17	0.45
1:A:203:GLN:HG2	1:A:233:VAL:CG1	2.48	0.44
1:A:138:VAL:HG11	1:A:222:PHE:CZ	2.51	0.44
1:A:203:GLN:HG2	1:A:233:VAL:HG11	1.99	0.44
1:A:84:ILE:HD12	1:A:86:LEU:HD11	2.00	0.44
1:A:33:ARG:HD2	1:A:337:PHE:HE2	1.83	0.44
1:A:90:PHE:CE1	1:A:201:TRP:CE2	3.07	0.43
1:A:153:LYS:O	1:A:156:TRP:HB2	2.18	0.43
1:A:134:LEU:O	1:A:210:TYR:HA	2.18	0.43
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.89	0.42
1:A:357:GLU:H	1:A:357:GLU:HG2	1.65	0.42
1:A:430:THR:CG2	1:A:456:LYS:HE3	2.49	0.42
1:A:145:HIS:HA	1:A:146:PRO:HD2	1.92	0.41
1:A:148:LEU:HB2	4:A:2160:HOH:O	2.20	0.41
1:A:389:SER:OG	1:A:416:THR:CG2	2.68	0.41
1:A:105:PHE:HD2	4:A:2108:HOH:O	2.03	0.41
1:A:236:ASP:OD1	1:A:236:ASP:N	2.50	0.40
1:A:145:HIS:CE1	1:A:147:TRP:CG	3.09	0.40

All (6) 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)
4:A:2082:HOH:O	4:A:2375:HOH:O[3_544]	1.85	0.35
1:A:246:ASP:OD2	1:A:451:ARG:NH2[3_554]	1.89	0.31
4:A:2112:HOH:O	4:A:2323:HOH:O[4_545]	1.99	0.21
1:A:50:ASP:CB	1:A:322:ARG:NH2[4_545]	2.00	0.20
1:A:437:GLN:NE2	4:A:2164:HOH:O[2_554]	2.15	0.05
4:A:2141:HOH:O	4:A:2397:HOH:O[3_554]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	452/454 (100%)	423 (94%)	25 (6%)	4 (1%)	14	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370[A]	ASP
1	A	370[B]	ASP
1	A	181	PRO
1	A	207	ILE

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	401/401 (100%)	390 (97%)	11 (3%)	39	34

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	92	ASN
1	A	94	LYS
1	A	154	LYS
1	A	161	LYS
1	A	170	GLN
1	A	181	PRO

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Mol	Chain	Res	Type
1	A	228	LYS
1	A	235	GLN
1	A	312	VAL
1	A	453	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	140	HIS
1	A	235	GLN
1	A	257	HIS
1	A	280	GLN
1	A	437	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 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
2	ACT	A	1479	-	3,3,3	1.26	0	3,3,3	0.90	0
2	ACT	A	1478	-	3,3,3	1.00	0	3,3,3	0.44	0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1479	ACT	2	0
2	A	1478	ACT	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 [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	452/454 (99%)	-0.09	4 (0%) 81 83	7, 18, 34, 47	3 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	GLY	3.7
1	A	322	ARG	2.8
1	A	477	LEU	2.8
1	A	166	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACT	A	1479	4/4	0.87	0.13	34,38,42,46	0
2	ACT	A	1478	4/4	0.90	0.11	31,33,35,35	0
3	CA	A	1480	1/1	0.99	0.04	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	1481	1/1	0.99	0.04	26,26,26,26	0
3	CA	A	1482	1/1	0.99	0.04	31,31,31,31	0
3	CA	A	1483	1/1	0.99	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.