



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:49 PM GMT

PDB ID : 3S5C
Title : Crystal Structure of a Hexachlorocyclohexane dehydrochlorinase (LinA)
Type2
Authors : Kukshal, V.; Macwan, A.S.; Kumar, A.; Ramachandran, R.
Deposited on : 2011-05-23
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

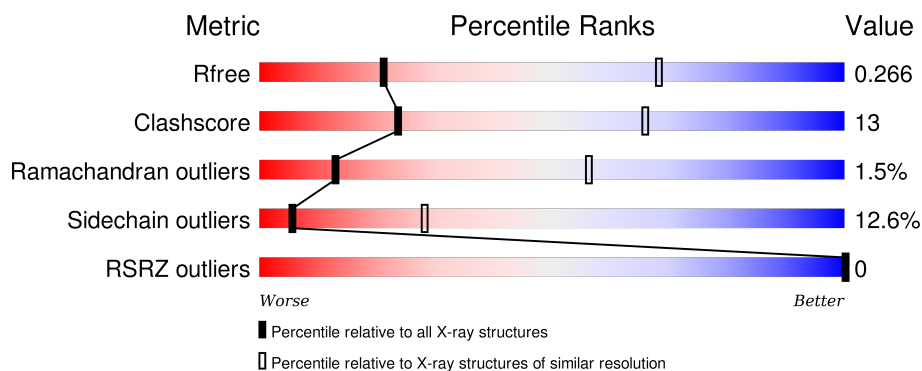
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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. 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	156	 63% 29% . . .
1	B	156	 65% 26% . 5%
1	C	156	 67% 24% 6% .
1	D	156	 60% 34% . . .
1	E	156	 71% 26% . .

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Mol	Chain	Length	Quality of chain
1	F	156	 58% 29% 5% • 6%
1	G	156	 62% 27% 7% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8266 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.

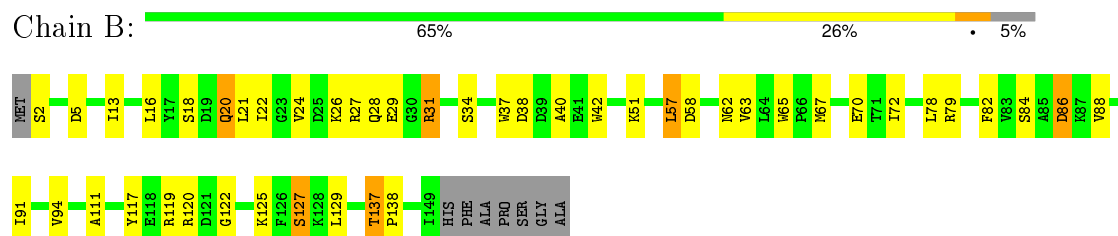
- Molecule 1 is a protein called LinA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	148	Total	C	N	O	S	0	0	0
			1166	743	198	221	4			
1	A	150	Total	C	N	O	S	0	0	0
			1176	749	200	223	4			
1	C	150	Total	C	N	O	S	0	0	0
			1183	756	202	221	4			
1	D	152	Total	C	N	O	S	0	0	0
			1199	766	204	225	4			
1	E	153	Total	C	N	O	S	0	0	0
			1205	769	205	227	4			
1	F	146	Total	C	N	O	S	0	0	0
			1154	735	196	219	4			
1	G	150	Total	C	N	O	S	0	0	0
			1183	756	202	221	4			

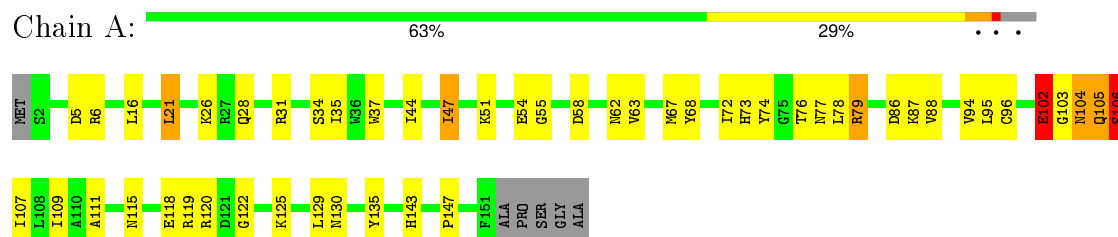
3 Residue-property plots

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.

