



Full wwPDB X-ray Structure Validation Report

Nov 7, 2014 – 12:57 PM EST

PDB ID : 4L1O
Title : Crystal structure of human ALDH3A1 with inhibitor 1-{[4-(1,3-benzodioxol-5-ylmethyl)piperazin-1-yl]methyl}-1H-indole-2,3-dione
Authors : Hurley, T.D.; Parajuli, B.
Deposited on : 2013-06-03
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

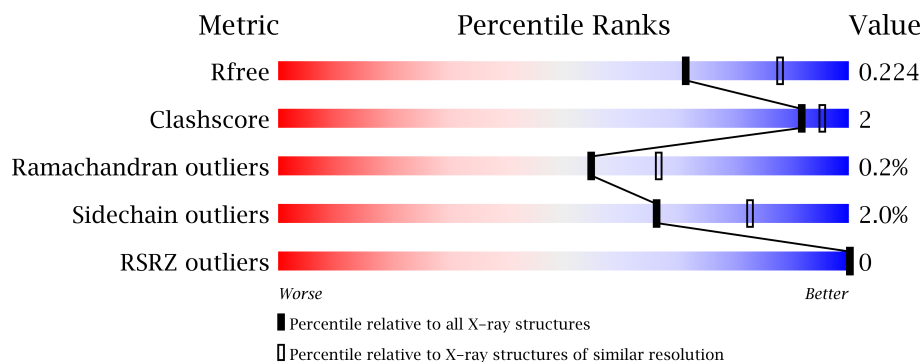
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : trunk24195
Percentile statistics : 23426
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk24195

1 Overall quality at a glance



The reported resolution of this entry is 2.30 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}	77520	3364 (2.30-2.30)
Clashscore	88313	3960 (2.30-2.30)
Ramachandran outliers	86584	3922 (2.30-2.30)
C α geometry	86677	3925 (2.30-2.30)
Sidechain outliers	86556	3921 (2.30-2.30)
RSRZ outliers	77580	3365 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	469	
1	B	469	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	1VL	A	601	-	X
2	1VL	B	601	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7809 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	10	0
			3550	2259	603	669	19			
1	B	452	Total	C	N	O	S	0	5	0
			3563	2266	609	668	20			

There are 34 discrepancies between the modelled and reference sequences:

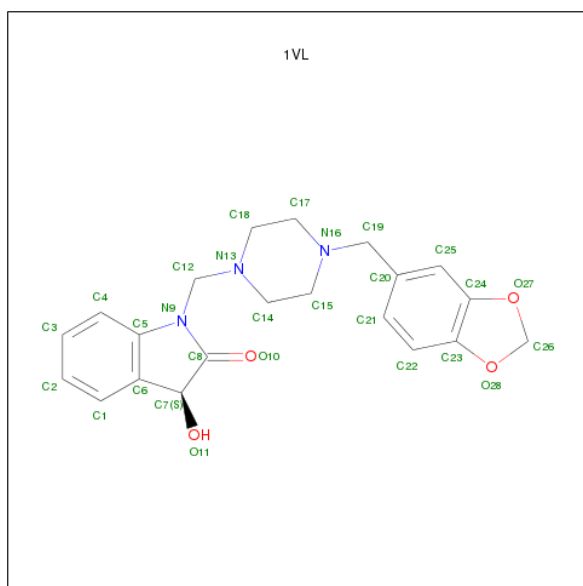
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	EXPRESSION TAG	UNP P30838
A	-15	HIS	-	EXPRESSION TAG	UNP P30838
A	-14	HIS	-	EXPRESSION TAG	UNP P30838
A	-13	HIS	-	EXPRESSION TAG	UNP P30838
A	-12	HIS	-	EXPRESSION TAG	UNP P30838
A	-11	HIS	-	EXPRESSION TAG	UNP P30838
A	-10	SER	-	EXPRESSION TAG	UNP P30838
A	-9	SER	-	EXPRESSION TAG	UNP P30838
A	-8	GLY	-	EXPRESSION TAG	UNP P30838
A	-7	LEU	-	EXPRESSION TAG	UNP P30838
A	-6	VAL	-	EXPRESSION TAG	UNP P30838
A	-5	PRO	-	EXPRESSION TAG	UNP P30838
A	-4	ARG	-	EXPRESSION TAG	UNP P30838
A	-3	GLY	-	EXPRESSION TAG	UNP P30838
A	-2	SER	-	EXPRESSION TAG	UNP P30838
A	-1	HIS	-	EXPRESSION TAG	UNP P30838
A	133	ALA	SER	NATURAL VARIANT	UNP P30838
B	-16	HIS	-	EXPRESSION TAG	UNP P30838
B	-15	HIS	-	EXPRESSION TAG	UNP P30838
B	-14	HIS	-	EXPRESSION TAG	UNP P30838
B	-13	HIS	-	EXPRESSION TAG	UNP P30838
B	-12	HIS	-	EXPRESSION TAG	UNP P30838
B	-11	HIS	-	EXPRESSION TAG	UNP P30838
B	-10	SER	-	EXPRESSION TAG	UNP P30838
B	-9	SER	-	EXPRESSION TAG	UNP P30838

