



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:25 AM GMT

PDB ID : 2R4P  
Title : Crystal structure of the long-chain fatty acid transporter FadL mutant G212E  
Authors : Hearn, E.M.; Patel, D.R.; Lepore, B.W.; Indic, M.; van den Berg, B.  
Deposited on : 2007-08-31  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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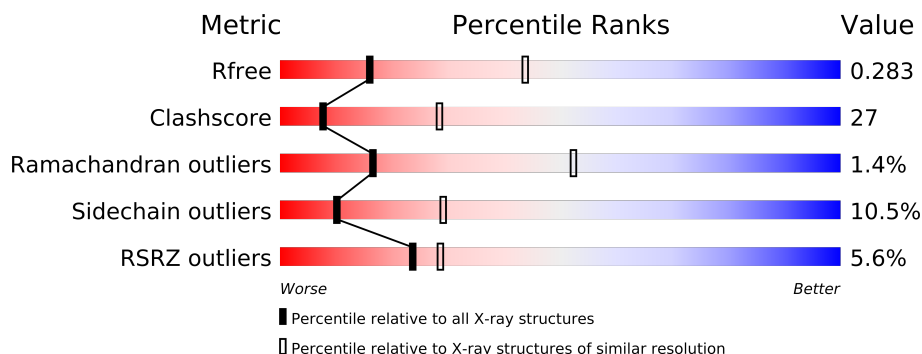
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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  $\geq 3$ , 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	427	
1	B	427	

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	LDA	A	501	-	X
2	LDA	B	502	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6496 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.

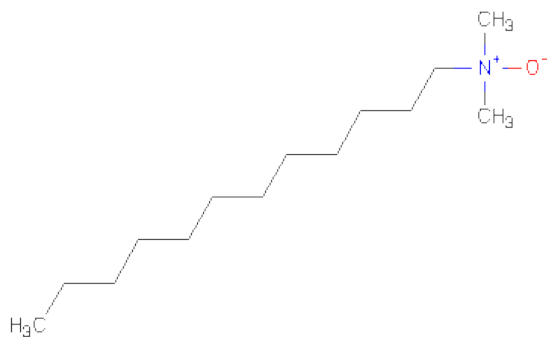
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3232	2043	548	635	6			
1	B	418	Total	C	N	O	S	0	0	0
			3232	2043	548	635	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	GLU	GLY	ENGINEERED	UNP P10384
A	197	THR	ILE	CONFLICT	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	212	GLU	GLY	ENGINEERED	UNP P10384
B	197	THR	ILE	CONFLICT	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<sub>14</sub>H<sub>31</sub>NO).



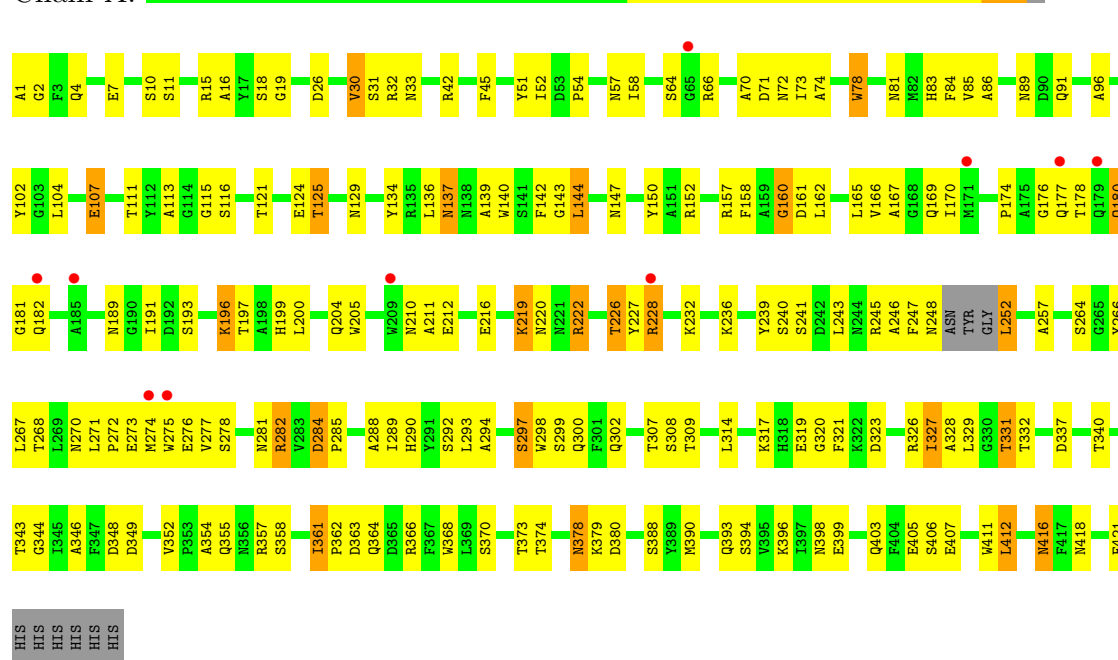
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		