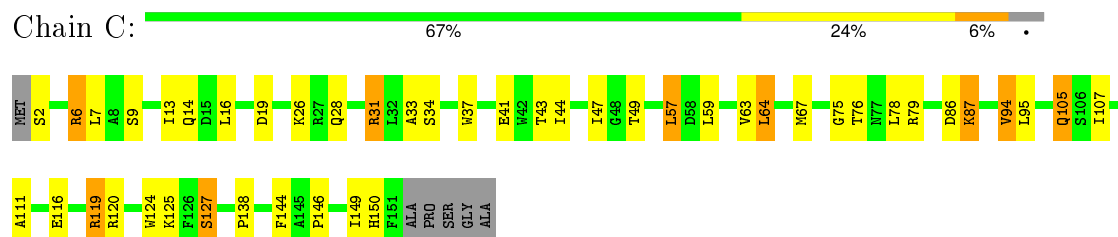
- Molecule 1: LinA



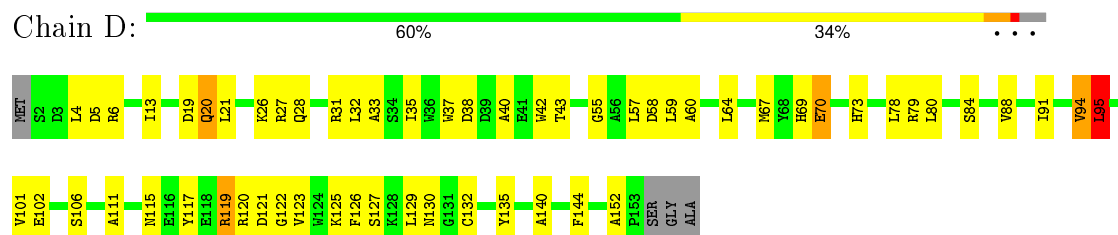
- Molecule 1: LinA



- Molecule 1: LinA

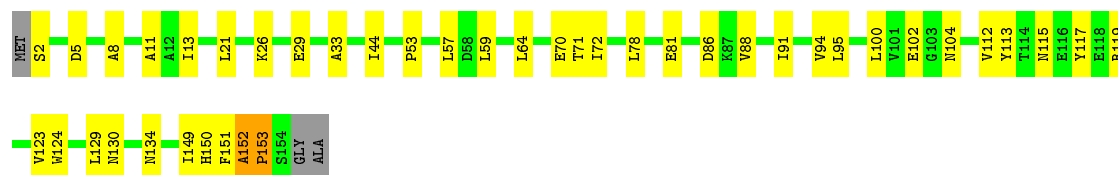


- Molecule 1: LinA



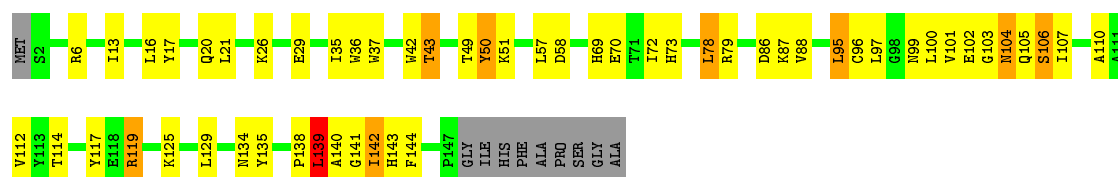
- Molecule 1: Lina

Chain E:  71% 26% ..



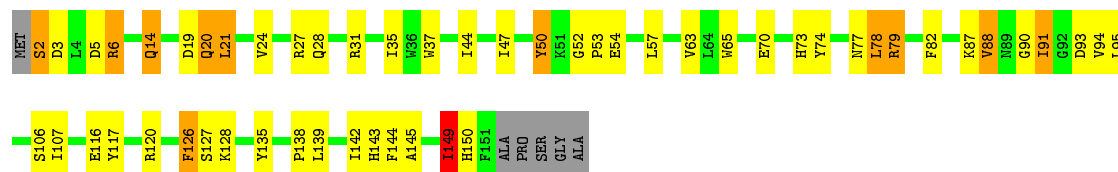
- Molecule 1: Lina

Chain F:  58% 29% 5% 6%



- Molecule 1: Lina

Chain G:  62% 27% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	162.53Å 162.53Å 186.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.72 – 3.50 30.72 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.72-3.50) 98.8 (30.72-3.50)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.179 , 0.271 0.179 , 0.266	Depositor DCC
R_{free} test set	969 reflections (5.47%)	DCC
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 26.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 18669 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8266	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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