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	EXPRESSION TAG	UNP P30838
B	-7	LEU	-	EXPRESSION TAG	UNP P30838
B	-6	VAL	-	EXPRESSION TAG	UNP P30838
B	-5	PRO	-	EXPRESSION TAG	UNP P30838
B	-4	ARG	-	EXPRESSION TAG	UNP P30838
B	-3	GLY	-	EXPRESSION TAG	UNP P30838
B	-2	SER	-	EXPRESSION TAG	UNP P30838
B	-1	HIS	-	EXPRESSION TAG	UNP P30838
B	133	ALA	SER	NATURAL VARIANT	UNP P30838

- Molecule 2 is (3S)-1-1-[4-(1,3-BENZODIOXOL-5-YLMETHYL)PIPERAZIN-1-YL]METHYL}-3-HYDROXY-1,3-DIHYDRO-2H-INDOL-2-ONE (three-letter code: 1VL) (formula: C₂₁H₂₃N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	13	3	2		
2	B	1	Total	C	N	O	0	0
			18	13	3	2		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

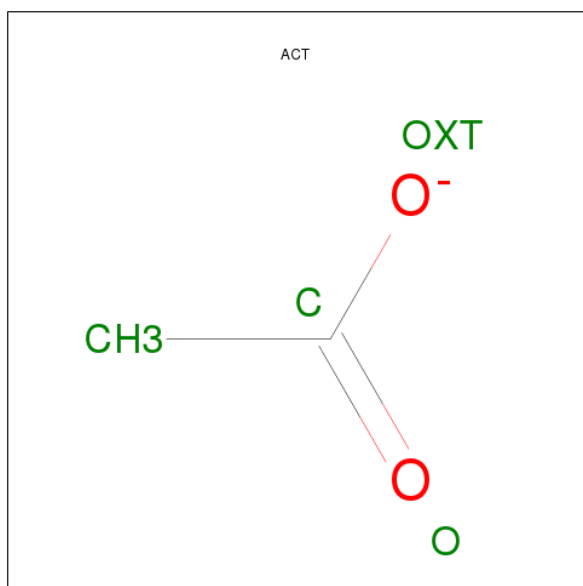
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	K	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is water.

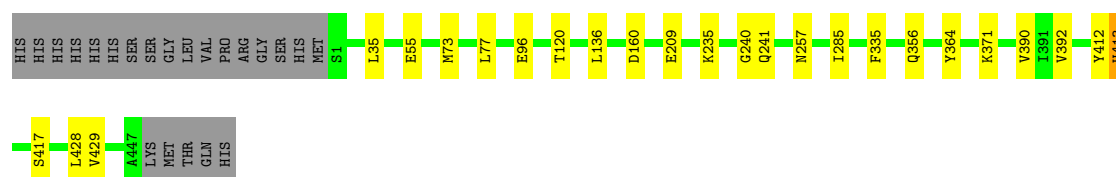
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	343	Total O 343 343	0	0
5	B	305	Total O 305 305	0	0

3 Residue-property plots

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.

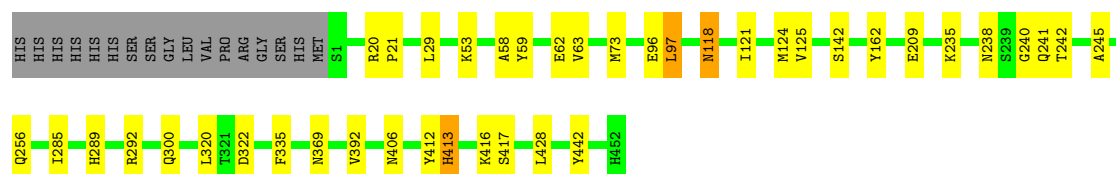
- Molecule 1: Aldehyde dehydrogenase

Chain A: 



