wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2024 – 08:04 AM EST

PDB ID	:	3PFB
Title	:	Crystal structure of the Lactobacillus johnsonii cinnamoyl esterase LJ0536 S106A mutant in complex with ethylferulate
Authors	:	Stogios, P.J.; Lai, K.K.; Vu, C.; Xu, X.; Cui, H.; Molloy, S.; Gonzalez, C.F.; Yakunin, A.; Savchenko, A.
Deposited on	:	2010-10-28
Resolution	:	1.58 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

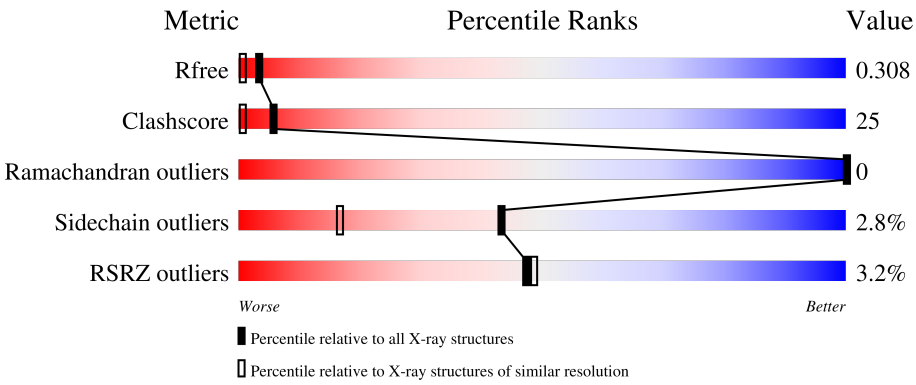
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 <=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	270	4% 58% 33% • 7%
1	B	270	2% 61% 29% • 7%

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	NH4	A	252	-	-	X	-
2	NH4	A	253	-	-	X	-
2	NH4	B	258	-	-	X	-
4	ZYC	A	256	-	X	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4898 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 Cinnamoyl esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1965	1246	332	381	6	0	2	0
1	B	250	1974	1253	331	384	6	0	4	0

There are 44 discrepancies between the modelled and reference sequences:

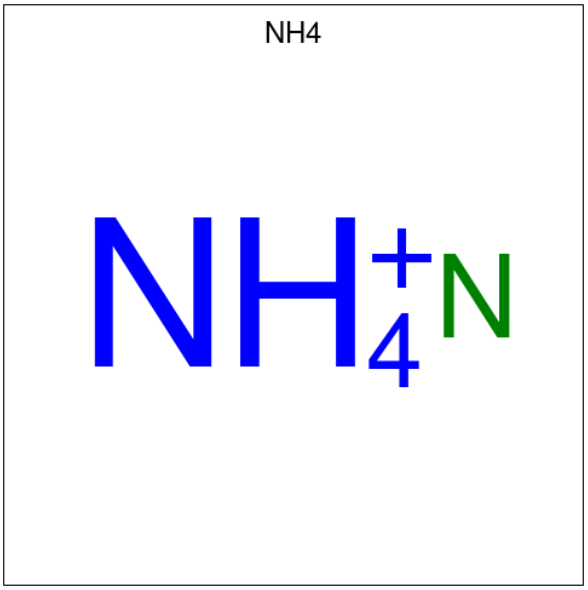
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP D3YEX6
A	-19	GLY	-	expression tag	UNP D3YEX6
A	-18	SER	-	expression tag	UNP D3YEX6
A	-17	SER	-	expression tag	UNP D3YEX6
A	-16	HIS	-	expression tag	UNP D3YEX6
A	-15	HIS	-	expression tag	UNP D3YEX6
A	-14	HIS	-	expression tag	UNP D3YEX6
A	-13	HIS	-	expression tag	UNP D3YEX6
A	-12	HIS	-	expression tag	UNP D3YEX6
A	-11	HIS	-	expression tag	UNP D3YEX6
A	-10	SER	-	expression tag	UNP D3YEX6
A	-9	SER	-	expression tag	UNP D3YEX6
A	-8	GLY	-	expression tag	UNP D3YEX6
A	-7	ARG	-	expression tag	UNP D3YEX6
A	-6	GLU	-	expression tag	UNP D3YEX6
A	-5	ASN	-	expression tag	UNP D3YEX6
A	-4	LEU	-	expression tag	UNP D3YEX6
A	-3	TYR	-	expression tag	UNP D3YEX6
A	-2	PHE	-	expression tag	UNP D3YEX6
A	-1	GLN	-	expression tag	UNP D3YEX6
A	0	GLY	-	expression tag	UNP D3YEX6
A	106	ALA	SER	engineered mutation	UNP D3YEX6
B	-20	MET	-	expression tag	UNP D3YEX6
B	-19	GLY	-	expression tag	UNP D3YEX6
B	-18	SER	-	expression tag	UNP D3YEX6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP D3YEX6
B	-16	HIS	-	expression tag	UNP D3YEX6
B	-15	HIS	-	expression tag	UNP D3YEX6
B	-14	HIS	-	expression tag	UNP D3YEX6
B	-13	HIS	-	expression tag	UNP D3YEX6
B	-12	HIS	-	expression tag	UNP D3YEX6
B	-11	HIS	-	expression tag	UNP D3YEX6
B	-10	SER	-	expression tag	UNP D3YEX6
B	-9	SER	-	expression tag	UNP D3YEX6
B	-8	GLY	-	expression tag	UNP D3YEX6
B	-7	ARG	-	expression tag	UNP D3YEX6
B	-6	GLU	-	expression tag	UNP D3YEX6
B	-5	ASN	-	expression tag	UNP D3YEX6
B	-4	LEU	-	expression tag	UNP D3YEX6
B	-3	TYR	-	expression tag	UNP D3YEX6
B	-2	PHE	-	expression tag	UNP D3YEX6
B	-1	GLN	-	expression tag	UNP D3YEX6
B	0	GLY	-	expression tag	UNP D3YEX6
B	106	ALA	SER	engineered mutation	UNP D3YEX6

- Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total N 1 1	0	0
2	A	1	Total N 1 1	0	0

Continued on next page...

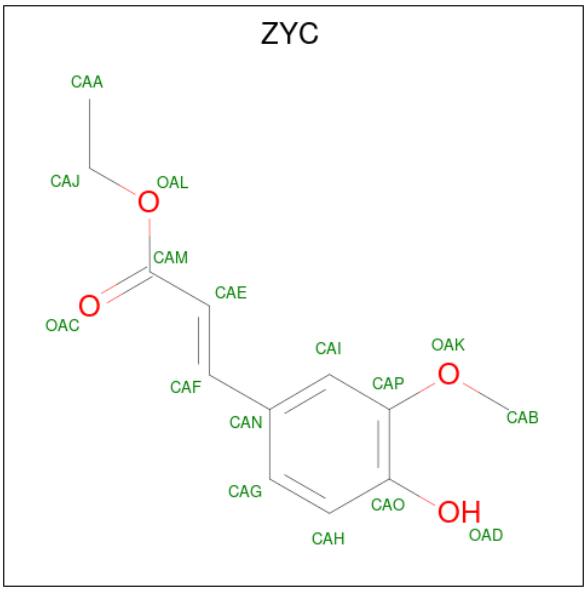
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total N 1 1	0	0
2	A	1	Total N 1 1	0	0
2	A	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	3	Total Cl 3 3	0	0

- Molecule 4 is ethyl (2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate (three-letter code: ZYC) (formula: $C_{12}H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	16	12	4	0	0
			Total	C	O		
4	B	1	16	12	4	0	0

- Molecule 5 is water.

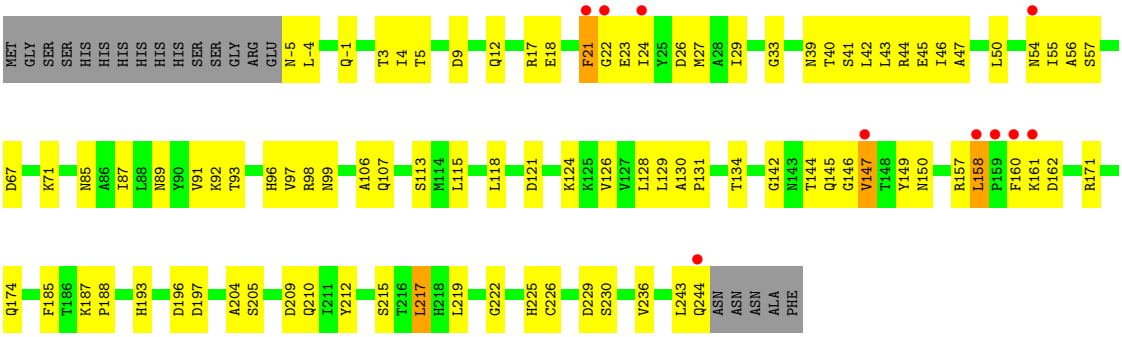
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	449	449	449	0	0
			Total	O		
5	B	458	458	458	0	0