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	0.54	0/1204	0.68	0/1638
1	B	0.55	0/1194	0.71	0/1624
1	C	0.53	0/1213	0.65	0/1650
1	D	0.50	0/1230	0.68	1/1674 (0.1%)
1	E	0.50	0/1236	0.70	0/1682
1	F	0.48	0/1182	0.68	1/1608 (0.1%)
1	G	0.52	0/1213	0.66	0/1650
All	All	0.52	0/8472	0.68	2/11526 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	95	LEU	CA-CB-CG	5.31	127.51	115.30
1	F	95	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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	1176	0	1127	37	0
1	B	1166	0	1123	28	0
1	C	1183	0	1135	27	0
1	D	1199	0	1151	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1205	0	1156	25	0
1	F	1154	0	1109	40	0
1	G	1183	0	1135	39	0
All	All	8266	0	7936	213	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 13.

The worst 5 of 213 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:F:42:TRP:CD1	1:F:129:LEU:HD22	2.00	0.94
1:C:107:ILE:HG22	1:C:138:PRO:HA	1.53	0.90
1:F:88:VAL:HG22	1:F:117:TYR:HB2	1.53	0.90
1:B:2:SER:HA	1:B:5:ASP:HB3	1.53	0.90
1:F:104:ASN:O	1:F:143:HIS:HE1	1.58	0.85

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	148/156 (95%)	130 (88%)	14 (10%)	4 (3%)	6	44
1	B	146/156 (94%)	140 (96%)	6 (4%)	0	100	100
1	C	148/156 (95%)	138 (93%)	10 (7%)	0	100	100
1	D	150/156 (96%)	133 (89%)	15 (10%)	2 (1%)	15	60
1	E	151/156 (97%)	140 (93%)	8 (5%)	3 (2%)	9	51
1	F	144/156 (92%)	128 (89%)	12 (8%)	4 (3%)	6	43
1	G	148/156 (95%)	132 (89%)	13 (9%)	3 (2%)	9	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1035/1092 (95%)	941 (91%)	78 (8%)	16 (2%)	13	56

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	D	140	ALA
1	E	152	ALA
1	F	141	GLY
1	E	102	GLU

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	121/126 (96%)	108 (89%)	13 (11%)	8	37
1	B	121/126 (96%)	107 (88%)	14 (12%)	7	33
1	C	122/126 (97%)	105 (86%)	17 (14%)	4	25
1	D	124/126 (98%)	108 (87%)	16 (13%)	5	27
1	E	125/126 (99%)	115 (92%)	10 (8%)	15	52
1	F	120/126 (95%)	102 (85%)	18 (15%)	3	21
1	G	122/126 (97%)	102 (84%)	20 (16%)	3	17
All	All	855/882 (97%)	747 (87%)	108 (13%)	5	28

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	26	LYS
1	E	21	LEU
1	G	88	VAL
1	D	38	ASP
1	D	94	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	115	ASN
1	E	28	GLN
1	G	28	GLN
1	D	130	ASN
1	E	77	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	150/156 (96%)	-0.69	0 100 100	25, 35, 59, 81	0
1	B	148/156 (94%)	-0.80	0 100 100	20, 30, 39, 53	0
1	C	150/156 (96%)	-0.53	0 100 100	34, 44, 51, 61	0
1	D	152/156 (97%)	-0.55	0 100 100	32, 45, 75, 81	0
1	E	153/156 (98%)	-0.34	0 100 100	30, 52, 67, 85	0
1	F	146/156 (93%)	-0.40	0 100 100	41, 62, 73, 78	0
1	G	150/156 (96%)	-0.11	0 100 100	47, 75, 102, 104	0
All	All	1049/1092 (96%)	-0.49	0 100 100	20, 47, 84, 104	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.