- Molecule 1: Aldehyde dehydrogenase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.26Å 86.40Å 170.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.95 – 2.30 47.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (47.95-2.30) 96.0 (47.95-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.65 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.177 , 0.225 0.184 , 0.224	Depositor DCC
R_{free} test set	1990 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 14.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 39389 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7809	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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, 0.375 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: 1VL, K, 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	0.35	0/3635	0.52	1/4927 (0.0%)
1	B	0.38	0/3647	0.52	0/4942
All	All	0.36	0/7282	0.52	1/9869 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3550	0	3583	14	0
1	B	3563	0	3593	23	0
2	A	18	0	0	0	0
2	B	18	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	3	0	0
4	B	4	0	3	1	0
5	A	343	0	0	0	0
5	B	305	0	0	1	0
All	All	7809	0	7182	34	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (34) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:412:TYR:O	1:A:413:HIS:HB2	2.00	0.60
1:A:120[B]:THR:HG22	1:A:136:LEU:HD21	1.84	0.58
1:B:289:HIS:HD2	1:B:292:ARG:HE	1.55	0.54
1:A:120[B]:THR:CG2	1:A:136:LEU:HD21	2.37	0.54
1:A:428:LEU:CD2	1:B:392:VAL:HG13	2.39	0.52
1:B:235:LYS:O	1:B:240:GLY:HA2	2.11	0.51
1:B:53:LYS:HE3	1:B:238:ASN:ND2	2.26	0.51
1:B:412:TYR:O	1:B:413:HIS:HB2	2.12	0.50
1:B:256:GLN:HE22	1:B:322:ASP:H	1.60	0.50
1:A:120[B]:THR:HG23	1:A:136:LEU:HD11	1.94	0.49
1:B:300:GLN:HG3	1:B:320:LEU:HD13	1.95	0.48
1:B:97:LEU:HD22	1:B:428:LEU:HD13	1.95	0.48
1:A:120[B]:THR:CG2	1:A:136:LEU:HD11	2.44	0.48
1:B:73:MET:HE1	1:B:417:SER:HB2	1.96	0.48
1:A:235:LYS:O	1:A:240:GLY:HA2	2.15	0.46
1:A:96:GLU:HB2	1:A:429:VAL:HB	1.99	0.45
1:B:442:TYR:HE2	4:B:604:ACT:H1	1.81	0.45
1:A:392[A]:VAL:HG23	1:B:428:LEU:HD23	1.98	0.44
1:A:392[A]:VAL:HG23	1:B:428:LEU:CD2	2.48	0.44
1:B:96:GLU:C	1:B:97:LEU:HD23	2.39	0.43
1:A:73:MET:HE1	1:A:417:SER:HB2	1.99	0.43
1:B:29:LEU:HD22	1:B:125:VAL:HG13	2.01	0.43
1:B:58:ALA:HA	5:B:1004:HOH:O	2.18	0.43
1:B:59:TYR:HA	1:B:63:VAL:HB	2.01	0.42
1:A:364:TYR:CE1	1:A:390:VAL:HA	2.54	0.42
1:B:242:THR:HB	1:B:245:ALA:HB2	2.01	0.42
1:B:241:GLN:HE22	1:B:285:ILE:H	1.65	0.42
1:B:124:MET:CE	1:B:162:TYR:HB3	2.49	0.42
1:B:62:GLU:HG3	1:B:118:ASN:HB2	2.02	0.42
1:B:121:ILE:O	1:B:125:VAL:HG23	2.19	0.42
1:A:241:GLN:HE22	1:A:285:ILE:H	1.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:20[A]:ARG:HB2	1:B:21:PRO:HD3	2.02	0.41
1:A:35:LEU:HD23	1:A:35:LEU:C	2.42	0.40
1:B:97:LEU:HD22	1:B:428:LEU:CD1	2.52	0.40

There are no symmetry-related clashes.

