Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:48 AM GMT

PDB ID	:	3Q16
Title	:	Linkage between the Bacterial Acid Stress and Stringent Responses: The Structure of the Inducible Lysine Decarboxylase
Authors	:	El Bakkouri, M.; Pai, E.F.; Houry, W.A.
Deposited on	:	2010-12-16
Resolution	:	4.10 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
http://wwpdb.org/validation/2016/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:

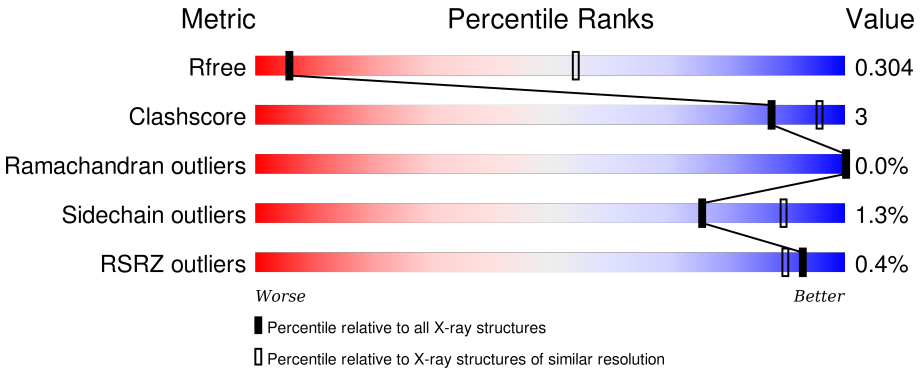
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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 <=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	715	92% 7%
1	B	715	% 90% 9%
1	C	715	91% 8%
1	D	715	90% 9%
1	E	715	91% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 28537 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 Lysine decarboxylase, inducible.

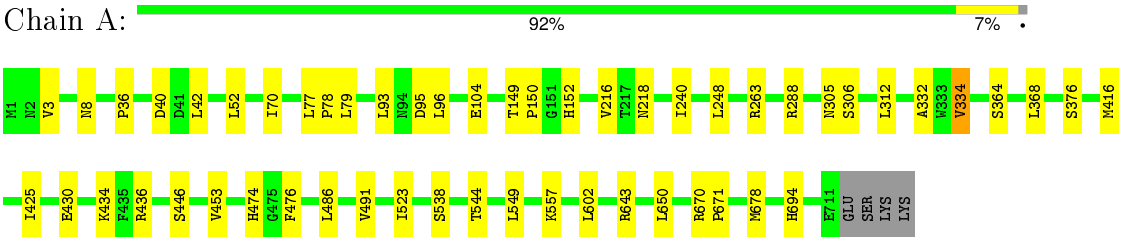
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	P	S	0	1	0
			5705	3650	953	1064	1	37			
1	B	711	Total	C	N	O	P	S	0	1	0
			5705	3650	953	1064	1	37			
1	C	711	Total	C	N	O	P	S	0	2	0
			5711	3654	953	1066	1	37			
1	D	711	Total	C	N	O	P	S	0	2	0
			5711	3654	953	1066	1	37			
1	E	711	Total	C	N	O	P	S	0	1	0
			5705	3650	953	1064	1	37			

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 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.

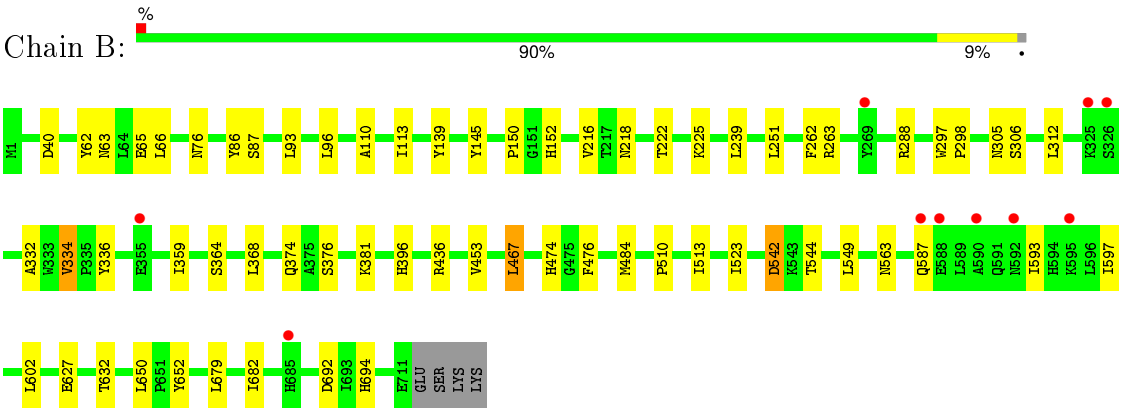
- Molecule 1: Lysine decarboxylase, inducible

