Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:14 AM GMT

PDB ID	:	3DWN
Title	:	Crystal structure of the long-chain fatty acid transporter FadL mutant A77E/S100R
Authors	:	Hearn, E.M.; Patel, D.R.; Lepore, B.W.; Indic, M.; van den Berg, B.
Deposited on	:	2008-07-22
Resolution	:	2.50 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:

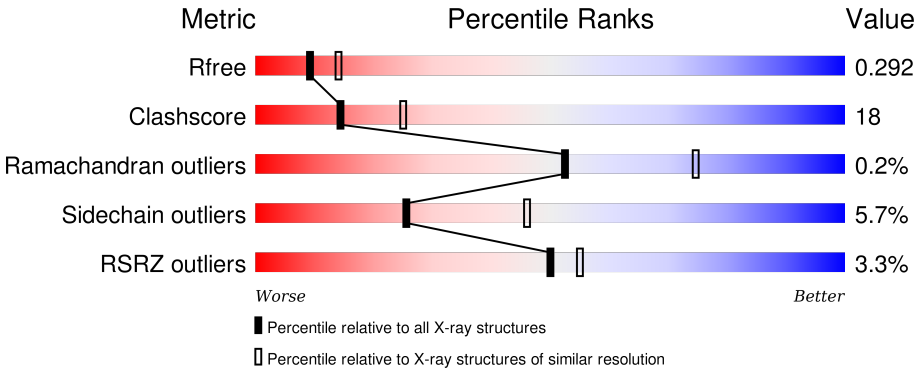
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	427	4% 65% 31%
1	B	427	2% 68% 27%

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	LDA	A	502	-	-	-	X
2	LDA	A	504	-	-	-	X
2	LDA	B	501	-	-	-	X
2	LDA	B	505	-	-	-	X
2	LDA	B	506	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6701 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.

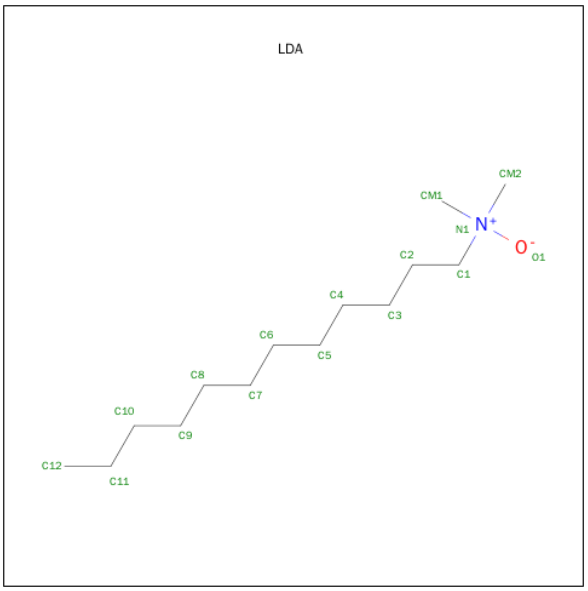
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3261	2062	555	638	6			
1	B	421	Total	C	N	O	S	0	0	0
			3261	2062	555	638	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLU	ALA	ENGINEERED	UNP P10384
A	100	ARG	SER	ENGINEERED	UNP P10384
A	422	HIS	-	EXPRESSION TAG	UNP P10384
A	423	HIS	-	EXPRESSION TAG	UNP P10384
A	424	HIS	-	EXPRESSION TAG	UNP P10384
A	425	HIS	-	EXPRESSION TAG	UNP P10384
A	426	HIS	-	EXPRESSION TAG	UNP P10384
A	427	HIS	-	EXPRESSION TAG	UNP P10384
B	77	GLU	ALA	ENGINEERED	UNP P10384
B	100	ARG	SER	ENGINEERED	UNP P10384
B	422	HIS	-	EXPRESSION TAG	UNP P10384
B	423	HIS	-	EXPRESSION TAG	UNP P10384
B	424	HIS	-	EXPRESSION TAG	UNP P10384
B	425	HIS	-	EXPRESSION TAG	UNP P10384
B	426	HIS	-	EXPRESSION TAG	UNP P10384
B	427	HIS	-	EXPRESSION TAG	UNP P10384

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 12 12	0	0
2	B	1	Total C N O 16 14 1 1	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 12 12	0	0

- Molecule 3 is water.

