Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 07:23 am BST

PDB ID	:	5IDI
Title	:	Structure of beta glucosidase 1A from Thermotoga neapolitana, mutant E349A
Authors	:	Kulkarni, T.; Nordberg Karlsson, E.; Logan, D.T.
Deposited on	:	2016-02-24
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 (i) symbol.

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

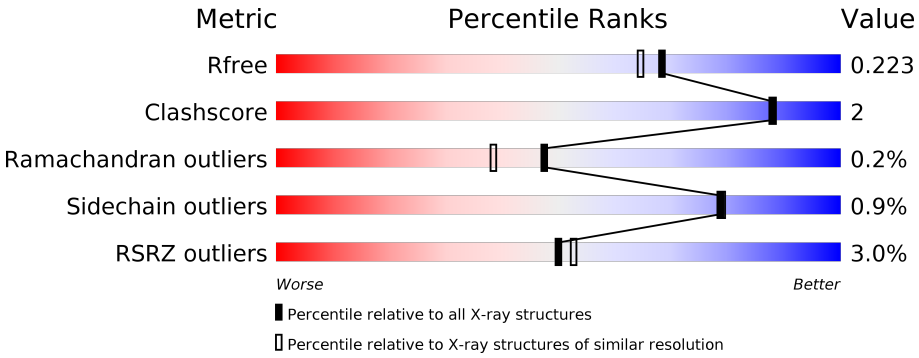
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on 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 <=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	452	2% 86% 12%
1	B	452	4% 87% 10%

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	501	-	-	X	-
2	ACT	A	502	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7747 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.

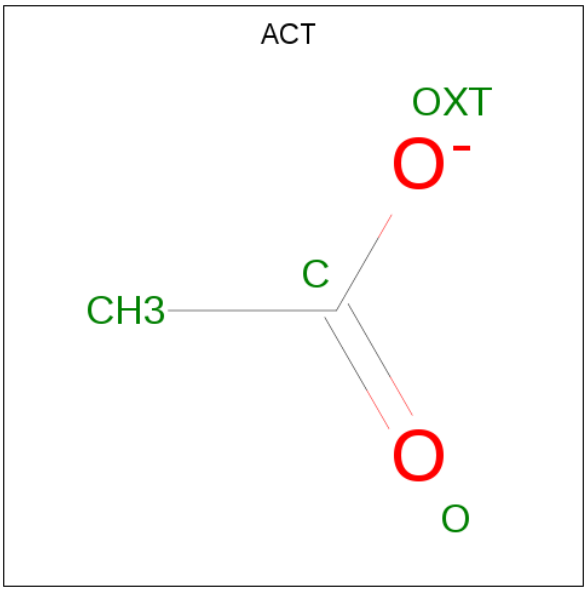
- Molecule 1 is a protein called 1,4-beta-D-glucan glucohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3646	2364	616	658	8			
1	B	444	Total	C	N	O	S	0	1	0
			3660	2372	617	663	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	LEU	PRO	conflict	UNP B9K7M5
A	349	GLY	GLU	engineered mutation	UNP B9K7M5
A	445	LEU	-	expression tag	UNP B9K7M5
A	446	GLU	-	expression tag	UNP B9K7M5
A	447	HIS	-	expression tag	UNP B9K7M5
A	448	HIS	-	expression tag	UNP B9K7M5
A	449	HIS	-	expression tag	UNP B9K7M5
A	450	HIS	-	expression tag	UNP B9K7M5
A	451	HIS	-	expression tag	UNP B9K7M5
A	452	HIS	-	expression tag	UNP B9K7M5
B	165	LEU	PRO	conflict	UNP B9K7M5
B	349	GLY	GLU	engineered mutation	UNP B9K7M5
B	445	LEU	-	expression tag	UNP B9K7M5
B	446	GLU	-	expression tag	UNP B9K7M5
B	447	HIS	-	expression tag	UNP B9K7M5
B	448	HIS	-	expression tag	UNP B9K7M5
B	449	HIS	-	expression tag	UNP B9K7M5
B	450	HIS	-	expression tag	UNP B9K7M5
B	451	HIS	-	expression tag	UNP B9K7M5
B	452	HIS	-	expression tag	UNP B9K7M5

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is water.