### 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.

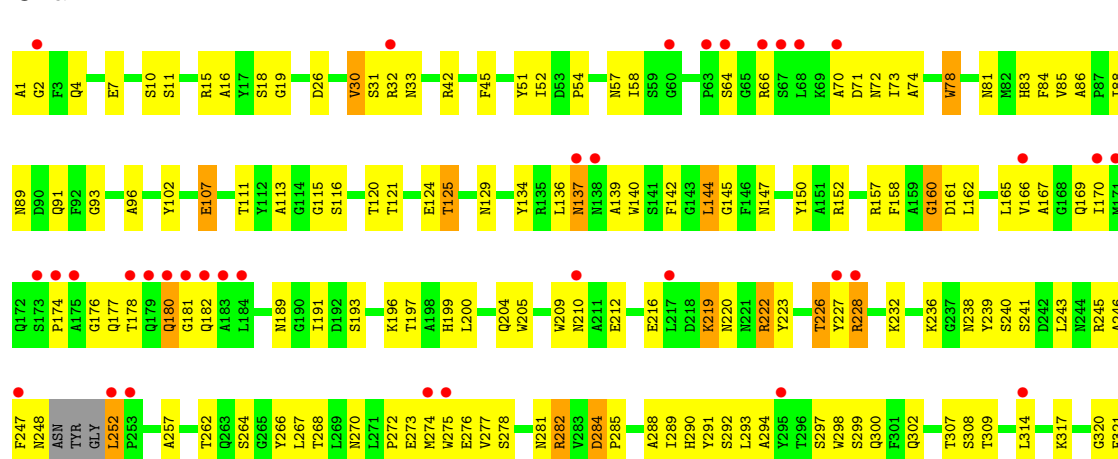
- Molecule 1: Long-chain fatty acid transport protein

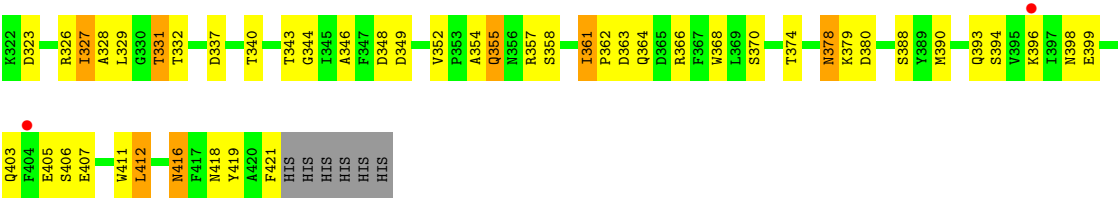
Chain A:



- Molecule 1: Long-chain fatty acid transport protein

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.51Å 69.97Å 84.15Å 90.00° 100.84° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 38.25 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (10.00-2.90) 98.4 (38.25-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.267 , 0.288 0.265 , 0.283	Depositor DCC
$R_{free}$ test set	2181 reflections (7.68%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 27.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 29131 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	6496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.46	0/3319	0.66	0/4518
1	B	0.42	0/3319	0.65	0/4518
All	All	0.44	0/6638	0.65	0/9036

There are no bond length outliers.

There are no bond angle outliers.

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	3232	0	3013	167	0
1	B	3232	0	3013	178	0
2	A	16	0	31	5	0
2	B	16	0	31	5	0
All	All	6496	0	6088	345	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 27.