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	455/469 (97%)	446 (98%)	8 (2%)	1 (0%)	55	67
1	B	455/469 (97%)	447 (98%)	7 (2%)	1 (0%)	55	67
All	All	910/938 (97%)	893 (98%)	15 (2%)	2 (0%)	55	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	HIS
1	B	413	HIS

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	390/400 (98%)	383 (98%)	7 (2%)	70	84
1	B	390/400 (98%)	382 (98%)	8 (2%)	64	81
All	All	780/800 (98%)	765 (98%)	15 (2%)	66	84

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

Mol	Chain	Res	Type
1	A	55	GLU
1	A	77	LEU
1	A	209	GLU
1	A	257	ASN
1	A	335	PHE
1	A	356	GLN
1	A	371	LYS
1	B	97	LEU
1	B	118	ASN
1	B	142	SER
1	B	209	GLU
1	B	335	PHE
1	B	369	ASN
1	B	406	ASN
1	B	416	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	37	GLN
1	A	118	ASN
1	A	241	GLN
1	A	257	ASN
1	A	393	HIS
1	A	406	ASN
1	B	27	GLN
1	B	33	GLN
1	B	118	ASN
1	B	122	GLN
1	B	238	ASN
1	B	241	GLN
1	B	256	GLN
1	B	289	HIS
1	B	369	ASN
1	B	406	ASN
1	B	423	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	1VL	A	601	1	20,20,32	4.07	6 (30%)	28,28,46	5.66	10 (35%)
4	ACT	A	604	-	1,3,3	1.17	0	0,3,3	0.00	-
2	1VL	B	601	1	20,20,32	4.08	5 (25%)	28,28,46	5.58	8 (28%)
4	ACT	B	604	-	1,3,3	1.07	0	0,3,3	0.00	-

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	1VL	A	601	1	-	0/4/28/40	0/3/3/5
4	ACT	A	604	-	-	0/0/0/0	0/0/0/0
2	1VL	B	601	1	-	0/4/28/40	0/3/3/5
4	ACT	B	604	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1VL	O10-C8	14.48	1.48	1.22
2	B	601	1VL	O10-C8	14.22	1.48	1.22
2	A	601	1VL	C5-C6	7.48	1.49	1.39
2	B	601	1VL	C5-C6	7.27	1.49	1.39
2	B	601	1VL	C7-C8	-6.84	1.46	1.52
2	A	601	1VL	C7-C8	-6.08	1.47	1.52
2	B	601	1VL	C6-C7	-3.84	1.45	1.51
2	A	601	1VL	C6-C7	-3.64	1.45	1.51
2	B	601	1VL	C5-N9	-2.42	1.34	1.39
2	A	601	1VL	C5-N9	-2.11	1.35	1.39
2	A	601	1VL	C12-N13	2.04	1.48	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	1VL	O10-C8-C7	-16.61	115.58	126.33
2	B	601	1VL	C7-C8-N9	16.32	122.96	107.04
2	A	601	1VL	C7-C8-N9	16.20	122.84	107.04
2	B	601	1VL	O10-C8-C7	-15.96	116.00	126.33
2	A	601	1VL	C6-C7-C8	-11.40	91.68	102.92
2	B	601	1VL	C6-C7-C8	-11.22	91.86	102.92
2	A	601	1VL	C5-N9-C8	-10.42	104.02	111.17
2	B	601	1VL	C5-N9-C8	-10.22	104.16	111.17
2	B	601	1VL	C12-N9-C8	7.51	130.33	123.51
2	A	601	1VL	C12-N9-C8	6.99	129.86	123.51
2	A	601	1VL	C12-N13-C18	-4.33	104.36	113.18
2	B	601	1VL	C12-N13-C18	-4.30	104.42	113.18
2	A	601	1VL	C6-C5-N9	-3.80	106.29	109.44
2	B	601	1VL	C6-C5-N9	-3.68	106.39	109.44
2	B	601	1VL	O10-C8-N9	-3.54	121.04	126.21
2	A	601	1VL	O10-C8-N9	-3.21	121.53	126.21
2	A	601	1VL	C5-C6-C7	2.12	115.08	108.66
2	A	601	1VL	C4-C5-N9	2.01	135.16	130.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	447/469 (95%)	-0.44	0 100 100	10, 15, 29, 45	0
1	B	452/469 (96%)	-0.36	0 100 100	11, 19, 31, 55	0
All	All	899/938 (95%)	-0.40	0 100 100	10, 17, 31, 55	0

There are no RSRZ outliers to report.

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	1VL	B	601	18/28	0.24	8.70	28,29,32,33	0
2	1VL	A	601	18/28	0.21	4.47	22,23,27,27	0
3	K	A	603	1/1	0.16	0.86	48,48,48,48	0
3	K	B	603	1/1	0.11	-0.05	33,33,33,33	0
4	ACT	A	604	4/4	0.14	-0.30	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	K	B	602	1/1	0.10	-1.15	41,41,41,41	0
3	K	A	602	1/1	0.06	-2.06	23,23,23,23	0
4	ACT	B	604	4/4	0.05	-2.20	18,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.