Chain A:



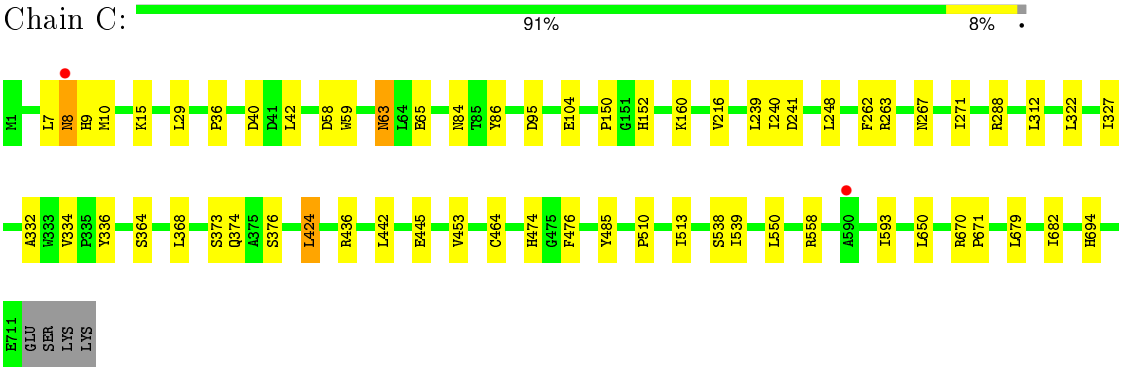
- Molecule 1: Lysine decarboxylase, inducible

Chain B:



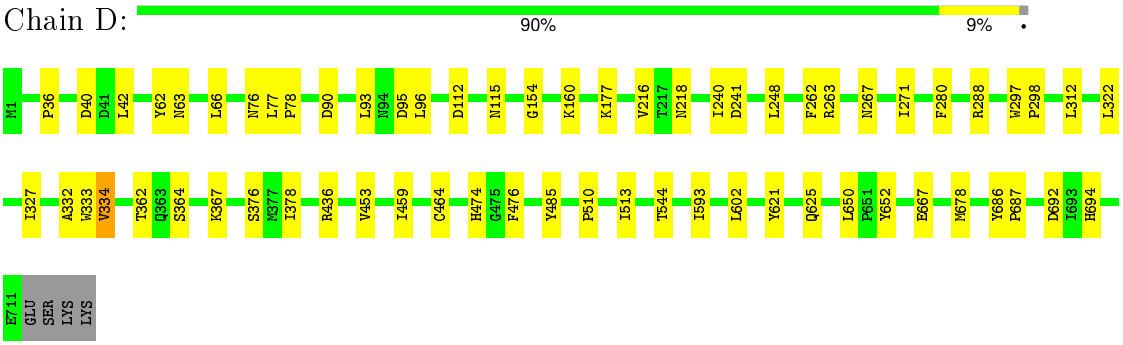
- Molecule 1: Lysine decarboxylase, inducible

Chain C:



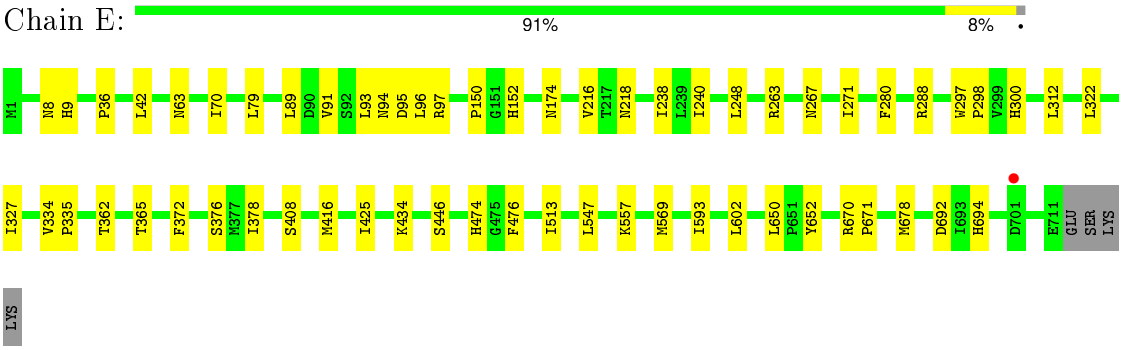
- Molecule 1: Lysine decarboxylase, inducible

Chain D:



- Molecule 1: Lysine decarboxylase, inducible

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	270.29Å 181.29Å 169.93Å 90.00° 125.06° 90.00°	Depositor
Resolution (Å)	68.00 – 4.10 66.05 – 4.10	Depositor EDS
% Data completeness (in resolution range)	77.6 (68.00-4.10) 77.6 (66.05-4.10)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.276 , 0.304 0.278 , 0.304	Depositor DCC
R_{free} test set	2077 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	87.7	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 18.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 40852 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	28537	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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, 0.375 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: LLP

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	0.31	0/5824	0.43	0/7893
1	B	0.32	0/5824	0.44	0/7893
1	C	0.30	0/5833	0.43	0/7905
1	D	0.30	0/5833	0.42	0/7905
1	E	0.30	0/5824	0.43	0/7893
All	All	0.31	0/29138	0.43	0/39489

There are no bond length outliers.

There are no bond angle outliers.

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	5705	0	5624	26	0
1	B	5705	0	5624	33	0
1	C	5711	0	5630	35	0
1	D	5711	0	5630	30	0
1	E	5705	0	5624	32	0
All	All	28537	0	28132	147	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 3.