All (345) close contacts within the same asymmetric unit are listed below.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:308:SER:HB3	1:B:314:LEU:HD21	1.28	1.13
1:A:308:SER:HB3	1:A:314:LEU:HD21	1.29	1.08
1:B:58:ILE:HB	1:B:70:ALA:HB3	1.39	1.02
1:A:58:ILE:HB	1:A:70:ALA:HB3	1.41	0.98
1:B:32:ARG:HD2	1:B:228:ARG:HH22	1.29	0.97
1:A:32:ARG:HD2	1:A:228:ARG:HH22	1.25	0.95
1:A:396:LYS:HE3	1:A:405:GLU:OE2	1.67	0.94
1:A:33:ASN:HD22	1:A:226:THR:HG21	1.31	0.94
1:A:248:ASN:HD21	1:A:257:ALA:H	1.15	0.93
1:B:33:ASN:HD22	1:B:226:THR:HG21	1.31	0.92
1:B:361:ILE:HG12	2:B:502:LDA:HM23	1.51	0.92
1:B:396:LYS:HE3	1:B:405:GLU:OE2	1.70	0.91
1:A:390:MET:HE3	1:A:412:LEU:HD21	1.52	0.91
1:B:326:ARG:HG3	1:B:348:ASP:HB3	1.53	0.90
1:A:326:ARG:HG3	1:A:348:ASP:HB3	1.52	0.90
1:B:248:ASN:HD21	1:B:257:ALA:H	1.14	0.89
1:B:390:MET:HE3	1:B:412:LEU:HD21	1.58	0.85
1:B:267:LEU:HD23	1:B:268:THR:N	1.94	0.83
1:A:32:ARG:HD2	1:A:228:ARG:NH2	1.93	0.83
1:A:267:LEU:HD23	1:A:268:THR:N	1.93	0.83
1:B:11:SER:HB3	1:B:15:ARG:NH2	1.94	0.82
1:A:302:GLN:HE22	1:A:320:GLY:HA2	1.44	0.82
1:A:11:SER:HB3	1:A:15:ARG:NH2	1.94	0.82
1:B:302:GLN:HE22	1:B:320:GLY:HA2	1.43	0.82
1:A:284:ASP:OD1	1:A:285:PRO:HD2	1.81	0.80
1:B:32:ARG:HD2	1:B:228:ARG:NH2	1.97	0.79
1:B:284:ASP:OD1	1:B:285:PRO:HD2	1.82	0.79
1:A:45:PHE:CE1	1:A:421:PHE:HE1	2.00	0.79
1:A:267:LEU:HD13	2:A:501:LDA:H81	1.64	0.78
1:B:45:PHE:CE1	1:B:421:PHE:HE1	2.01	0.78
1:B:281:ASN:HB2	1:B:289:ILE:HG22	1.64	0.78
1:B:212:GLU:HG3	1:B:226:THR:HG22	1.67	0.77
1:A:378:ASN:O	1:A:379:LYS:HB2	1.85	0.76
1:A:281:ASN:HB2	1:A:289:ILE:HG22	1.67	0.76
1:A:232:LYS:HG2	1:A:270:ASN:ND2	2.01	0.74
1:A:248:ASN:ND2	1:A:257:ALA:H	1.86	0.74
1:B:248:ASN:ND2	1:B:257:ALA:H	1.85	0.74
1:B:33:ASN:ND2	1:B:226:THR:HG21	2.03	0.74
1:A:33:ASN:ND2	1:A:226:THR:HG21	2.03	0.74
1:A:212:GLU:HG3	1:A:226:THR:HG22	1.69	0.74
1:B:252:LEU:HD12	1:B:252:LEU:N	2.03	0.74
1:B:232:LYS:HG2	1:B:270:ASN:ND2	2.02	0.73
1:A:252:LEU:N	1:A:252:LEU:HD12	2.05	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:58:ILE:HD13	1:A:406:SER:HB3	1.71	0.72
1:A:102:TYR:O	1:A:125:THR:HB	1.89	0.72
1:B:308:SER:CB	1:B:314:LEU:HD21	2.15	0.71
1:B:134:TYR:CE1	1:B:136:LEU:HD23	2.25	0.71
1:B:378:ASN:O	1:B:379:LYS:HB2	1.90	0.71
1:B:52:ILE:HG12	1:B:412:LEU:CD1	2.20	0.71
1:B:52:ILE:HG12	1:B:412:LEU:HD13	1.73	0.70
1:A:343:THR:HG22	1:A:344:GLY:N	2.06	0.70
1:A:200:LEU:HB3	2:A:501:LDA:H111	1.73	0.70
1:A:113:ALA:O	1:A:160:GLY:HA3	1.92	0.70
1:A:308:SER:CB	1:A:314:LEU:HD21	2.16	0.70
1:A:45:PHE:HE1	1:A:421:PHE:CE1	2.09	0.70
1:B:113:ALA:O	1:B:160:GLY:HA3	1.91	0.70
1:B:343:THR:HG22	1:B:344:GLY:N	2.06	0.69
1:B:58:ILE:HD13	1:B:406:SER:HB3	1.74	0.69
1:B:302:GLN:NE2	1:B:320:GLY:HA2	2.07	0.69
1:A:178:THR:HG22	1:A:180:GLN:H	1.57	0.69
1:A:52:ILE:HG12	1:A:412:LEU:CD1	2.22	0.68
1:A:45:PHE:HE1	1:A:421:PHE:HE1	1.40	0.68
1:B:102:TYR:O	1:B:125:THR:HB	1.93	0.68
1:A:134:TYR:CE1	1:A:136:LEU:HD23	2.29	0.68
1:B:45:PHE:HE1	1:B:421:PHE:CE1	2.12	0.67
1:B:150:TYR:CE2	1:B:152:ARG:HG3	2.30	0.67
1:B:178:THR:HG22	1:B:180:GLN:H	1.61	0.66
1:A:52:ILE:HG12	1:A:412:LEU:HD13	1.75	0.66
1:A:302:GLN:NE2	1:A:320:GLY:HA2	2.09	0.65
1:A:361:ILE:HG12	2:A:501:LDA:O1	1.95	0.65
1:B:398:ASN:OD1	1:B:403:GLN:HG2	1.97	0.64
1:A:150:TYR:CE2	1:A:152:ARG:HG3	2.32	0.64
1:B:45:PHE:HE1	1:B:421:PHE:HE1	1.42	0.64
1:B:19:GLY:HA2	1:B:278:SER:HB2	1.79	0.64
1:B:45:PHE:CE1	1:B:421:PHE:CE1	2.85	0.64
1:B:248:ASN:HD21	1:B:257:ALA:N	1.93	0.63
1:A:378:ASN:OD1	1:A:380:ASP:HB2	2.00	0.62
1:A:398:ASN:OD1	1:A:403:GLN:HG2	2.00	0.62
1:B:81:ASN:HD22	1:B:83:HIS:CE1	2.18	0.62
1:A:232:LYS:HG2	1:A:270:ASN:HD22	1.64	0.61
1:B:232:LYS:HG2	1:B:270:ASN:HD22	1.66	0.61
1:A:19:GLY:HA2	1:A:278:SER:HB2	1.82	0.61
1:A:107:GLU:O	1:A:107:GLU:HG2	2.00	0.61
1:A:45:PHE:CE1	1:A:421:PHE:CE1	2.84	0.60
1:A:245:ARG:HB2	1:A:245:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:ASN:HD22	1:A:83:HIS:CE1	2.19	0.60