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.

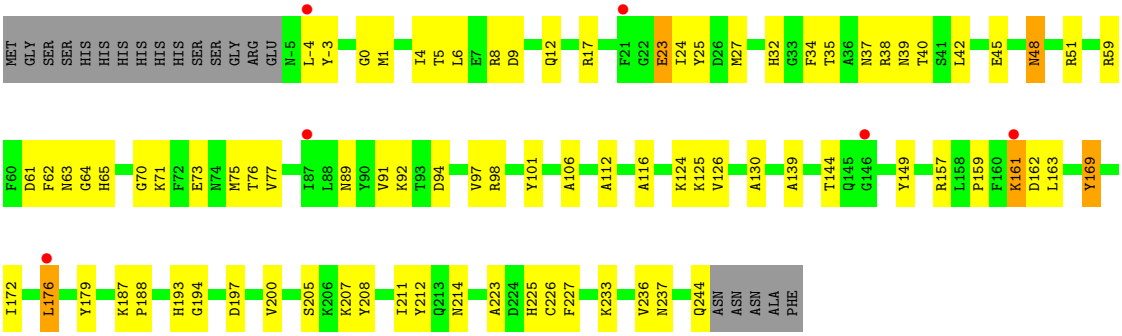
- Molecule 1: Cinnamoyl esterase

Chain A:



- Molecule 1: Cinnamoyl esterase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	72.26Å 83.89Å 88.95Å 90.00° 98.21° 90.00°	Depositor
Resolution (Å)	44.20 – 1.58 36.20 – 1.58	Depositor EDS
% Data completeness (in resolution range)	73.1 (44.20-1.58) 73.1 (36.20-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.304 0.218 , 0.308	Depositor DCC
R_{free} test set	2673 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4898	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2515e-03.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZYC, CL, NH4

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	0.99	1/2011 (0.0%)	0.92	2/2732 (0.1%)
1	B	1.03	2/2026 (0.1%)	0.98	2/2753 (0.1%)
All	All	1.01	3/4037 (0.1%)	0.95	4/5485 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	TYR	CE1-CZ	5.17	1.45	1.38
1	B	116	ALA	CA-CB	-5.11	1.41	1.52
1	A	185	PHE	CE2-CZ	5.05	1.47	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	176	LEU	CB-CG-CD2	-6.60	99.78	111.00
1	A	171	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	129	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	B	8	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	1965	0	1926	97	0
1	B	1974	0	1937	102	0
2	A	5	0	0	6	0
2	B	11	0	0	2	0
3	A	1	0	0	0	0
3	B	3	0	0	2	0
4	A	16	0	13	13	0
4	B	16	0	13	3	0
5	A	449	0	0	39	0
5	B	458	0	0	42	0
All	All	4898	0	3889	200	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 25.

The worst 5 of 200 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:B:6:LEU:HG	5:B:1785:HOH:O	1.42	1.19
2:B:258:NH4:N	3:B:261:CL:CL	2.28	1.02
1:A:26:ASP:HA	5:A:2076:HOH:O	1.60	1.01
1:B:161:LYS:O	1:B:161:LYS:HG2	1.57	1.00
1:B:65:HIS:HB3	5:B:1620:HOH:O	1.63	0.99

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	250/270 (93%)	240 (96%)	10 (4%)	0	100	100
1	B	252/270 (93%)	237 (94%)	15 (6%)	0	100	100
All	All	502/540 (93%)	477 (95%)	25 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	214/229 (93%)	205 (96%)	9 (4%)	30 7
1	B	216/229 (94%)	213 (99%)	3 (1%)	67 45
All	All	430/458 (94%)	418 (97%)	12 (3%)	43 17