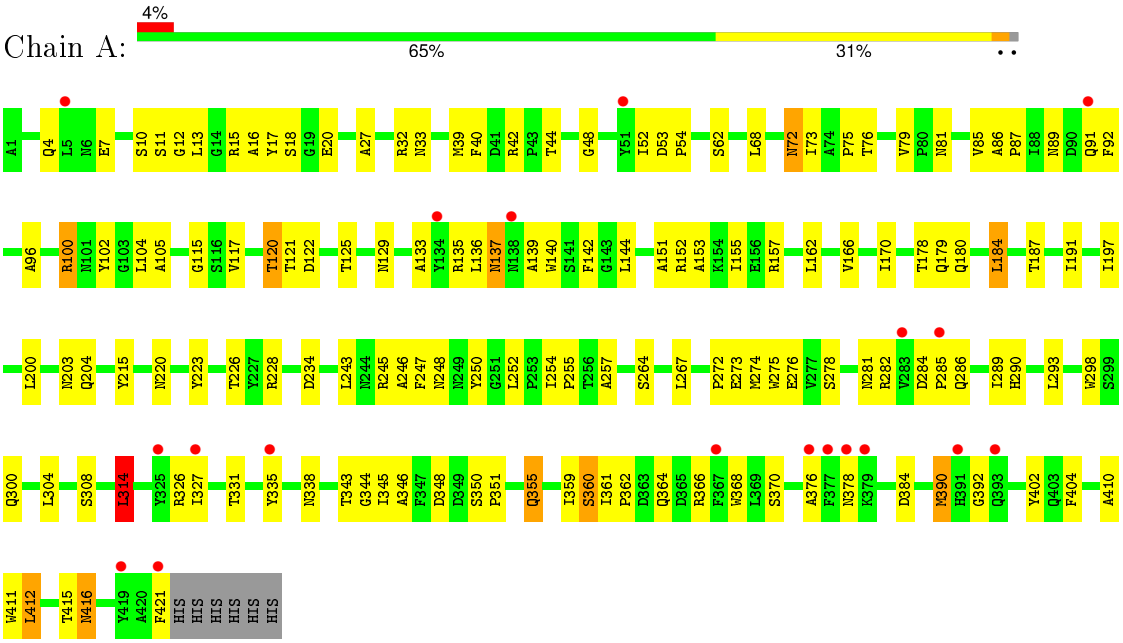
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	52	Total O 52 52	0	0
3	B	53	Total O 53 53	0	0

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.

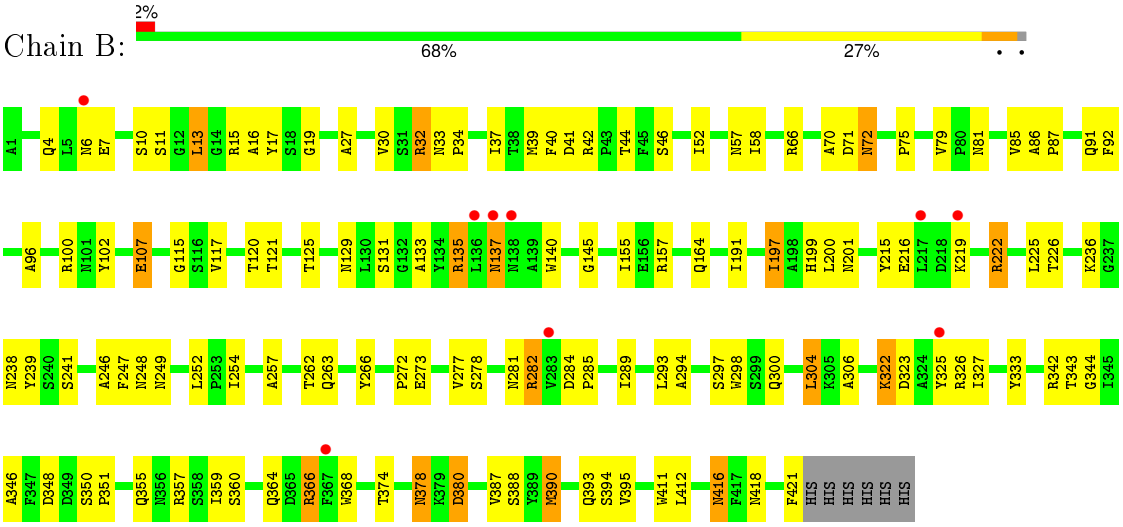
- Molecule 1: Long-chain fatty acid transport protein

Chain A:



- Molecule 1: Long-chain fatty acid transport protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.09Å 147.05Å 151.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 35.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (10.00-2.50) 97.5 (35.73-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.289 0.243 , 0.292	Depositor DCC
R_{free} test set	2440 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.0	EDS
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 48653 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6701	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.24% 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: LDA

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	0.41	0/3350	0.65	1/4560 (0.0%)
1	B	0.40	0/3350	0.64	0/4560
All	All	0.40	0/6700	0.64	1/9120 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	314	LEU	CA-CB-CG	5.63	128.26	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	3261	0	3042	122	0
1	B	3261	0	3042	110	0
2	A	36	0	69	11	0
2	B	38	0	73	6	0
3	A	52	0	0	6	0
3	B	53	0	0	2	0
All	All	6701	0	6226	231	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 18.