All (147) 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:467:LEU:HD11	1:B:484:MET:HB2	1.58	0.85
1:C:7:LEU:O	1:C:8:ASN:HB2	1.98	0.64
1:E:474:HIS:HD2	1:E:476:PHE:H	1.49	0.59
1:D:312:LEU:HD21	1:D:334:VAL:HG11	1.85	0.57
1:C:332:ALA:HA	1:C:364:SER:H	1.71	0.56
1:E:312:LEU:HD21	1:E:334:VAL:HG11	1.88	0.56
1:C:216:VAL:HB	1:C:376:SER:HB3	1.88	0.56
1:E:650:LEU:HB3	1:E:694:HIS:HB2	1.89	0.55
1:B:312:LEU:HD21	1:B:334:VAL:HG11	1.90	0.54
1:E:446:SER:HB3	1:E:557:LYS:HZ3	1.72	0.54
1:C:312:LEU:HD21	1:C:334:VAL:HG11	1.88	0.54
1:A:216:VAL:HB	1:A:376:SER:HB3	1.89	0.54
1:A:312:LEU:HD21	1:A:334:VAL:HG11	1.90	0.53
1:A:474:HIS:HD2	1:A:476:PHE:H	1.56	0.53
1:E:240:ILE:HD11	1:E:248:LEU:HB3	1.90	0.53
1:C:267:ASN:HD21	1:C:271:ILE:HD12	1.73	0.53
1:C:550:LEU:HD23	1:E:89:LEU:HD12	1.91	0.53
1:A:602:LEU:HG	1:A:678:MET:HE1	1.90	0.53
1:E:216:VAL:HB	1:E:376:SER:HB3	1.90	0.52
1:C:442:LEU:HD22	1:E:94:ASN:HD21	1.75	0.51
1:D:650:LEU:HB3	1:D:694:HIS:HB2	1.92	0.51
1:C:7:LEU:HG	1:C:8:ASN:N	2.26	0.51
1:E:216:VAL:HG12	1:E:218:ASN:H	1.75	0.51
1:C:322:LEU:HD23	1:C:327:ILE:HG12	1.93	0.50
1:A:650:LEU:HB3	1:A:694:HIS:HB2	1.91	0.50
1:A:332:ALA:HA	1:A:364:SER:H	1.76	0.50
1:B:93:LEU:HA	1:B:96:LEU:HD12	1.94	0.49
1:D:216:VAL:HB	1:D:376:SER:HB3	1.95	0.49
1:C:368:LEU:HD23	1:C:538:SER:HB3	1.94	0.49
1:B:216:VAL:HB	1:B:376:SER:HB3	1.93	0.49
1:D:36:PRO:HG3	1:D:42:LEU:HD13	1.95	0.49
1:B:597:ILE:HG23	1:B:602:LEU:HB3	1.94	0.49
1:A:436:ARG:HG2	1:A:453:VAL:HG11	1.95	0.48
1:B:650:LEU:HB3	1:B:694:HIS:HB2	1.95	0.48
1:D:332:ALA:HA	1:D:364:SER:H	1.78	0.48
1:D:602:LEU:HG	1:D:678:MET:HE1	1.95	0.48
1:E:263:ARG:HD2	1:E:288:ARG:HH22	1.79	0.47
1:B:332:ALA:HA	1:B:364:SER:H	1.79	0.47
1:C:513:ILE:HD11	1:C:593:ILE:HD12	1.96	0.47
1:D:267:ASN:HD21	1:D:271:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ILE:HG22	1:E:300:HIS:HB3	1.96	0.47
1:A:36:PRO:HG3	1:A:42:LEU:HD13	1.96	0.47
1:D:241:ASP:HA	1:D:262:PHE:HB2	1.96	0.47
1:D:263:ARG:HD2	1:D:288:ARG:HH22	1.79	0.47
1:A:93:LEU:HA	1:A:96:LEU:HD12	1.96	0.47
1:C:150:PRO:HB2	1:C:152:HIS:CD2	2.50	0.47
1:B:474:HIS:HD2	1:B:476:PHE:H	1.62	0.47
1:C:650:LEU:HB3	1:C:694:HIS:HB2	1.97	0.46
1:B:359:ILE:HB	1:B:381:LYS:HB3	1.97	0.46
1:A:77:LEU:HA	1:A:78:PRO:HD3	1.84	0.46
1:A:70:ILE:HG21	1:A:79:LEU:HD21	1.96	0.46