1:B:361:ILE:HD11	2:B:502:LDA:HM12	1.84	0.60
1:B:191:ILE:H	1:B:191:ILE:HD12	1.67	0.60
1:B:378:ASN:OD1	1:B:380:ASP:HB2	2.02	0.60
1:A:343:THR:CG2	1:A:344:GLY:N	2.65	0.60
1:B:42:ARG:HD2	1:B:421:PHE:O	2.02	0.59
1:B:343:THR:CG2	1:B:344:GLY:N	2.65	0.59
1:B:199:HIS:C	1:B:200:LEU:HD12	2.23	0.59
1:A:236:LYS:HD3	1:A:266:TYR:CE2	2.37	0.59
1:A:191:ILE:HD12	1:A:191:ILE:H	1.68	0.58
1:B:245:ARG:NH1	1:B:245:ARG:HB2	2.18	0.58
1:B:276:GLU:HG3	1:B:294:ALA:HB2	1.84	0.58
1:A:267:LEU:C	1:A:267:LEU:HD23	2.23	0.58
1:B:219:LYS:HA	1:B:219:LYS:HE2	1.85	0.58
1:B:177:GLN:HA	1:B:182:GLN:HE21	1.69	0.58
1:B:236:LYS:HD3	1:B:266:TYR:CE2	2.38	0.58
1:B:370:SER:HB3	1:B:388:SER:OG	2.03	0.57
1:A:326:ARG:CG	1:A:348:ASP:HB3	2.31	0.57
1:B:11:SER:HB3	1:B:15:ARG:HH22	1.68	0.57
1:A:199:HIS:C	1:A:200:LEU:HD12	2.24	0.57
1:A:58:ILE:HD13	1:A:406:SER:CB	2.33	0.57
1:A:42:ARG:HD2	1:A:421:PHE:O	2.05	0.57
1:A:393:GLN:HE21	1:A:394:SER:H	1.52	0.57
1:B:176:GLY:O	1:B:182:GLN:HG3	2.05	0.57
1:B:107:GLU:O	1:B:107:GLU:HG2	2.04	0.57
1:B:121:THR:HG21	2:B:502:LDA:HM22	1.86	0.57
1:B:30:VAL:HG11	1:B:85:VAL:HG21	1.86	0.56
1:B:393:GLN:HE21	1:B:394:SER:H	1.52	0.56
1:B:57:ASN:ND2	1:B:72:ASN:H	2.04	0.56
1:A:248:ASN:HD21	1:A:257:ALA:N	1.94	0.56
1:B:169:GLN:OE1	1:B:169:GLN:HA	2.06	0.56
1:B:267:LEU:HD23	1:B:267:LEU:C	2.25	0.56
1:A:177:GLN:HA	1:A:182:GLN:HE21	1.71	0.55
1:A:30:VAL:HG11	1:A:85:VAL:HG21	1.87	0.55
1:B:10:SER:HB2	1:B:416:ASN:HB2	1.87	0.55
1:B:136:LEU:HD12	1:B:140:TRP:HB2	1.88	0.55
1:A:290:HIS:HE1	1:A:332:THR:OG1	1.90	0.55
1:A:144:LEU:HD23	1:A:210:ASN:O	2.06	0.55
1:A:219:LYS:HE2	1:A:219:LYS:HA	1.88	0.55
1:B:134:TYR:CD1	1:B:136:LEU:HD23	2.41	0.55
1:B:243:LEU:O	1:B:257:ALA:HB1	2.07	0.55
1:A:176:GLY:O	1:A:182:GLN:HG3	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:137:ASN:ND2	1:A:140:TRP:H	2.05	0.54
1:A:57:ASN:ND2	1:A:72:ASN:H	2.06	0.54
1:A:134:TYR:CD1	1:A:136:LEU:HD23	2.41	0.54
1:B:346:ALA:HB3	1:B:368:TRP:HB2	1.89	0.54
1:A:81:ASN:HD22	1:A:83:HIS:HE1	1.55	0.54
1:A:10:SER:HB2	1:A:416:ASN:HB2	1.89	0.54
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.07	0.54
1:A:276:GLU:HG3	1:A:294:ALA:HB2	1.89	0.54
1:A:239:TYR:CG	1:A:240:SER:N	2.76	0.54
1:B:239:TYR:CG	1:B:240:SER:N	2.76	0.54
1:A:11:SER:HB3	1:A:15:ARG:HH22	1.72	0.54
1:B:167:ALA:CB	1:B:189:ASN:HB2	2.37	0.54
1:A:297:SER:HA	1:A:323:ASP:CG	2.28	0.54
1:B:58:ILE:HD13	1:B:406:SER:CB	2.36	0.54
1:A:246:ALA:O	1:A:248:ASN:N	2.41	0.53
1:B:144:LEU:HD23	1:B:210:ASN:O	2.07	0.53
1:B:297:SER:HA	1:B:323:ASP:CG	2.29	0.53
1:A:167:ALA:CB	1:A:189:ASN:HB2	2.39	0.53
1:A:104:LEU:HD23	2:A:501:LDA:H12	1.90	0.53
1:B:137:ASN:ND2	1:B:140:TRP:H	2.05	0.53
1:A:346:ALA:HB3	1:A:368:TRP:HB2	1.91	0.53
1:A:136:LEU:HD12	1:A:140:TRP:HB2	1.90	0.53
1:B:81:ASN:HD22	1:B:83:HIS:HE1	1.56	0.52
1:B:1:ALA:HB1	1:B:4:GLN:HB3	1.91	0.52
1:B:246:ALA:O	1:B:248:ASN:N	2.42	0.52
1:A:89:ASN:ND2	1:A:91:GLN:H	2.07	0.52
1:B:326:ARG:CG	1:B:348:ASP:HB3	2.32	0.52
1:A:227:TYR:HD1	1:A:275:TRP:NE1	2.08	0.52
1:B:292:SER:O	1:B:327:ILE:HD13	2.09	0.52
1:A:292:SER:O	1:A:327:ILE:HD13	2.09	0.52
1:A:166:VAL:O	1:A:170:ILE:HG13	2.10	0.51
1:B:354:ALA:HA	1:B:357:ARG:HG3	1.92	0.51
1:A:243:LEU:O	1:A:257:ALA:HB1	2.10	0.51
1:B:89:ASN:ND2	1:B:91:GLN:H	2.09	0.51
1:B:178:THR:HG22	1:B:180:GLN:HB2	1.92	0.51
1:B:220:ASN:HB3	1:B:282:ARG:HB3	1.93	0.51
1:A:26:ASP:HB2	1:A:418:ASN:ND2	2.25	0.51
1:B:26:ASP:HB2	1:B:418:ASN:ND2	2.26	0.51
1:A:178:THR:HB	1:A:181:GLY:H	1.76	0.51
1:A:273:GLU:HG3	1:A:297:SER:OG	2.11	0.51
1:A:178:THR:HG22	1:A:180:GLN:HB2	1.92	0.50
1:B:18:SER:HB3	1:B:328:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:361:ILE:O	1:A:363:ASP:N	2.44	0.50
1:B:216:GLU:HB3	1:B:222:ARG:HB3	1.93	0.50
1:A:18:SER:HB3	1:A:328:ALA:HB1	1.92	0.50
1:A:1:ALA:HB1	1:A:4:GLN:HB3	1.94	0.50
1:B:58:ILE:HB	1:B:70:ALA:CB	2.27	0.50