All (231) 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:30:VAL:HG21	1:B:85:VAL:HG11	1.40	0.99
1:A:137:ASN:HD21	1:A:140:TRP:H	1.11	0.97
1:A:355:GLN:NE2	1:A:355:GLN:H	1.64	0.95
1:B:57:ASN:HD22	1:B:71:ASP:HA	1.32	0.92
1:A:355:GLN:HE21	1:A:355:GLN:H	0.93	0.89
1:B:19:GLY:HA2	1:B:278:SER:HB2	1.55	0.86
1:A:355:GLN:HB3	1:B:355:GLN:HB3	1.56	0.86
1:A:355:GLN:N	1:A:355:GLN:HE21	1.72	0.86
1:A:42:ARG:HD2	1:A:421:PHE:O	1.77	0.84
1:B:137:ASN:HD21	1:B:140:TRP:H	1.22	0.83
1:B:137:ASN:ND2	1:B:140:TRP:H	1.76	0.82
1:A:304:LEU:HD11	2:A:502:LDA:H11	1.62	0.80
1:A:248:ASN:HD21	1:A:257:ALA:H	1.28	0.78
1:A:137:ASN:ND2	1:A:140:TRP:H	1.80	0.77
1:B:248:ASN:HD21	1:B:257:ALA:H	1.29	0.77
1:A:344:GLY:C	1:A:345:ILE:HD12	2.05	0.77
1:B:42:ARG:HD2	1:B:421:PHE:O	1.86	0.76
1:B:30:VAL:HG21	1:B:85:VAL:CG1	2.16	0.76
1:B:236:LYS:HD3	1:B:266:TYR:CE2	2.23	0.73
1:A:100:ARG:HG3	1:A:125:THR:O	1.88	0.73
1:B:364:GLN:NE2	1:B:366:ARG:HH11	1.89	0.71
1:B:102:TYR:O	1:B:125:THR:HB	1.91	0.71
1:B:304:LEU:HD13	2:B:501:LDA:HM23	1.73	0.71
1:A:121:THR:HG21	2:A:502:LDA:HM22	1.73	0.71
1:A:197:ILE:HD11	1:A:243:LEU:HD11	1.74	0.70
1:A:366:ARG:HG2	1:A:390:MET:CE	2.21	0.70
1:A:52:ILE:HG12	1:A:412:LEU:CD1	2.21	0.70
1:A:246:ALA:HB3	2:A:504:LDA:H92	1.74	0.70
1:A:368:TRP:CZ3	1:A:390:MET:HB2	2.28	0.69
1:B:52:ILE:HG23	1:B:412:LEU:CD2	2.24	0.68
1:B:364:GLN:HE21	1:B:366:ARG:HH11	1.40	0.68
1:A:191:ILE:HD11	1:A:247:PHE:HZ	1.58	0.68
1:A:220:ASN:HB3	1:A:282:ARG:HB3	1.77	0.67
1:A:191:ILE:HD11	1:A:247:PHE:CZ	2.30	0.67
1:A:153:ALA:HB1	2:A:502:LDA:H62	1.76	0.66
1:A:81:ASN:HD21	1:A:416:ASN:HD21	1.44	0.66
1:B:293:LEU:HD13	1:B:327:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLN:NE2	1:B:366:ARG:NH1	2.43	0.66
1:A:326:ARG:HG3	1:A:348:ASP:HB3	1.79	0.65
1:B:81:ASN:HD21	1:B:416:ASN:HD21	1.45	0.64
1:B:326:ARG:HG3	1:B:348:ASP:HB3	1.79	0.64
1:B:293:LEU:HD13	1:B:327:ILE:CD1	2.26	0.64
1:A:308:SER:HB3	1:A:314:LEU:HD21	1.80	0.64
1:B:282:ARG:HG3	1:B:282:ARG:HH11	1.61	0.64
1:A:338:ASN:HA	1:A:376:ALA:HB3	1.81	0.63
1:B:57:ASN:ND2	1:B:72:ASN:H	1.97	0.62
1:B:66:ARG:HD2	1:B:164:GLN:HE22	1.63	0.62
1:A:12:GLY:HA2	1:A:15:ARG:HB2	1.82	0.61
1:B:30:VAL:CG2	1:B:85:VAL:HG11	2.24	0.61
1:A:32:ARG:HD3	1:A:276:GLU:OE2	1.99	0.61
1:A:366:ARG:HG2	1:A:390:MET:HE3	1.81	0.61
1:B:41:ASP:OD1	1:B:42:ARG:HG2	2.01	0.61
1:B:357:ARG:NH1	1:B:395:VAL:HB	2.16	0.61
1:A:102:TYR:O	1:A:125:THR:HB	2.02	0.60
1:A:197:ILE:HG12	1:A:254:ILE:HD11	1.83	0.60
1:B:121:THR:OG1	1:B:157:ARG:NH2	2.35	0.60
1:A:117:VAL:HG23	1:A:359:ILE:HD11	1.84	0.59
1:A:293:LEU:HD13	1:A:327:ILE:HD11	1.84	0.59
1:B:57:ASN:ND2	1:B:71:ASP:HA	2.11	0.59