1:D:216:VAL:HG12	1:D:218:ASN:H	1.81	0.46
1:B:652:TYR:HB2	1:B:692:ASP:HB3	1.96	0.46
1:B:510:PRO:HD2	1:B:513:ILE:HD12	1.97	0.46
1:B:336:TYR:HE2	1:B:368:LEU:HD13	1.79	0.46
1:A:436:ARG:HE	1:A:491:VAL:HG22	1.81	0.46
1:C:59:TRP:O	1:C:63:ASN:HB3	2.16	0.45
1:C:8:ASN:ND2	1:C:58:ASP:H	2.14	0.45
1:C:336:TYR:HE2	1:C:368:LEU:HD13	1.82	0.45
1:E:150:PRO:HB2	1:E:152:HIS:CD2	2.51	0.45
1:A:3:VAL:HB	1:A:52:LEU:HA	1.98	0.45
1:A:434:LYS:HE3	1:C:86:TYR:HA	1.97	0.45
1:A:104:GLU:HG3	1:D:544:THR:HG23	1.98	0.45
1:E:267:ASN:HD21	1:E:271:ILE:HD12	1.81	0.45
1:D:322:LEU:HD23	1:D:327:ILE:HG12	1.99	0.45
1:B:86:TYR:HA	1:E:434:LYS:HE3	1.99	0.45
1:D:436:ARG:HG2	1:D:453:VAL:HG11	1.99	0.45
1:D:93:LEU:HA	1:D:96:LEU:HD12	1.99	0.45
1:B:139:TYR:HE1	1:B:145:TYR:HD2	1.65	0.44
1:A:523:ILE:HG21	1:A:549:LEU:HD13	1.99	0.44
1:B:263:ARG:HD2	1:B:288:ARG:HH22	1.83	0.44
1:B:563:ASN:HB2	1:B:587:GLN:HE21	1.83	0.44
1:E:36:PRO:HG3	1:E:42:LEU:HD13	1.99	0.44
1:A:446:SER:HB3	1:A:557:LYS:HE2	2.00	0.44
1:B:436:ARG:HG2	1:B:453:VAL:HG11	1.99	0.44
1:C:474:HIS:HD2	1:C:476:PHE:H	1.66	0.43
1:C:510:PRO:HD2	1:C:513:ILE:HD12	1.99	0.43
1:B:523:ILE:HG21	1:B:549:LEU:HD13	1.99	0.43
1:D:240:ILE:HD11	1:D:248:LEU:HB3	1.99	0.43
1:D:652:TYR:HB2	1:D:692:ASP:HB3	1.99	0.43
1:B:513:ILE:HD11	1:B:593:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:HG12	1:A:218:ASN:H	1.84	0.43
1:D:90:ASP:H	1:D:93:LEU:HD12	1.84	0.43
1:E:652:TYR:HB2	1:E:692:ASP:HB3	2.01	0.43
1:D:333:TRP:HE1	1:D:367:LLP:H2'1	1.84	0.43
1:C:36:PRO:HG3	1:C:42:LEU:HD13	2.00	0.43
1:B:62:TYR:HB3	1:B:66:LEU:HD12	1.99	0.43
1:B:150:PRO:HB2	1:B:152:HIS:CD2	2.53	0.43
1:C:240:ILE:HD11	1:C:248:LEU:HB3	2.00	0.43
1:A:240:ILE:HD11	1:A:248:LEU:HB3	2.00	0.43
1:E:474:HIS:CD2	1:E:476:PHE:H	2.34	0.43
1:D:510:PRO:HD2	1:D:513:ILE:HD12	2.00	0.42
1:A:263:ARG:HG3	1:A:288:ARG:HH22	1.84	0.42
1:D:362:THR:HG22	1:D:378:ILE:HG12	2.01	0.42
1:D:280:PHE:HD1	1:D:322:LEU:HD13	1.84	0.42
1:C:464:CYS:HB3	1:C:485:TYR:HB3	2.02	0.42
1:C:263:ARG:HG3	1:C:288:ARG:HH22	1.85	0.42
1:E:93:LEU:HA	1:E:96:LEU:HD12	2.02	0.42
1:B:218:ASN:HA	1:B:374:GLN:HE21	1.85	0.42
1:C:436:ARG:HG2	1:C:453:VAL:HG11	2.01	0.42
1:E:297:TRP:HA	1:E:298:PRO:HD3	1.94	0.42
1:C:241:ASP:HA	1:C:262:PHE:HB2	2.01	0.42
1:B:542:ASP:OD1	1:B:544:THR:HB	2.20	0.42
1:D:686:TYR:HA	1:D:687:PRO:HD3	1.92	0.42
