Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2023 – 05:11 pm GMT

PDB ID	:	5LVK
Title	:	Human Lysozyme co-crystallized with [H2Ind][trans-RuCl4(DMSO)(HInd)]
Authors	:	Kurpiewska, K.; Szura, A.; Lewinski, K.
Deposited on	:	2016-09-14
Resolution	:	2.49 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

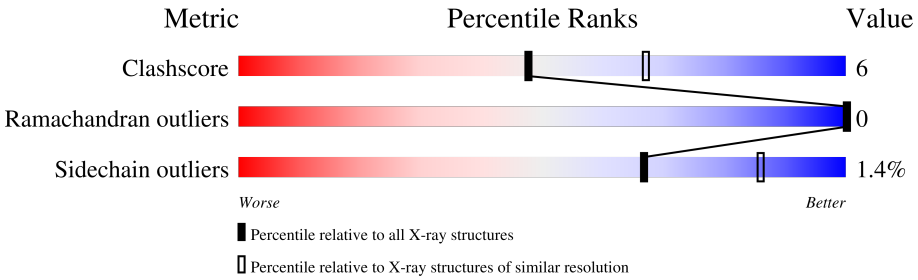
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.49 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

2 Entry composition

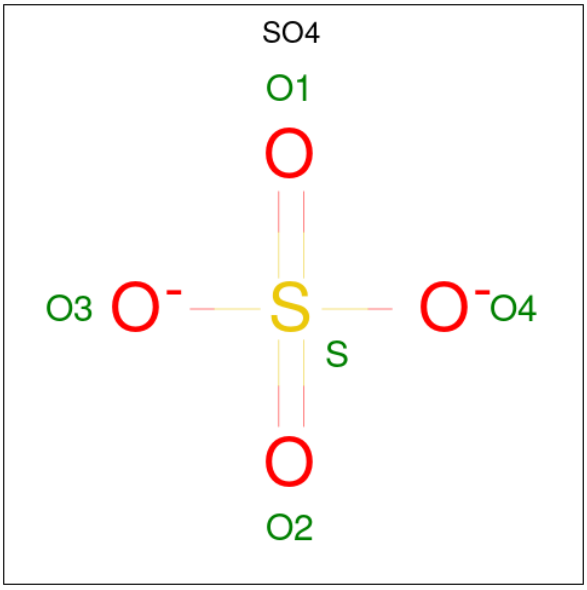
There are 7 unique types of molecules in this entry. The entry contains 2354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	1	0
			1036	638	201	187	10			
1	B	130	Total	C	N	O	S	0	1	0
			1037	638	203	186	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Cl 4 4	0	0
3	B	1	Total Cl 1 1	0	0

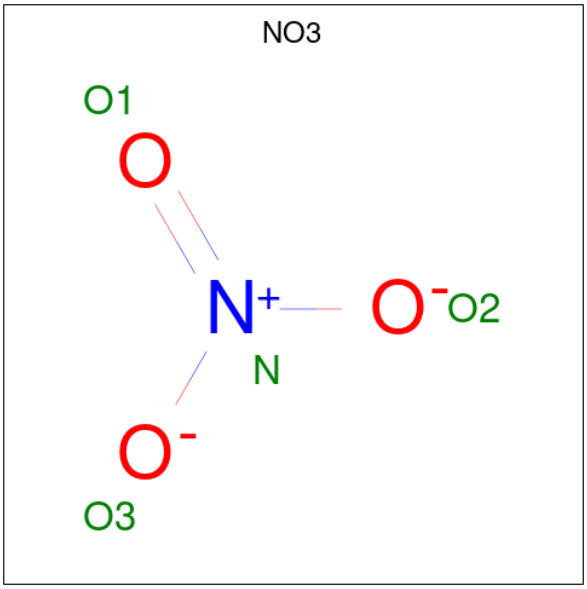
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is RUTHENIUM ION (three-letter code: RU) (formula: Ru).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Ru 2 2	0	0

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total N O 4 1 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	125	Total O 125 125	0	0
7	B	127	Total O 127 127	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.04Å 64.10Å 111.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.37 – 2.49	Depositor
% Data completeness (in resolution range)	99.3 (14.37-2.49)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.177 , 0.281	Depositor
Wilson B-factor (Å^2)	10.3	Xtriage
Anisotropy	0.908	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2354	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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.