1:B:322:LYS:HD2	1:B:322:LYS:C	2.22	0.59
1:B:191:ILE:HD11	1:B:247:PHE:CZ	2.38	0.58
1:B:216:GLU:HB3	1:B:222:ARG:HB3	1.84	0.58
1:B:52:ILE:HG23	1:B:412:LEU:HD22	1.85	0.58
1:A:137:ASN:C	1:A:137:ASN:HD22	2.05	0.57
1:B:155:ILE:HD11	2:B:501:LDA:H61	1.87	0.57
1:B:197:ILE:HG13	1:B:254:ILE:HD11	1.85	0.57
1:A:62:SER:HB2	1:A:68:LEU:HD21	1.87	0.56
1:A:162:LEU:O	1:A:166:VAL:HG23	2.05	0.56
1:A:170:ILE:HD13	1:A:184:LEU:HB3	1.87	0.56
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.70	0.56
1:B:191:ILE:HD11	1:B:247:PHE:HZ	1.69	0.56
1:A:18:SER:OG	1:A:290:HIS:HD2	1.89	0.56
1:B:282:ARG:NH1	1:B:282:ARG:HG3	2.19	0.56
1:A:366:ARG:HG2	1:A:390:MET:HE2	1.86	0.56
1:A:293:LEU:HD13	1:A:327:ILE:CD1	2.35	0.56
1:A:390:MET:HE1	1:A:392:GLY:N	2.21	0.55
1:A:348:ASP:OD2	1:A:366:ARG:HB2	2.06	0.55
1:A:273:GLU:HG2	1:A:300:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:MET:CE	1:A:135:ARG:HH22	2.20	0.55
1:A:53:ASP:OD2	1:A:76:THR:HG22	2.07	0.55
1:A:152:ARG:HG3	1:A:203:ASN:OD1	2.07	0.55
1:A:254:ILE:HD12	3:A:516:HOH:O	2.07	0.54
1:B:368:TRP:CZ3	1:B:390:MET:HB3	2.42	0.54
1:B:272:PRO:HA	1:B:300:GLN:NE2	2.23	0.54
1:A:137:ASN:ND2	1:A:139:ALA:H	2.05	0.54
1:A:115:GLY:HA3	3:A:529:HOH:O	2.07	0.54
1:B:37:ILE:HB	1:B:133:ALA:CB	2.38	0.53
1:A:75:PRO:HD2	1:A:105:ALA:O	2.09	0.53
1:A:197:ILE:CG1	1:A:254:ILE:HD11	2.39	0.53
1:A:48:GLY:HA3	1:A:416:ASN:ND2	2.24	0.53
1:B:378:ASN:OD1	1:B:380:ASP:HB2	2.09	0.53
1:B:100:ARG:HG2	1:B:125:THR:O	2.09	0.53
1:A:91:GLN:HB3	1:A:92:PHE:CD1	2.44	0.53
1:B:346:ALA:HB3	1:B:368:TRP:HB2	1.90	0.52
1:B:411:TRP:O	1:B:412:LEU:HD23	2.10	0.52
1:B:7:GLU:HA	1:B:17:TYR:OH	2.09	0.52
1:A:361:ILE:HD11	2:A:502:LDA:CM1	2.40	0.52
1:B:40:PHE:O	1:B:87:PRO:HG3	2.09	0.52
1:A:10:SER:O	1:A:13:LEU:HB3	2.09	0.52
1:A:281:ASN:HB2	1:A:289:ILE:CG2	2.39	0.52
1:A:89:ASN:OD1	1:A:91:GLN:HB2	2.10	0.52
1:B:284:ASP:CG	1:B:285:PRO:HD2	2.31	0.52
1:B:157:ARG:HB2	1:B:197:ILE:HG22	1.92	0.51
1:A:245:ARG:HD3	3:A:532:HOH:O	2.10	0.51
1:B:37:ILE:HB	1:B:133:ALA:HB3	1.93	0.51
1:B:135:ARG:NH2	1:B:216:GLU:OE2	2.44	0.51
1:B:266:TYR:O	1:B:306:ALA:HA	2.11	0.51
1:A:304:LEU:CD1	2:A:502:LDA:HM13	2.42	0.50
1:B:10:SER:HB2	1:B:416:ASN:HB2	1.93	0.50
1:B:39:MET:CE	1:B:135:ARG:HH12	2.24	0.50
1:B:199:HIS:O	1:B:239:TYR:HA	2.10	0.50
1:A:73:ILE:O	1:A:75:PRO:HD3	2.12	0.50
1:B:411:TRP:C	1:B:412:LEU:HD23	2.32	0.50
1:B:225:LEU:HD13	1:B:277:VAL:HG12	1.94	0.50
1:B:66:ARG:HH11	1:B:164:GLN:HE22	1.58	0.49
1:A:52:ILE:O	1:A:54:PRO:HD3	2.12	0.49
1:B:39:MET:HE2	1:B:39:MET:HA	1.95	0.49
1:A:304:LEU:HD11	2:A:502:LDA:HM13	1.94	0.49
1:B:272:PRO:HG2	1:B:298:TRP:CE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:TRP:C	1:A:412:LEU:HD22	2.33	0.49