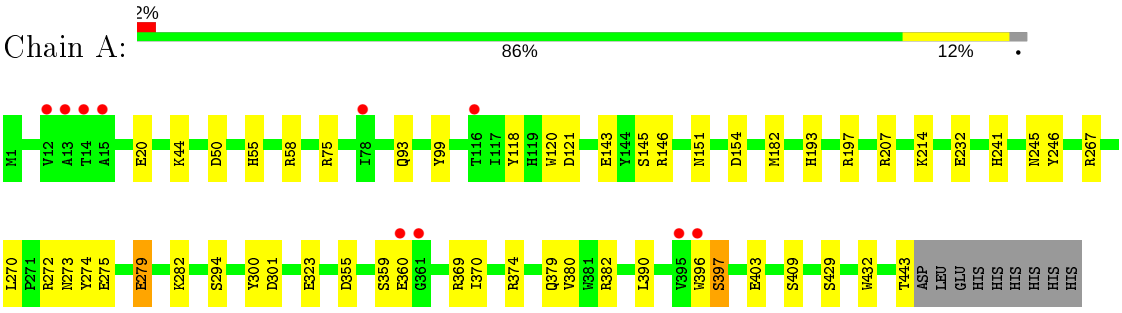
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	193	Total O 193 193	0	0
3	B	236	Total O 236 236	0	0

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 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.

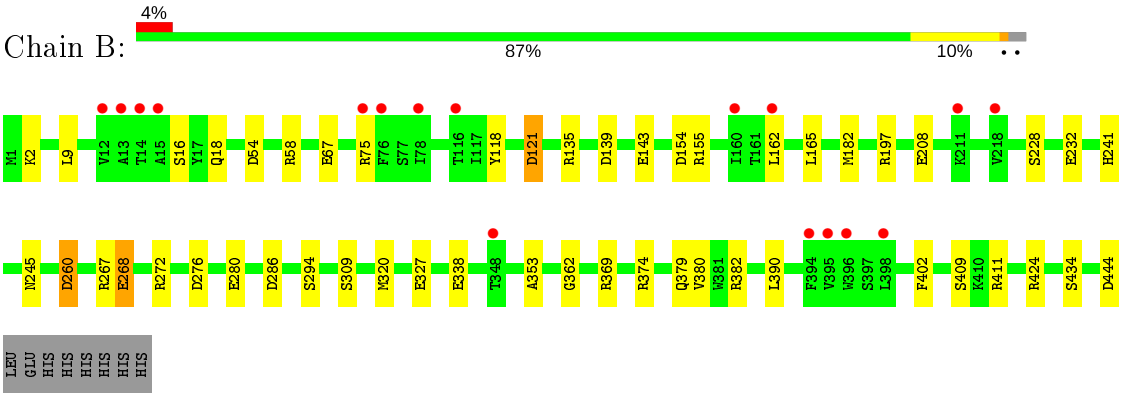
- Molecule 1: 1,4-beta-D-glucan glucohydrolase

Chain A:



- Molecule 1: 1,4-beta-D-glucan glucohydrolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.28Å 98.73Å 154.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-1.90) 98.9 (29.56-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	11.63 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.169 , 0.215 0.179 , 0.223	Depositor DCC
R_{free} test set	4096 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7747	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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, 0.333 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: ACT

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	1.37	15/3759 (0.4%)	1.24	25/5104 (0.5%)
1	B	1.44	20/3776 (0.5%)	1.18	22/5127 (0.4%)
All	All	1.40	35/7535 (0.5%)	1.21	47/10231 (0.5%)