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NO3, CL, NA, RU, SO4

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	0.40	0/1056	0.63	0/1426
1	B	0.40	0/1060	0.58	0/1430
All	All	0.40	0/2116	0.60	0/2856

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-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 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	1036	0	1000	10	0
1	B	1037	0	1005	15	0
2	A	15	0	0	0	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	B	2	0	0	0	0
6	B	4	0	0	0	0
7	A	125	0	0	3	0
7	B	127	0	0	4	0
All	All	2354	0	2005	25	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 6.

All (25) 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:49:ASP:O	1:B:62:ARG:NH2	2.18	0.77
1:A:50:ARG:NH2	7:A:301:HOH:O	2.18	0.74
1:B:113[A]:ARG:NH1	7:B:305:HOH:O	2.32	0.63
1:A:21:ARG:NH1	7:A:304:HOH:O	2.35	0.59
1:B:12:LEU:HD12	1:B:29:MET:HE2	1.89	0.55
1:A:1:LYS:NZ	1:A:7:GLU:OE2	2.40	0.55
1:B:8:LEU:HG	1:B:29:MET:HE1	1.90	0.54
1:B:12:LEU:HD12	1:B:29:MET:CE	2.38	0.54
1:A:122:ARG:O	1:A:126:GLN:HG2	2.09	0.52
1:B:63:TYR:HB2	7:B:380:HOH:O	2.12	0.49
1:A:31:LEU:HD22	1:A:106:ILE:HD11	1.95	0.49
1:B:13:LYS:NZ	1:B:130:VAL:OXT	2.37	0.48
1:A:39:ASN:ND2	1:A:41:ARG:H	2.12	0.48
1:B:33:LYS:NZ	7:B:309:HOH:O	2.47	0.46
1:B:67:ASP:HB3	1:B:81:CYS:SG	2.56	0.45
1:B:31:LEU:HD13	1:B:112:TRP:HB2	1.97	0.45
1:B:62:ARG:NH2	1:B:71:PRO:HD2	2.32	0.45
1:B:112:TRP:CZ3	1:B:117:GLN:HB2	2.51	0.44
1:A:64:TRP:CD2	1:A:99:VAL:HG22	2.53	0.44
1:B:110:VAL:HA	1:B:113[A]:ARG:HG3	2.00	0.43
1:A:107:ARG:HB3	1:A:113:ARG:HD3	1.99	0.43
1:A:113:ARG:NH1	7:A:305:HOH:O	2.36	0.41
1:A:54:TYR:HE1	1:A:61:SER:HB3	1.86	0.41
1:B:14:ARG:NH2	7:B:301:HOH:O	2.18	0.41
1:B:64:TRP:CE2	1:B:99:VAL:HG22	2.56	0.41

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	129/130 (99%)	122 (95%)	7 (5%)	0	100	100
1	B	129/130 (99%)	123 (95%)	6 (5%)	0	100	100
All	All	258/260 (99%)	245 (95%)	13 (5%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	106/105 (101%)	103 (97%)	3 (3%)	43	70
1	B	106/105 (101%)	104 (98%)	2 (2%)	57	80
All	All	212/210 (101%)	207 (98%)	5 (2%)	67	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74[A]	VAL
1	A	74[B]	VAL
1	A	91	ASP
1	B	113[A]	ARG
1	B	113[B]	ARG

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

Mol	Chain	Res	Type
1	A	39	ASN
1	A	86	GLN
1	B	88	ASN

4.3.3 RNA

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.