1:A:204:GLN:HG2	1:A:234:ASP:O	2.13	0.48
1:A:15:ARG:O	1:A:16:ALA:HB3	2.13	0.48
1:B:297:SER:HA	1:B:323:ASP:OD2	2.13	0.48
1:A:223:TYR:HA	1:A:278:SER:O	2.13	0.48
1:A:289:ILE:HA	1:A:331:THR:HG22	1.95	0.48
1:A:4:GLN:NE2	1:A:274:MET:HE1	2.29	0.48
1:B:6:ASN:ND2	1:B:32:ARG:HH21	2.11	0.48
1:B:304:LEU:HD21	2:B:501:LDA:H32	1.94	0.47
1:A:96:ALA:HA	1:A:129:ASN:O	2.14	0.47
1:B:15:ARG:O	1:B:16:ALA:HB3	2.14	0.47
1:A:89:ASN:OD1	1:A:91:GLN:N	2.42	0.47
1:A:360:SER:C	1:A:362:PRO:HD3	2.35	0.47
1:B:58:ILE:HB	1:B:70:ALA:HB3	1.96	0.47
1:B:238:ASN:HB3	1:B:262:THR:HG23	1.96	0.47
1:A:121:THR:OG1	1:A:157:ARG:NH2	2.47	0.47
1:A:362:PRO:HA	3:A:551:HOH:O	2.15	0.47
1:B:131:SER:HB3	1:B:145:GLY:CA	2.45	0.47
1:B:342:ARG:NH2	1:B:374:THR:OG1	2.36	0.47
1:A:11:SER:HB2	1:A:15:ARG:HH12	1.80	0.47
1:B:273:GLU:HG2	1:B:300:GLN:OE1	2.15	0.47
1:B:11:SER:HB2	1:B:15:ARG:HH12	1.79	0.47
1:A:178:THR:HG22	1:A:179:GLN:N	2.29	0.47
1:A:286:GLN:NE2	1:A:335:TYR:O	2.47	0.47
1:A:151:ALA:O	1:A:203:ASN:HA	2.14	0.46
1:A:402:TYR:HB2	1:A:404:PHE:CE1	2.49	0.46
1:B:137:ASN:N	1:B:137:ASN:HD22	2.12	0.46
1:A:254:ILE:HG13	1:A:255:PRO:HD2	1.97	0.46
1:A:20:GLU:HB2	1:A:32:ARG:HD2	1.98	0.46
1:A:40:PHE:CD2	1:A:85:VAL:HG11	2.51	0.46
1:A:361:ILE:HD11	2:A:502:LDA:HM11	1.97	0.46
1:A:52:ILE:HA	1:A:412:LEU:HD13	1.98	0.46
1:B:6:ASN:ND2	1:B:32:ARG:NH2	2.64	0.46
1:A:39:MET:CE	1:A:135:ARG:NH2	2.79	0.46
1:A:178:THR:HG22	3:A:554:HOH:O	2.16	0.46
1:A:104:LEU:HD23	2:A:502:LDA:H21	1.98	0.46
1:A:267:LEU:C	1:A:267:LEU:HD23	2.37	0.46
1:B:44:THR:HB	1:B:85:VAL:CG2	2.46	0.45
1:B:27:ALA:HB2	1:B:44:THR:HG22	1.99	0.45
1:A:345:ILE:N	1:A:345:ILE:HD12	2.30	0.45
1:A:343:THR:HG23	1:A:370:SER:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:CD2	1:B:388:SER:HB2	2.45	0.45
1:A:284:ASP:OD1	1:A:285:PRO:HD2	2.17	0.45
1:A:100:ARG:NH1	1:A:100:ARG:HG2	2.31	0.45
1:A:187:THR:HG21	2:A:504:LDA:H82	1.98	0.45
1:A:384:ASP:O	1:A:415:THR:HA	2.16	0.45
1:A:140:TRP:CE2	1:A:215:TYR:HD2	2.34	0.45
1:A:33:ASN:HB2	1:A:226:THR:HG21	1.99	0.45
1:B:393:GLN:HG2	1:B:394:SER:O	2.17	0.45
1:B:52:ILE:HG23	1:B:412:LEU:HD21	1.95	0.44
1:B:115:GLY:HA3	3:B:556:HOH:O	2.17	0.44
1:A:137:ASN:C	1:A:137:ASN:ND2	2.71	0.44
1:B:79:VAL:HG13	1:B:100:ARG:HD2	1.99	0.44
1:A:52:ILE:HG12	1:A:412:LEU:HD13	1.99	0.44
1:A:7:GLU:HA	1:A:17:TYR:OH	2.18	0.43
1:A:272:PRO:HG2	1:A:298:TRP:CE3	2.54	0.43
1:A:27:ALA:HB2	1:A:44:THR:HG22	2.00	0.43
1:B:86:ALA:HA	1:B:87:PRO:HD3	1.81	0.43
1:A:133:ALA:HA	1:A:142:PHE:O	2.19	0.43
1:B:343:THR:HG22	1:B:344:GLY:H	1.83	0.43
1:A:308:SER:HB3	1:A:314:LEU:CD2	2.47	0.43