1:B:273:GLU:HG3	1:B:297:SER:OG	2.10	0.50
1:B:289:ILE:HD12	1:B:331:THR:HB	1.93	0.50
1:A:66:ARG:HH11	1:A:161:ASP:HB3	1.76	0.50
1:A:220:ASN:HB3	1:A:282:ARG:HB3	1.93	0.50
1:A:216:GLU:HB3	1:A:222:ARG:HB3	1.94	0.50
1:A:111:THR:HA	1:A:193:SER:HB3	1.93	0.50
1:B:378:ASN:O	1:B:379:LYS:CB	2.60	0.49
1:B:66:ARG:HH11	1:B:161:ASP:HB3	1.77	0.49
1:A:354:ALA:HA	1:A:357:ARG:HG3	1.93	0.49
1:A:137:ASN:ND2	1:A:139:ALA:H	2.10	0.49
1:B:111:THR:HA	1:B:193:SER:HB3	1.95	0.49
1:A:358:SER:HB2	1:A:399:GLU:OE1	2.11	0.49
1:A:54:PRO:HG2	1:A:74:ALA:O	2.12	0.49
1:B:4:GLN:NE2	1:B:274:MET:CE	2.76	0.49
1:B:361:ILE:HG12	2:B:502:LDA:CM2	2.32	0.49
1:B:361:ILE:O	1:B:363:ASP:N	2.44	0.49
1:A:289:ILE:HD12	1:A:331:THR:HB	1.92	0.49
1:B:73:ILE:HD11	1:B:362:PRO:HG2	1.94	0.49
1:B:54:PRO:HG2	1:B:74:ALA:O	2.13	0.49
1:A:370:SER:HB3	1:A:388:SER:OG	2.11	0.49
1:A:212:GLU:CG	1:A:226:THR:HG22	2.42	0.49
1:B:113:ALA:C	1:B:160:GLY:HA3	2.33	0.49
1:B:200:LEU:N	1:B:200:LEU:HD12	2.28	0.48
1:B:411:TRP:C	1:B:412:LEU:HD22	2.34	0.48
1:B:31:SER:HB3	1:B:83:HIS:HD2	1.78	0.48
1:B:290:HIS:HE1	1:B:332:THR:OG1	1.95	0.48
1:B:166:VAL:O	1:B:170:ILE:HG13	2.13	0.48
1:B:293:LEU:HD13	1:B:327:ILE:HG12	1.95	0.48
1:A:137:ASN:HD21	1:A:140:TRP:H	1.61	0.48
1:B:178:THR:HB	1:B:181:GLY:H	1.78	0.48
1:A:4:GLN:NE2	1:A:274:MET:CE	2.77	0.48
1:B:239:TYR:CE2	1:B:314:LEU:HB3	2.48	0.48
1:A:64:SER:HB3	1:A:165:LEU:HD21	1.96	0.48
1:B:51:TYR:HD1	1:B:78:TRP:HD1	1.60	0.48
1:A:51:TYR:HD1	1:A:78:TRP:CD1	2.32	0.47
1:B:51:TYR:HD1	1:B:78:TRP:CD1	2.32	0.47
1:B:212:GLU:CG	1:B:226:THR:HG22	2.40	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:274:MET:HE3	1:B:274:MET:HB2	1.78	0.47
1:A:298:TRP:HB3	1:A:321:PHE:HB3	1.97	0.47
1:B:137:ASN:ND2	1:B:139:ALA:H	2.12	0.47
1:B:137:ASN:HD21	1:B:140:TRP:H	1.61	0.47
1:B:147:ASN:ND2	1:B:210:ASN:OD1	2.46	0.47
1:A:51:TYR:HD1	1:A:78:TRP:HD1	1.61	0.47
1:B:31:SER:HB3	1:B:83:HIS:CD2	2.49	0.47
1:B:7:GLU:N	1:B:7:GLU:CD	2.68	0.47
1:B:177:GLN:HA	1:B:182:GLN:NE2	2.29	0.47
1:B:1:ALA:HB1	1:B:4:GLN:CB	2.45	0.47
1:B:358:SER:HB2	1:B:399:GLU:OE1	2.14	0.47
1:A:200:LEU:N	1:A:200:LEU:HD12	2.30	0.46
1:B:30:VAL:O	1:B:30:VAL:HG23	2.16	0.46
1:B:30:VAL:CG1	1:B:85:VAL:HG21	2.44	0.46
1:A:378:ASN:O	1:A:379:LYS:CB	2.56	0.46
1:A:227:TYR:HD1	1:A:275:TRP:CD1	2.33	0.46
1:A:113:ALA:C	1:A:160:GLY:HA3	2.34	0.46
1:A:137:ASN:C	1:A:137:ASN:HD22	2.19	0.46
1:B:16:ALA:HB2	1:B:370:SER:OG	2.16	0.46
1:A:58:ILE:CD1	1:A:406:SER:HB3	2.42	0.46
1:A:364:GLN:HG3	1:A:393:GLN:O	2.16	0.46
1:A:31:SER:HB3	1:A:83:HIS:HD2	1.79	0.46
1:A:66:ARG:NH1	1:A:161:ASP:HB3	2.30	0.46
1:A:411:TRP:C	1:A:412:LEU:HD22	2.36	0.46
1:B:298:TRP:HB3	1:B:321:PHE:HB3	1.96	0.46
1:B:64:SER:HB3	1:B:165:LEU:HD21	1.98	0.46
1:B:199:HIS:O	1:B:239:TYR:HA	2.16	0.46
1:A:227:TYR:CD1	1:A:275:TRP:NE1	2.84	0.46
1:B:66:ARG:NH1	1:B:161:ASP:HB3	2.30	0.46
1:A:281:ASN:O	1:A:288:ALA:HA	2.16	0.46
1:B:137:ASN:C	1:B:137:ASN:HD22	2.18	0.46
1:B:58:ILE:CD1	1:B:406:SER:HB3	2.44	0.45
1:A:232:LYS:NZ	1:A:270:ASN:HD21	2.14	0.45
1:A:73:ILE:HD11	1:A:362:PRO:HG2	1.98	0.45
1:A:191:ILE:HD12	1:A:191:ILE:N	2.32	0.45
1:A:177:GLN:HA	1:A:182:GLN:NE2	2.31	0.45
1:A:319:GLU:OE1	2:A:501:LDA:HM23	2.16	0.45
1:B:227:TYR:HD1	1:B:275:TRP:NE1	2.15	0.45
1:B:228:ARG:HB3	1:B:274:MET:HB3	1.98	0.45
1:A:246:ALA:C	1:A:248:ASN:H	2.20	0.45
1:A:89:ASN:CG	1:A:91:GLN:H	2.20	0.45
1:B:116:SER:HA	1:B:158:PHE:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:30:VAL:CG1	1:A:85:VAL:HG21	2.46	0.45
1:B:241:SER:HB3	1:B:257:ALA:HA	1.99	0.45
1:A:340:THR:HB	1:A:374:THR:HB	1.99	0.45
1:B:121:THR:OG1	1:B:157:ARG:NH2	2.50	0.45
1:A:252:LEU:CD1	1:A:252:LEU:N	2.76	0.45
1:A:1:ALA:HB1	1:A:4:GLN:CB	2.47	0.44
1:A:239:TYR:CE2	1:A:314:LEU:HB3	2.51	0.44
1:B:348:ASP:OD2	1:B:366:ARG:HB2	2.16	0.44
1:A:31:SER:HB3	1:A:83:HIS:CD2	2.52	0.44
1:B:157:ARG:HA	1:B:157:ARG:HD3	1.74	0.44