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	SER	CB-OG	-9.55	1.29	1.42
1	B	327	GLU	CD-OE1	9.17	1.35	1.25
1	B	232	GLU	CD-OE1	9.13	1.35	1.25
1	B	327	GLU	CG-CD	8.56	1.64	1.51
1	B	409	SER	CB-OG	7.94	1.52	1.42
1	A	232	GLU	CD-OE1	7.89	1.34	1.25
1	A	93	GLN	CA-CB	7.38	1.70	1.53
1	A	197	ARG	CZ-NH1	7.21	1.42	1.33
1	B	67	GLU	CD-OE2	-7.10	1.17	1.25
1	B	444	ASP	CB-CG	6.92	1.66	1.51
1	B	143	GLU	CD-OE1	6.50	1.32	1.25
1	A	409	SER	CB-OG	6.50	1.50	1.42
1	A	143	GLU	CD-OE1	6.45	1.32	1.25
1	B	228	SER	CB-OG	6.22	1.50	1.42
1	B	268	GLU	CG-CD	5.93	1.60	1.51
1	B	338	GLU	CD-OE2	-5.81	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	260	ASP	CB-CG	5.61	1.63	1.51
1	A	355	ASP	CB-CG	5.60	1.63	1.51
1	A	397	SER	CB-OG	5.50	1.49	1.42
1	B	118	TYR	CE1-CZ	5.49	1.45	1.38
1	A	279	GLU	CD-OE2	5.49	1.31	1.25
1	B	208	GLU	CD-OE1	5.49	1.31	1.25
1	A	275	GLU	CD-OE1	5.41	1.31	1.25
1	A	145	SER	CB-OG	5.36	1.49	1.42
1	B	280	GLU	CD-OE2	-5.30	1.19	1.25
1	B	409	SER	CA-CB	5.29	1.60	1.52
1	A	99	TYR	CG-CD1	-5.24	1.32	1.39
1	A	374	ARG	CZ-NH1	5.20	1.39	1.33
1	B	434	SER	CB-OG	-5.19	1.35	1.42
1	A	151	ASN	C-O	5.14	1.33	1.23
1	A	300	TYR	CZ-OH	-5.13	1.29	1.37
1	B	16	SER	CB-OG	5.12	1.49	1.42
1	A	246	TYR	CD1-CE1	5.06	1.47	1.39
1	B	294	SER	CB-OG	-5.03	1.35	1.42
1	B	327	GLU	CD-OE2	5.01	1.31	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	197	ARG	NE-CZ-NH2	-13.87	113.36	120.30
1	A	146	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	A	374	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	A	374	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	A	146	ARG	NE-CZ-NH1	10.95	125.77	120.30
1	B	75	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	A	75	ARG	NE-CZ-NH1	-9.78	115.41	120.30
1	A	197	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	A	355	ASP	CB-CG-OD1	9.00	126.40	118.30
1	A	75	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	B	75	ARG	NE-CZ-NH2	7.95	124.27	120.30
1	B	424	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	154	ASP	CB-CG-OD1	7.56	125.10	118.30
1	B	424	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	154	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	121	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	374	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	58	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	155	ARG	NE-CZ-NH1	6.36	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	58	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	139	ASP	CB-CG-OD1	6.12	123.80	118.30
1	B	320	MET	CG-SD-CE	6.10	109.96	100.20
1	A	50	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	121	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	301	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	B	54	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	369	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	146	ARG	CD-NE-CZ	5.83	131.76	123.60
1	B	121	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	355	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	B	286	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	207	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	276	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	267	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	369	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	267	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	232	GLU	CG-CD-OE2	-5.46	107.39	118.30
1	A	282	LYS	CD-CE-NZ	-5.43	99.21	111.70
1	A	121	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	443	THR	CA-CB-OG1	-5.39	97.68	109.00
1	B	197	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	374	ARG	CG-CD-NE	-5.35	100.57	111.80
1	A	443	THR	CA-CB-CG2	5.26	119.77	112.40
1	B	320	MET	CA-CB-CG	5.22	122.18	113.30
1	B	67	GLU	CG-CD-OE1	5.18	128.67	118.30
1	B	9	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	A	270	LEU	CB-CG-CD2	5.16	119.77	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	SER	Peptide