1:B:75:PRO:HD3	1:B:107:GLU:HG2	2.00	0.43
1:B:33:ASN:HB2	1:B:226:THR:HG21	2.01	0.43
1:A:359:ILE:O	1:A:362:PRO:HG3	2.19	0.43
1:B:390:MET:C	1:B:390:MET:SD	2.97	0.43
1:B:343:THR:HG22	1:B:344:GLY:N	2.34	0.43
1:A:89:ASN:C	1:A:91:GLN:H	2.22	0.43
1:A:157:ARG:HB2	1:A:197:ILE:HG22	2.01	0.42
1:A:86:ALA:HA	1:A:87:PRO:HD3	1.85	0.42
1:B:91:GLN:HG3	1:B:92:PHE:CD1	2.54	0.42
1:A:79:VAL:HG13	1:A:100:ARG:HB2	2.01	0.42
1:B:117:VAL:HG23	1:B:359:ILE:HD11	2.01	0.42
1:B:200:LEU:HB3	2:B:501:LDA:H101	2.00	0.42
1:B:246:ALA:HB3	2:B:506:LDA:H92	2.02	0.42
1:B:350:SER:HA	1:B:351:PRO:HD3	1.83	0.42
1:A:184:LEU:HD13	1:A:184:LEU:HA	1.87	0.42
1:B:7:GLU:CD	1:B:7:GLU:H	2.23	0.42
1:B:32:ARG:HA	1:B:32:ARG:HD3	1.89	0.42
1:B:131:SER:HB3	1:B:145:GLY:HA2	2.02	0.42
1:B:236:LYS:HD3	1:B:266:TYR:CZ	2.53	0.42
1:A:72:ASN:HA	1:A:72:ASN:HD22	1.65	0.42
1:A:390:MET:HB3	1:A:410:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LEU:HD13	2:B:501:LDA:H12	2.02	0.41
1:B:39:MET:HE2	1:B:135:ARG:HH12	1.84	0.41
1:B:96:ALA:HA	1:B:129:ASN:O	2.20	0.41
1:B:238:ASN:HB3	1:B:262:THR:CG2	2.50	0.41
1:B:33:ASN:HA	1:B:34:PRO:HD2	1.93	0.41
1:A:180:GLN:HE21	2:A:503:LDA:H62	1.86	0.41
1:B:294:ALA:HB3	1:B:326:ARG:HB3	2.02	0.41
1:B:293:LEU:HD11	1:B:325:TYR:HD2	1.85	0.41
1:A:4:GLN:HB2	1:A:298:TRP:HZ2	1.85	0.41
1:B:281:ASN:HB2	1:B:289:ILE:CG2	2.50	0.41
1:A:284:ASP:CG	1:A:285:PRO:HD2	2.41	0.41
1:A:155:ILE:HB	1:A:200:LEU:HB2	2.03	0.41
1:B:140:TRP:CE2	1:B:215:TYR:HD2	2.39	0.41
1:A:157:ARG:HA	1:A:157:ARG:HD3	1.83	0.41
1:A:346:ALA:HB3	1:A:368:TRP:HB2	2.02	0.41
1:B:249:ASN:HA	3:B:520:HOH:O	2.21	0.41
1:B:241:SER:HB3	1:B:257:ALA:HA	2.02	0.41
1:A:120:THR:HG23	1:A:122:ASP:OD1	2.21	0.40
1:A:350:SER:HA	1:A:351:PRO:HD3	1.82	0.40
1:A:344:GLY:O	1:A:345:ILE:HD12	2.21	0.40
1:B:252:LEU:HB2	1:B:254:ILE:HG22	2.03	0.40
1:A:250:TYR:HB2	3:A:505:HOH:O	2.21	0.40
1:B:322:LYS:HD2	1:B:323:ASP:O	2.20	0.40
1:A:7:GLU:CD	1:A:7:GLU:N	2.75	0.40
1:B:4:GLN:HA	1:B:102:TYR:CD1	2.57	0.40
1:B:387:VAL:HA	1:B:412:LEU:O	2.21	0.40
1:B:348:ASP:OD2	1:B:366:ARG:HB2	2.21	0.40
1:B:284:ASP:OD1	1:B:285:PRO:HD2	2.21	0.40
1:A:228:ARG:HH11	1:A:228:ARG:HG3	1.86	0.40
1:B:46:SER:OG	1:B:418:ASN:ND2	2.55	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	419/427 (98%)	405 (97%)	13 (3%)	1 (0%)	52	75
1	B	419/427 (98%)	398 (95%)	20 (5%)	1 (0%)	52	75
All	All	838/854 (98%)	803 (96%)	33 (4%)	2 (0%)	52	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	ASN
1	B	378	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	332/338 (98%)	315 (95%)	17 (5%)	29	52
1	B	332/338 (98%)	311 (94%)	21 (6%)	22	40
All	All	664/676 (98%)	626 (94%)	38 (6%)	25	46