1:A:302:GLN:NE2	1:A:302:GLN:HA	2.33	0.44
1:B:227:TYR:HD1	1:B:275:TRP:CD1	2.36	0.44
1:A:121:THR:OG1	1:A:157:ARG:NH2	2.51	0.44
1:B:364:GLN:O	1:B:366:ARG:HG3	2.18	0.44
1:B:246:ALA:C	1:B:248:ASN:H	2.21	0.44
1:B:162:LEU:HA	1:B:162:LEU:HD23	1.88	0.44
1:A:378:ASN:OD1	1:A:380:ASP:N	2.50	0.44
1:A:16:ALA:HB2	1:A:370:SER:OG	2.18	0.44
1:A:7:GLU:CD	1:A:7:GLU:N	2.71	0.44
1:B:302:GLN:HA	1:B:302:GLN:NE2	2.33	0.44
1:A:199:HIS:O	1:A:239:TYR:HA	2.18	0.43
1:A:364:GLN:O	1:A:366:ARG:HG3	2.17	0.43
1:A:299:SER:HA	1:A:321:PHE:O	2.18	0.43
1:A:228:ARG:HB3	1:A:274:MET:HB3	2.00	0.43
1:B:136:LEU:HD12	1:B:140:TRP:CB	2.48	0.43
1:A:293:LEU:HD13	1:A:327:ILE:HG12	1.99	0.43
1:A:174:PRO:C	1:A:176:GLY:H	2.22	0.43
1:B:299:SER:HA	1:B:321:PHE:O	2.18	0.43
1:B:355:GLN:HB2	1:B:355:GLN:HE21	1.64	0.43
1:A:96:ALA:HA	1:A:129:ASN:O	2.19	0.43
1:B:348:ASP:O	1:B:348:ASP:OD2	2.37	0.43
1:A:30:VAL:HG23	1:A:30:VAL:O	2.18	0.43
1:A:241:SER:HB3	1:A:257:ALA:HA	2.01	0.43
1:A:162:LEU:O	1:A:166:VAL:HG23	2.19	0.43
1:B:96:ALA:HA	1:B:129:ASN:O	2.19	0.43
1:B:340:THR:HB	1:B:374:THR:HB	2.01	0.43
1:A:348:ASP:OD2	1:A:366:ARG:HB2	2.19	0.43
1:B:134:TYR:CE1	1:B:136:LEU:CD2	2.99	0.43
1:A:116:SER:HA	1:A:158:PHE:O	2.19	0.43
1:A:274:MET:HE3	1:A:274:MET:HB2	1.79	0.43
1:B:30:VAL:CG2	1:B:30:VAL:O	2.67	0.43
1:B:321:PHE:CZ	1:B:352:VAL:HG22	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:89:ASN:CG	1:B:91:GLN:H	2.22	0.42
1:A:84:PHE:CZ	1:A:86:ALA:HB2	2.54	0.42
1:B:19:GLY:HA2	1:B:292:SER:HB3	2.01	0.42
1:A:136:LEU:HD12	1:A:140:TRP:CB	2.49	0.42
1:A:321:PHE:CZ	1:A:352:VAL:HG22	2.55	0.42
1:B:88:ILE:HG13	1:B:93:GLY:HA2	2.02	0.42
1:B:4:GLN:NE2	1:B:274:MET:HE1	2.35	0.42
1:B:272:PRO:HG2	1:B:298:TRP:CD2	2.54	0.42
1:B:355:GLN:HG3	1:B:355:GLN:H	1.40	0.42
1:A:196:LYS:HB2	1:A:196:LYS:HE3	1.89	0.42
1:B:281:ASN:O	1:B:288:ALA:HA	2.20	0.42
1:B:232:LYS:NZ	1:B:270:ASN:HD21	2.18	0.42
1:A:191:ILE:H	1:A:191:ILE:CD1	2.33	0.42
1:A:272:PRO:HG2	1:A:298:TRP:CD2	2.54	0.42
1:A:204:GLN:HG3	1:A:205:TRP:N	2.34	0.42
1:B:145:GLY:O	1:B:209:TRP:HA	2.20	0.42
1:A:282:ARG:HH11	1:A:282:ARG:HG3	1.85	0.42
1:B:238:ASN:HB3	1:B:262:THR:CG2	2.50	0.42
1:B:137:ASN:C	1:B:137:ASN:ND2	2.73	0.42
1:A:273:GLU:H	1:A:300:GLN:HE22	1.68	0.42
1:A:246:ALA:C	1:A:248:ASN:N	2.73	0.41
1:B:364:GLN:HG3	1:B:393:GLN:O	2.20	0.41
1:B:291:TYR:N	1:B:291:TYR:CD2	2.88	0.41
1:B:7:GLU:CD	1:B:7:GLU:H	2.24	0.41
1:B:84:PHE:CZ	1:B:86:ALA:HB2	2.56	0.41
1:A:157:ARG:HD3	1:A:157:ARG:HA	1.75	0.41
1:B:378:ASN:OD1	1:B:380:ASP:N	2.53	0.41
1:B:162:LEU:O	1:B:166:VAL:HG23	2.21	0.41
1:B:191:ILE:N	1:B:191:ILE:HD12	2.31	0.41
1:A:147:ASN:ND2	1:A:210:ASN:OD1	2.46	0.41
1:B:282:ARG:HG3	1:B:282:ARG:HH11	1.85	0.41
1:B:58:ILE:CB	1:B:70:ALA:HB3	2.28	0.41
1:B:239:TYR:O	1:B:240:SER:HB3	2.20	0.41
1:B:174:PRO:C	1:B:176:GLY:H	2.22	0.41
1:B:227:TYR:CD1	1:B:275:TRP:NE1	2.89	0.41
1:B:361:ILE:CD1	2:B:502:LDA:HM12	2.49	0.41
1:B:246:ALA:C	1:B:248:ASN:N	2.74	0.41
1:B:273:GLU:HG2	1:B:300:GLN:OE1	2.21	0.41
1:B:204:GLN:HG3	1:B:205:TRP:N	2.35	0.41
1:B:380:ASP:O	1:B:419:TYR:HA	2.21	0.41
1:A:271:LEU:HA	1:A:272:PRO:HD3	1.83	0.41
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:ASN:HB3	1:A:282:ARG:CB	2.51	0.40
1:A:284:ASP:CG	1:A:285:PRO:HD2	2.41	0.40
1:B:177:GLN:H	1:B:177:GLN:CD	2.25	0.40
1:B:272:PRO:HA	1:B:300:GLN:NE2	2.36	0.40
1:A:348:ASP:O	1:A:348:ASP:OD2	2.39	0.40
1:A:19:GLY:HA2	1:A:292:SER:HB3	2.03	0.40
1:B:223:TYR:CD1	1:B:223:TYR:N	2.88	0.40
1:A:143:GLY:O	1:A:211:ALA:HA	2.22	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	414/427 (97%)	382 (92%)	26 (6%)	6 (1%)	16	52
1	B	414/427 (97%)	376 (91%)	32 (8%)	6 (1%)	16	52
All	All	828/854 (97%)	758 (92%)	58 (7%)	12 (1%)	16	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	PHE
1	A	378	ASN
1	B	247	PHE
1	B	378	ASN
1	A	2	GLY
1	B	2	GLY
1	B	160	GLY
1	A	160	GLY
1	B	196	LYS
1	A	196	LYS
1	A	115	GLY
1	B	115	GLY