1:E:602:LEU:HG	1:E:678:MET:HE1	2.01	0.42
1:E:322:LEU:HD23	1:E:327:ILE:HG12	2.00	0.42
1:B:679:LEU:HA	1:B:682:ILE:HG22	2.01	0.42
1:B:87:SER:HB2	1:E:547:LEU:HD11	2.02	0.42
1:B:216:VAL:HG12	1:B:218:ASN:H	1.85	0.42
1:B:297:TRP:HA	1:B:298:PRO:HD3	1.93	0.42
1:D:77:LEU:HA	1:D:78:PRO:HD3	1.92	0.42
1:B:627:GLU:HG3	1:B:632:THR:HG21	2.02	0.41
1:E:334:VAL:N	1:E:335:PRO:HD3	2.35	0.41
1:C:679:LEU:HA	1:C:682:ILE:HG22	2.01	0.41
1:E:280:PHE:HD1	1:E:322:LEU:HD13	1.85	0.41
1:C:445:GLU:HB3	1:E:91:VAL:HG21	2.03	0.41
1:A:150:PRO:HB2	1:A:152:HIS:CD2	2.56	0.41
1:E:70:ILE:HG21	1:E:79:LEU:HD21	2.02	0.41
1:A:670:ARG:N	1:A:671:PRO:CD	2.83	0.41
1:B:305:ASN:HA	1:B:306:SER:HA	1.73	0.41
1:C:670:ARG:N	1:C:671:PRO:CD	2.83	0.41
1:E:670:ARG:N	1:E:671:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:ARG:HD2	1:E:97:ARG:HG2	2.02	0.41
1:E:513:ILE:HD11	1:E:593:ILE:HD12	2.02	0.41
1:A:368:LEU:HD23	1:A:538:SER:HB3	2.02	0.41
1:C:424:LEU:HD22	1:C:539:ILE:HB	2.03	0.41
1:B:222:THR:HG22	1:B:396:HIS:HB3	2.02	0.41
1:E:372:PHE:HD2	1:E:408:SER:HB3	1.86	0.41
1:C:15:LYS:HE2	1:C:84:ASN:HD21	1.85	0.41
1:D:297:TRP:HA	1:D:298:PRO:HD3	1.92	0.41
1:D:464:CYS:HB3	1:D:485:TYR:HB3	2.02	0.41
1:B:110:ALA:HA	1:B:113:ILE:HD12	2.03	0.41
1:D:474:HIS:HD2	1:D:476:PHE:H	1.69	0.41
1:D:621:TYR:O	1:D:625:GLN:HG2	2.21	0.40
1:A:544:THR:OG1	1:C:104:GLU:HG3	2.21	0.40
1:A:416:MET:SD	1:A:425:ILE:HD11	2.60	0.40
1:D:154:GLY:HA2	1:D:177:LYS:HA	2.03	0.40
1:D:513:ILE:HD11	1:D:593:ILE:HD12	2.03	0.40
1:C:7:LEU:HG	1:C:8:ASN:H	1.85	0.40
1:C:239:LEU:HB3	1:C:262:PHE:CE1	2.56	0.40
1:E:416:MET:SD	1:E:425:ILE:HD11	2.61	0.40
1:D:62:TYR:HB3	1:D:66:LEU:HD12	2.03	0.40
1:B:239:LEU:HB3	1:B:262:PHE:CE1	2.57	0.40
1:C:373:SER:O	1:C:374:GLN:HB2	2.22	0.40
1:B:225:LYS:HA	1:B:251:LEU:HD13	2.02	0.40
1:E:362:THR:HG22	1:E:378:ILE:HG12	2.03	0.40
1:A:305:ASN:HA	1:A:306:SER:HA	1.71	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	709/715 (99%)	678 (96%)	31 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	709/715 (99%)	673 (95%)	36 (5%)	0	100	100
1	C	710/715 (99%)	673 (95%)	36 (5%)	1 (0%)	56	90
1	D	710/715 (99%)	675 (95%)	35 (5%)	0	100	100
1	E	709/715 (99%)	671 (95%)	38 (5%)	0	100	100
All	All	3547/3575 (99%)	3370 (95%)	176 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	8	ASN