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	100	ARG
1	A	120	THR
1	A	136	LEU
1	A	137	ASN
1	A	144	LEU
1	A	184	LEU
1	A	252	LEU
1	A	264	SER
1	A	275	TRP
1	A	314	LEU

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Mol	Chain	Res	Type
1	A	355	GLN
1	A	360	SER
1	A	364	GLN
1	A	390	MET
1	A	412	LEU
1	A	416	ASN
1	B	13	LEU
1	B	32	ARG
1	B	72	ASN
1	B	107	GLU
1	B	120	THR
1	B	135	ARG
1	B	137	ASN
1	B	197	ILE
1	B	201	ASN
1	B	219	LYS
1	B	222	ARG
1	B	263	GLN
1	B	282	ARG
1	B	304	LEU
1	B	322	LYS
1	B	333	TYR
1	B	360	SER
1	B	366	ARG
1	B	380	ASP
1	B	390	MET
1	B	416	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	72	ASN
1	A	127	ASN
1	A	129	ASN
1	A	137	ASN
1	A	180	GLN
1	A	238	ASN
1	A	248	ASN
1	A	263	GLN
1	A	270	ASN
1	A	281	ASN

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Mol	Chain	Res	Type
1	A	290	HIS
1	A	302	GLN
1	A	303	GLN
1	A	316	GLN
1	A	355	GLN
1	A	356	ASN
1	A	416	ASN
1	A	418	ASN
1	B	6	ASN
1	B	29	ASN
1	B	57	ASN
1	B	72	ASN
1	B	83	HIS
1	B	89	ASN
1	B	127	ASN
1	B	129	ASN
1	B	137	ASN
1	B	164	GLN
1	B	180	GLN
1	B	248	ASN
1	B	270	ASN
1	B	281	ASN
1	B	290	HIS
1	B	300	GLN
1	B	303	GLN
1	B	356	ASN
1	B	364	GLN
1	B	416	ASN
1	B	418	ASN