### 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	330/338 (98%)	295 (89%)	35 (11%)	10	28
1	B	330/338 (98%)	296 (90%)	34 (10%)	10	30
All	All	660/676 (98%)	591 (90%)	69 (10%)	10	29

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	71	ASP
1	A	78	TRP
1	A	107	GLU
1	A	124	GLU
1	A	125	THR
1	A	137	ASN
1	A	142	PHE
1	A	144	LEU
1	A	180	GLN
1	A	197	THR
1	A	219	LYS
1	A	222	ARG
1	A	226	THR
1	A	228	ARG
1	A	252	LEU
1	A	264	SER
1	A	277	VAL
1	A	282	ARG
1	A	284	ASP
1	A	297	SER
1	A	307	THR
1	A	309	THR
1	A	317	LYS
1	A	327	ILE
1	A	329	LEU
1	A	331	THR
1	A	337	ASP
1	A	349	ASP

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Mol	Chain	Res	Type
1	A	355	GLN
1	A	361	ILE
1	A	373	THR
1	A	407	GLU
1	A	412	LEU
1	A	416	ASN
1	B	30	VAL
1	B	71	ASP
1	B	78	TRP
1	B	107	GLU
1	B	120	THR
1	B	124	GLU
1	B	125	THR
1	B	137	ASN
1	B	142	PHE
1	B	144	LEU
1	B	180	GLN
1	B	197	THR
1	B	219	LYS
1	B	222	ARG
1	B	226	THR
1	B	228	ARG
1	B	252	LEU
1	B	264	SER
1	B	277	VAL
1	B	282	ARG
1	B	284	ASP
1	B	307	THR
1	B	309	THR
1	B	317	LYS
1	B	327	ILE
1	B	329	LEU
1	B	331	THR
1	B	337	ASP
1	B	349	ASP
1	B	355	GLN
1	B	361	ILE
1	B	407	GLU
1	B	412	LEU
1	B	416	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	33	ASN
1	A	57	ASN
1	A	72	ASN
1	A	83	HIS
1	A	129	ASN
1	A	137	ASN
1	A	138	ASN
1	A	182	GLN
1	A	194	ASN
1	A	248	ASN
1	A	270	ASN
1	A	281	ASN
1	A	290	HIS
1	A	300	GLN
1	A	302	GLN
1	A	303	GLN
1	A	316	GLN
1	A	355	GLN
1	A	356	ASN
1	A	393	GLN
1	A	418	ASN
1	B	4	GLN
1	B	33	ASN
1	B	57	ASN
1	B	72	ASN
1	B	83	HIS
1	B	129	ASN
1	B	137	ASN
1	B	138	ASN
1	B	182	GLN
1	B	248	ASN
1	B	270	ASN
1	B	281	ASN
1	B	290	HIS
1	B	300	GLN
1	B	302	GLN
1	B	303	GLN
1	B	316	GLN
1	B	355	GLN
1	B	356	ASN
1	B	393	GLN
1	B	418	ASN