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASP
1	A	230	SER
1	B	161	LYS
1	B	23	GLU
1	A	147	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	HIS
1	B	203	ASN
1	B	237	ASN
1	B	225	HIS
1	A	210	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 16 are modelled with single atom and 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	$\#\|Z\| > 2$
4	ZYC	A	256	-	16,16,16	1.85	4 (25%)	20,20,20	3.32	10 (50%)
4	ZYC	B	264	-	16,16,16	1.54	2 (12%)	20,20,20	2.63	7 (35%)

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
4	ZYC	A	256	-	-	6/10/10/10	0/1/1/1
4	ZYC	B	264	-	-	5/10/10/10	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	256	ZYC	CAE-CAM	-4.99	1.36	1.48
4	A	256	ZYC	CAN-CAF	-3.90	1.36	1.47
4	B	264	ZYC	CAE-CAM	-3.87	1.39	1.48
4	B	264	ZYC	CAN-CAF	-2.73	1.39	1.47
4	A	256	ZYC	CAE-CAF	2.19	1.38	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	256	ZYC	CAN-CAF-CAE	-9.48	105.21	126.91
4	B	264	ZYC	CAJ-OAL-CAM	6.45	129.14	116.42
4	A	256	ZYC	OAK-CAP-CAO	6.37	123.80	114.57
4	B	264	ZYC	OAL-CAJ-CAA	5.56	128.86	108.42
4	A	256	ZYC	CAB-OAK-CAP	-5.42	109.36	117.53

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	264	ZYC	CAA-CAJ-OAL-CAM
4	A	256	ZYC	CAO-CAP-OAK-CAB
4	A	256	ZYC	CAE-CAF-CAN-CAI
4	A	256	ZYC	CAI-CAP-OAK-CAB
4	A	256	ZYC	CAE-CAF-CAN-CAG

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	256	ZYC	13	0
4	B	264	ZYC	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 (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	250/270 (92%)	0.50	10 (4%) 38 39	17, 23, 33, 40	0
1	B	250/270 (92%)	0.45	6 (2%) 59 60	17, 22, 29, 34	0
All	All	500/540 (92%)	0.48	16 (3%) 47 49	17, 23, 32, 40	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	4.1
1	A	21	PHE	3.8
1	B	146	GLY	3.2
1	A	160	PHE	3.0
1	A	158	LEU	3.0

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 monosaccharides 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
4	ZYC	A	256	16/16	0.75	0.23	20,39,45,45	16
4	ZYC	B	264	16/16	0.86	0.16	20,31,33,34	0
2	NH4	B	258	1/1	0.88	0.13	26,26,26,26	0
2	NH4	A	254	1/1	0.94	0.10	30,30,30,30	0
2	NH4	B	259	1/1	0.95	0.19	25,25,25,25	0
3	CL	B	261	1/1	0.96	0.07	48,48,48,48	0
2	NH4	B	256	1/1	0.96	0.08	22,22,22,22	0
2	NH4	B	260	1/1	0.96	0.20	26,26,26,26	0
2	NH4	A	253	1/1	0.97	0.12	17,17,17,17	0
3	CL	B	263	1/1	0.97	0.06	53,53,53,53	0
2	NH4	B	252	1/1	0.98	0.17	14,14,14,14	0
2	NH4	B	254	1/1	0.98	0.20	14,14,14,14	0
3	CL	A	255	1/1	0.98	0.08	49,49,49,49	0
2	NH4	B	255	1/1	0.98	0.08	17,17,17,17	0
3	CL	B	262	1/1	0.98	0.04	44,44,44,44	0
2	NH4	A	252	1/1	0.98	0.22	15,15,15,15	0
2	NH4	B	257	1/1	0.98	0.11	25,25,25,25	0
2	NH4	B	251	1/1	0.98	0.30	22,22,22,22	0
2	NH4	A	251	1/1	0.99	0.27	15,15,15,15	0
2	NH4	A	250	1/1	0.99	0.21	14,14,14,14	0
2	NH4	B	253	1/1	0.99	0.15	16,16,16,16	0
2	NH4	B	250	1/1	0.99	0.20	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.