5.3.3 RNA

There are no RNA molecules 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 (i)

6 ligands 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	$\#\|Z\| > 2$
2	LDA	A	502	-	15,15,15	3.66	2 (13%)	16,17,17	2.18	4 (25%)
2	LDA	A	503	-	7,7,15	0.46	0	6,6,17	1.09	1 (16%)
2	LDA	A	504	-	11,11,15	0.53	0	10,10,17	1.07	1 (10%)
2	LDA	B	501	-	15,15,15	4.24	3 (20%)	16,17,17	8.09	6 (37%)
2	LDA	B	505	-	9,9,15	0.46	0	8,8,17	1.06	1 (12%)
2	LDA	B	506	-	11,11,15	0.52	0	10,10,17	1.09	1 (10%)

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	LDA	A	502	-	-	0/13/13/13	0/0/0/0
2	LDA	A	503	-	-	0/5/5/13	0/0/0/0
2	LDA	A	504	-	-	0/9/9/13	0/0/0/0
2	LDA	B	501	-	-	0/13/13/13	0/0/0/0
2	LDA	B	505	-	-	0/7/7/13	0/0/0/0
2	LDA	B	506	-	-	0/9/9/13	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	LDA	O1-N1	-15.67	1.24	1.39
2	A	502	LDA	O1-N1	-13.22	1.27	1.39
2	A	502	LDA	CM2-N1	-4.68	1.42	1.49
2	B	501	LDA	CM2-N1	-2.90	1.45	1.49
2	B	501	LDA	C1-N1	2.65	1.56	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	LDA	O1-N1-C1	-22.86	84.55	110.27
2	B	501	LDA	CM1-N1-C1	-10.97	74.43	109.77
2	A	502	LDA	CM2-N1-CM1	-6.36	101.65	108.83
2	B	501	LDA	CM2-N1-C1	-4.53	95.19	109.77
2	A	502	LDA	C9-C8-C7	-2.32	102.54	114.53
2	B	501	LDA	C9-C8-C7	-2.31	102.62	114.53
2	A	503	LDA	C9-C8-C7	-2.24	102.97	114.53
2	B	505	LDA	C9-C8-C7	-2.20	103.17	114.53
2	B	506	LDA	C9-C8-C7	-2.15	103.44	114.53
2	A	504	LDA	C9-C8-C7	-2.09	103.72	114.53
2	A	502	LDA	O1-N1-C1	2.85	113.48	110.27
2	A	502	LDA	O1-N1-CM2	2.90	112.93	109.05
2	B	501	LDA	O1-N1-CM2	5.10	115.87	109.05
2	B	501	LDA	O1-N1-CM1	18.50	133.78	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	LDA	8	0
2	A	503	LDA	1	0
2	A	504	LDA	2	0
2	B	501	LDA	5	0
2	B	506	LDA	1	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

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	421/427 (98%)	0.12	19 (4%) 37 42	22, 35, 55, 63	1 (0%)
1	B	421/427 (98%)	0.08	9 (2%) 67 71	24, 37, 55, 62	0
All	All	842/854 (98%)	0.10	28 (3%) 50 55	22, 36, 55, 63	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	ASN	3.6
1	A	419	TYR	3.6
1	B	283	VAL	3.5
1	A	367	PHE	3.4
1	A	91	GLN	3.4
1	B	217	LEU	3.1
1	B	219	LYS	2.8
1	A	283	VAL	2.7
1	A	335	TYR	2.7
1	A	138	ASN	2.6
1	B	136	LEU	2.6
1	A	378	ASN	2.5
1	A	393	GLN	2.4
1	A	421	PHE	2.4
1	A	5	LEU	2.4
1	A	376	ALA	2.4
1	A	134	TYR	2.3
1	A	51	TYR	2.3
1	B	6	ASN	2.3
1	A	379	LYS	2.2
1	A	285	PRO	2.2
1	A	377	PHE	2.1
1	B	367	PHE	2.1
1	B	325	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	137	ASN	2.1
1	A	325	TYR	2.1
1	A	327	ILE	2.1
1	A	391	HIS	2.0

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 carbohydrates 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. 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
2	LDA	B	501	16/16	0.78	0.36	7.17	38,44,66,67	0
2	LDA	A	502	16/16	0.82	0.36	6.55	35,43,65,65	0
2	LDA	B	505	10/16	0.82	0.40	5.60	70,72,75,75	0
2	LDA	B	506	12/16	0.87	0.29	4.53	54,56,58,59	0
2	LDA	A	504	12/16	0.84	0.28	3.49	47,50,57,57	0
2	LDA	A	503	8/16	0.76	0.28	1.88	53,55,59,61	0

6.5 Other polymers (i)

There are no such residues in this entry.