### 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 ⓘ

2 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	501	-	15,15,15	4.06	2 (13%)	17,17,17	2.23	6 (35%)
2	LDA	B	502	-	15,15,15	3.99	2 (13%)	17,17,17	2.05	5 (29%)

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	501	-	-	0/13/13/13	0/0/0/0
2	LDA	B	502	-	-	0/13/13/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LDA	O1-N1	-14.76	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	LDA	O1-N1	-14.45	1.25	1.39
2	B	502	LDA	CM2-N1	-4.87	1.41	1.49
2	A	501	LDA	CM2-N1	-4.63	1.42	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LDA	CM2-N1-CM1	-5.59	102.46	108.85
2	B	502	LDA	CM2-N1-CM1	-4.85	103.31	108.85
2	A	501	LDA	C2-C1-N1	3.82	120.39	113.80
2	B	502	LDA	C2-C1-N1	3.77	120.30	113.80
2	A	501	LDA	O1-N1-C1	3.07	114.46	110.19
2	B	502	LDA	O1-N1-C1	2.82	114.11	110.19
2	A	501	LDA	O1-N1-CM2	2.65	112.57	109.01
2	B	502	LDA	O1-N1-CM2	2.60	112.51	109.01
2	A	501	LDA	CM1-N1-C1	-2.45	101.85	109.86
2	B	502	LDA	C9-C8-C7	-2.31	102.11	114.61
2	A	501	LDA	C9-C8-C7	-2.06	103.49	114.61

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	418/427 (97%)	0.11	10 (2%) 56 65	7, 31, 63, 92	0
1	B	418/427 (97%)	0.52	37 (8%) 10 12	16, 47, 90, 108	0
All	All	836/854 (97%)	0.32	47 (5%) 24 28	7, 38, 84, 108	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	7.8
1	B	181	GLY	6.3
1	B	180	GLN	5.1
1	B	184	LEU	5.0
1	B	138	ASN	4.9
1	B	275	TRP	4.9
1	A	177	GLN	4.5
1	B	174	PRO	4.1
1	B	183	ALA	4.0
1	A	182	GLN	3.8
1	B	228	ARG	3.8
1	A	275	TRP	3.6
1	B	178	THR	3.4
1	B	70	ALA	3.3
1	B	227	TYR	3.2
1	B	170	ILE	3.1
1	B	396	LYS	3.1
1	B	64	SER	3.1
1	B	166	VAL	3.0
1	B	32	ARG	2.9
1	A	171	MET	2.9
1	B	274	MET	2.8
1	B	60	GLY	2.8
1	A	228	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	66	ARG	2.6
1	B	179	GLN	2.6
1	B	171	MET	2.5
1	B	252	LEU	2.5
1	A	185	ALA	2.4
1	B	295	TYR	2.4
1	B	2	GLY	2.4
1	B	67	SER	2.4
1	B	217	LEU	2.4
1	B	404	PHE	2.4
1	B	68	LEU	2.3
1	B	314	LEU	2.3
1	B	247	PHE	2.3
1	A	179	GLN	2.3
1	B	253	PRO	2.2
1	B	137	ASN	2.2
1	A	209	TRP	2.2
1	B	210	ASN	2.1
1	B	182	GLN	2.1
1	A	65	GLY	2.1
1	B	63	PRO	2.0
1	A	274	MET	2.0
1	B	173	SER	2.0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	LDA	B	502	16/16	0.47	5.72	70,71,77,78	0
2	LDA	A	501	16/16	0.35	4.26	67,70,76,76	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.