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	3646	0	3504	17	0
1	B	3660	0	3514	8	0
2	A	8	0	6	5	0
2	B	4	0	3	1	0
3	A	193	0	0	4	0
3	B	236	0	0	2	0
All	All	7747	0	7027	28	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 (28) 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:370:ILE:HD11	1:A:429:SER:HA	1.52	0.88
2:B:501:ACT:H1	3:B:665:HOH:O	1.73	0.86
1:B:379:GLN:HE22	1:B:382:ARG:HH11	1.24	0.84
1:A:370:ILE:CD1	1:A:429:SER:HA	2.15	0.76
2:A:501:ACT:H1	3:A:669:HOH:O	1.85	0.75
1:A:379:GLN:HE22	1:A:382:ARG:HH11	1.36	0.73
1:B:380:VAL:HG13	1:B:390:LEU:CD2	2.29	0.62
1:A:182:MET:HG2	1:B:182:MET:HG2	1.82	0.62
1:A:294:SER:OG	2:A:502:ACT:H2	2.05	0.57
2:A:502:ACT:H1	3:A:769:HOH:O	2.13	0.48
1:B:162:LEU:HB2	1:B:165:LEU:HD11	1.97	0.47
1:A:193:HIS:CE1	1:A:274:TYR:HB2	2.50	0.46
1:B:241:HIS:O	1:B:245:ASN:HB2	2.14	0.46
1:A:403:GLU:OE1	2:A:501:ACT:OXT	2.34	0.45
1:A:214:LYS:HE3	3:A:731:HOH:O	2.17	0.45
1:B:268:GLU:HB2	3:B:796:HOH:O	2.18	0.44
1:A:272:ARG:HA	1:A:272:ARG:HD3	1.93	0.42
2:A:501:ACT:H2	3:A:667:HOH:O	2.18	0.42
1:B:18:GLN:HA	1:B:402:PHE:HB3	2.02	0.42
1:A:118:TYR:CZ	1:A:120:TRP:HA	2.55	0.42
1:A:294:SER:HB2	1:A:323:GLU:O	2.20	0.41
1:B:353:ALA:HA	1:B:411:ARG:O	2.20	0.41
1:A:272:ARG:O	1:A:273:ASN:HB2	2.21	0.41
1:A:370:ILE:HD12	1:A:432:TRP:CB	2.50	0.41
1:A:241:HIS:O	1:A:245:ASN:HB2	2.21	0.41
1:A:20:GLU:HA	1:A:55:HIS:HB3	2.03	0.41
1:A:380:VAL:HG13	1:A:390:LEU:CD2	2.51	0.41
1:A:396:TRP:HA	1:A:397:SER:HA	1.91	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	441/452 (98%)	429 (97%)	11 (2%)	1 (0%)	47 38
1	B	443/452 (98%)	432 (98%)	10 (2%)	1 (0%)	47 38
All	All	884/904 (98%)	861 (97%)	21 (2%)	2 (0%)	47 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLU
1	B	362	GLY

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	380/389 (98%)	378 (100%)	2 (0%)	88 89
1	B	382/389 (98%)	377 (99%)	5 (1%)	69 68
All	All	762/778 (98%)	755 (99%)	7 (1%)	78 79

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS

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Mol	Chain	Res	Type
1	A	279	GLU
1	B	2	LYS
1	B	121	ASP
1	B	135	ARG
1	B	260	ASP
1	B	272	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	379	GLN
1	B	379	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 carbohydrates in this entry.

5.6 Ligand geometry

3 ligands are 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	ACT	B	501	-	1,3,3	3.09	1 (100%)	0,3,3	0.00	-
2	ACT	A	502	-	1,3,3	2.79	1 (100%)	0,3,3	0.00	-
2	ACT	A	501	-	1,3,3	3.34	1 (100%)	0,3,3	0.00	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ACT	CH3-C	-3.34	1.44	1.48
2	B	501	ACT	CH3-C	-3.09	1.44	1.48
2	A	502	ACT	CH3-C	2.79	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ACT	1	0
2	A	502	ACT	2	0
2	A	501	ACT	3	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	443/452 (98%)	-0.04	10 (2%) 60 63	20, 26, 41, 68	0
1	B	444/452 (98%)	-0.11	17 (3%) 40 43	18, 24, 40, 56	0
All	All	887/904 (98%)	-0.08	27 (3%) 50 53	18, 25, 41, 68	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	VAL	3.3
1	A	360	GLU	3.3
1	A	13	ALA	3.3
1	B	211	LYS	3.1
1	B	396	TRP	3.1
1	B	13	ALA	2.9
1	A	395	VAL	2.8
1	B	348	THR	2.7
1	B	12	VAL	2.6
1	A	12	VAL	2.5
1	B	162	LEU	2.5
1	A	14	THR	2.5
1	B	395	VAL	2.5
1	B	75	ARG	2.4
1	A	15	ALA	2.3
1	A	78	ILE	2.3
1	B	160	ILE	2.2
1	A	361	GLY	2.2
1	A	396	TRP	2.2
1	B	14	THR	2.2
1	B	15	ALA	2.2
1	B	76	PHE	2.2
1	B	78	ILE	2.1
1	A	116	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	116	THR	2.1
1	B	394	PHE	2.0
1	B	398	LEU	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 carbohydrates 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, 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	B-factors(Å^2)	Q<0.9
2	ACT	A	502	4/4	0.82	0.17	37,38,44,48	0
2	ACT	B	501	4/4	0.84	0.18	19,23,24,34	0
2	ACT	A	501	4/4	0.89	0.15	23,25,26,32	0

6.5 Other polymers (i)

There are no such residues in this entry.