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	621/624 (100%)	613 (99%)	8 (1%)	76	89
1	B	621/624 (100%)	614 (99%)	7 (1%)	80	90
1	C	622/624 (100%)	613 (99%)	9 (1%)	74	89
1	D	622/624 (100%)	612 (98%)	10 (2%)	70	88
1	E	621/624 (100%)	614 (99%)	7 (1%)	80	90
All	All	3107/3120 (100%)	3066 (99%)	41 (1%)	76	89

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	40	ASP
1	A	95	ASP
1	A	149	THR
1	A	334	VAL
1	A	430	GLU
1	A	486	LEU

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Mol	Chain	Res	Type
1	A	643	ARG
1	B	40	ASP
1	B	63	ASN
1	B	65	GLU
1	B	76	ASN
1	B	334	VAL
1	B	467	LEU
1	B	542	ASP
1	C	9	HIS
1	C	10	MET
1	C	29	LEU
1	C	40	ASP
1	C	63	ASN
1	C	65	GLU
1	C	95	ASP
1	C	160	LYS
1	C	424	LEU
1	D	40	ASP
1	D	63	ASN
1	D	76	ASN
1	D	95	ASP
1	D	112	ASP
1	D	115	ASN
1	D	160	LYS
1	D	334	VAL
1	D	459	ILE
1	D	667	GLU
1	E	8	ASN
1	E	9	HIS
1	E	63	ASN
1	E	95	ASP
1	E	174	ASN
1	E	365	THR
1	E	569	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	23	HIS
1	A	174	ASN
1	A	224	ASN

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Mol	Chain	Res	Type
1	A	338	ASN
1	A	474	HIS
1	A	594	HIS
1	B	8	ASN
1	B	23	HIS
1	B	63	ASN
1	B	99	GLN
1	B	174	ASN
1	B	218	ASN
1	B	224	ASN
1	B	328	HIS
1	B	374	GLN
1	B	455	GLN
1	B	474	HIS
1	B	587	GLN
1	B	625	GLN
1	C	23	HIS
1	C	63	ASN
1	C	99	GLN
1	C	174	ASN
1	C	224	ASN
1	C	328	HIS
1	C	374	GLN
1	C	455	GLN
1	C	474	HIS
1	C	478	ASN
1	C	594	HIS
1	C	625	GLN
1	D	23	HIS
1	D	63	ASN
1	D	99	GLN
1	D	174	ASN
1	D	218	ASN
1	D	224	ASN
1	D	328	HIS
1	D	374	GLN
1	D	426	ASN
1	D	455	GLN
1	D	474	HIS
1	D	587	GLN
1	D	594	HIS
1	D	625	GLN

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Mol	Chain	Res	Type
1	D	699	GLN
1	E	23	HIS
1	E	63	ASN
1	E	99	GLN
1	E	174	ASN
1	E	224	ASN
1	E	328	HIS
1	E	455	GLN
1	E	474	HIS
1	E	625	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	A	367	1	23,24,25	1.69	5 (21%)	28,32,34	1.85	5 (17%)
1	LLP	B	367	1	23,24,25	1.69	5 (21%)	28,32,34	1.76	5 (17%)
1	LLP	C	367	1	23,24,25	1.69	5 (21%)	28,32,34	1.83	5 (17%)
1	LLP	D	367	1	23,24,25	1.69	5 (21%)	28,32,34	1.82	5 (17%)
1	LLP	E	367	1	23,24,25	1.68	4 (17%)	28,32,34	1.82	5 (17%)

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
1	LLP	A	367	1	-	0/15/17/19	0/1/1/1
1	LLP	B	367	1	-	0/15/17/19	0/1/1/1
1	LLP	C	367	1	-	0/15/17/19	0/1/1/1
1	LLP	D	367	1	-	0/15/17/19	0/1/1/1
1	LLP	E	367	1	-	0/15/17/19	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	367	LLP	O3-C3	-5.73	1.23	1.37
1	A	367	LLP	O3-C3	-5.72	1.23	1.37
1	C	367	LLP	O3-C3	-5.72	1.23	1.37
1	E	367	LLP	O3-C3	-5.71	1.23	1.37
1	B	367	LLP	O3-C3	-5.68	1.23	1.37
1	B	367	LLP	C6-N1	2.00	1.38	1.34
1	D	367	LLP	C6-N1	2.01	1.38	1.34
1	C	367	LLP	C4'-NZ	2.01	1.33	1.27
1	A	367	LLP	C6-N1	2.02	1.38	1.34
1	D	367	LLP	C4'-NZ	2.03	1.33	1.27
1	C	367	LLP	C6-N1	2.04	1.38	1.34
1	B	367	LLP	C4'-NZ	2.06	1.33	1.27
1	E	367	LLP	C6-N1	2.07	1.38	1.34
1	A	367	LLP	C4'-NZ	2.08	1.33	1.27
1	C	367	LLP	C2-N1	2.24	1.38	1.34
1	D	367	LLP	C2-N1	2.25	1.38	1.34
1	E	367	LLP	C2-N1	2.26	1.38	1.34
1	A	367	LLP	C2-N1	2.29	1.38	1.34
1	B	367	LLP	C2-N1	2.34	1.39	1.34
1	E	367	LLP	C4-C4'	2.51	1.51	1.46
1	C	367	LLP	C4-C4'	2.55	1.51	1.46
1	A	367	LLP	C4-C4'	2.57	1.51	1.46
1	D	367	LLP	C4-C4'	2.57	1.51	1.46
1	B	367	LLP	C4-C4'	2.64	1.51	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	367	LLP	CE-NZ-C4'	-3.01	110.29	118.97
1	C	367	LLP	CE-NZ-C4'	-2.96	110.41	118.97
1	B	367	LLP	CE-NZ-C4'	-2.91	110.56	118.97
1	A	367	LLP	CE-NZ-C4'	-2.81	110.85	118.97
1	D	367	LLP	CE-NZ-C4'	-2.79	110.91	118.97
1	E	367	LLP	C4-C4'-NZ	-2.62	110.49	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	367	LLP	C4-C4'-NZ	-2.60	110.61	125.06
1	A	367	LLP	C4-C4'-NZ	-2.58	110.67	125.06
1	C	367	LLP	C4-C4'-NZ	-2.58	110.71	125.06
1	D	367	LLP	C4-C4'-NZ	-2.56	110.82	125.06
1	B	367	LLP	C5-C6-N1	-2.21	120.03	123.86
1	D	367	LLP	C5-C6-N1	-2.17	120.10	123.86
1	D	367	LLP	O-C-CA	-2.13	119.94	125.49
1	C	367	LLP	C5-C6-N1	-2.12	120.17	123.86
1	A	367	LLP	C5-C6-N1	-2.10	120.21	123.86
1	E	367	LLP	C5-C6-N1	-2.10	120.22	123.86
1	E	367	LLP	O-C-CA	-2.09	120.03	125.49
1	A	367	LLP	O-C-CA	-2.07	120.09	125.49
1	C	367	LLP	O-C-CA	-2.06	120.12	125.49
1	B	367	LLP	O-C-CA	-2.05	120.14	125.49
1	B	367	LLP	OP4-C5'-C5	6.62	119.94	108.99
1	E	367	LLP	OP4-C5'-C5	7.04	120.63	108.99
1	D	367	LLP	OP4-C5'-C5	7.11	120.74	108.99
1	C	367	LLP	OP4-C5'-C5	7.12	120.75	108.99
1	A	367	LLP	OP4-C5'-C5	7.40	121.22	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	367	LLP	1	0

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

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	710/715 (99%)	-0.06	0 100 100	87, 99, 111, 118	0
1	B	710/715 (99%)	0.07	10 (1%) 78 69	87, 100, 111, 122	0
1	C	710/715 (99%)	-0.25	2 (0%) 94 92	88, 99, 111, 117	0
1	D	710/715 (99%)	-0.22	0 100 100	89, 99, 111, 116	0
1	E	710/715 (99%)	-0.24	1 (0%) 95 95	86, 99, 111, 116	0
All	All	3550/3575 (99%)	-0.14	13 (0%) 93 90	86, 99, 111, 122	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	GLN	3.2
1	B	595	LYS	2.6
1	B	590	ALA	2.4
1	B	325	LYS	2.4
1	B	588	GLU	2.3
1	C	590	ALA	2.2
1	B	269	TYR	2.2
1	E	701	ASP	2.2
1	B	685	HIS	2.2
1	B	326	SER	2.1
1	C	8	ASN	2.1
1	B	592	ASN	2.1
1	B	355	GLU	2.0

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

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, 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	LLDF	B-factors(Å^2)	Q<0.9
1	LLP	D	367	24/25	0.93	0.20	-	95,99,100,100	0
1	LLP	C	367	24/25	0.92	0.22	-	95,99,100,100	0
1	LLP	B	367	24/25	0.84	0.28	-	95,99,100,100	0
1	LLP	A	367	24/25	0.85	0.26	-	95,99,100,100	0
1	LLP	E	367	24/25	0.92	0.23	-	95,99,100,100	0

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.