



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:18 PM GMT

PDB ID : 1T16  
Title : Crystal structure of the bacterial fatty acid transporter FadL from Escherichia coli  
Authors : van den Berg, B.; Black, P.N.; Clemons Jr., W.M.; Rapoport, T.A.  
Deposited on : 2004-04-15  
Resolution : 2.60 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](mailto: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.

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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 : 1.7 (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

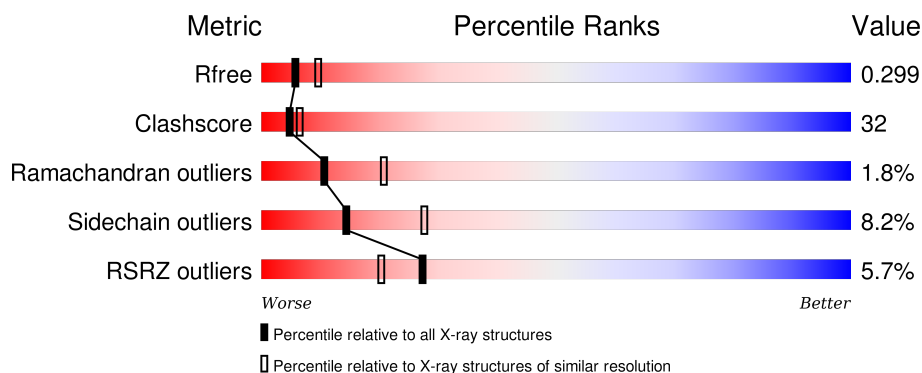
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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  $\geq 3$ , 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	427	<div> <div>4%</div> <div>54%</div> <div>41%</div> <div>5%</div> </div>
1	B	427	<div> <div>8%</div> <div>51%</div> <div>44%</div> <div>.</div> </div>

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
3	LDA	A	431	-	-	-	X
3	LDA	A	432	-	-	-	X
3	LDA	B	431	-	-	X	X
3	LDA	B	432	-	-	-	X
4	C8E	A	433	-	-	-	X
4	C8E	B	433	-	-	-	X
4	C8E	B	434	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6909 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	427	Total	C	N	O	S	0	0	0
			3313	2093	570	644	6			
1	B	427	Total	C	N	O	S	0	0	0
			3313	2093	570	644	6			

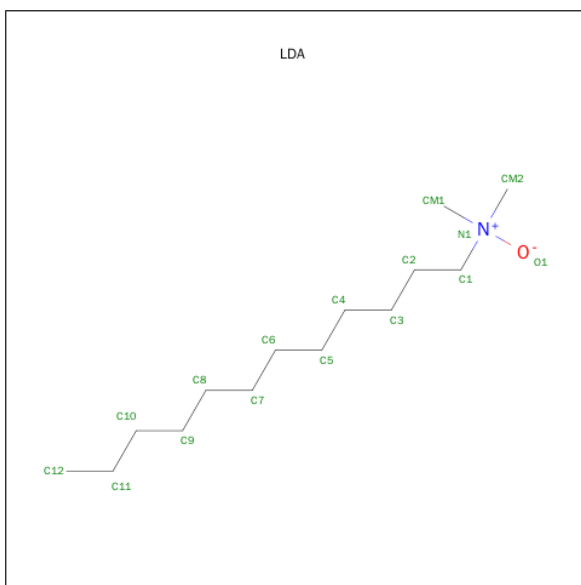
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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 COPPER (II) ION (three-letter code: CU) (formula: Cu).

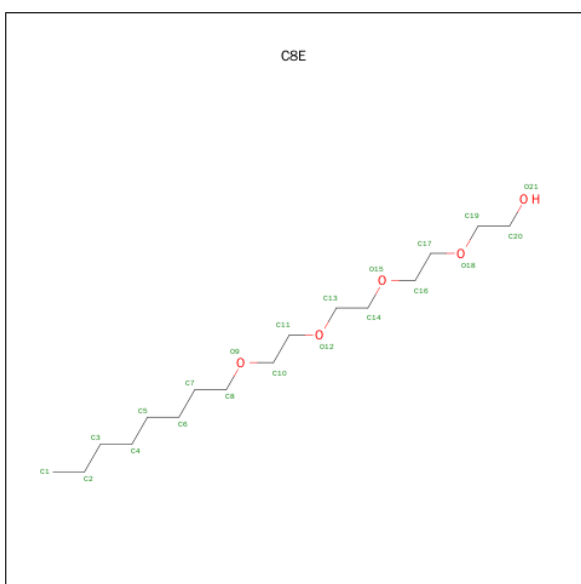
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cu	0	0
			3	3		
2	A	3	Total	Cu	0	0
			3	3		

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula:  $C_{16}H_{34}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			21	16	5		
4	B	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		

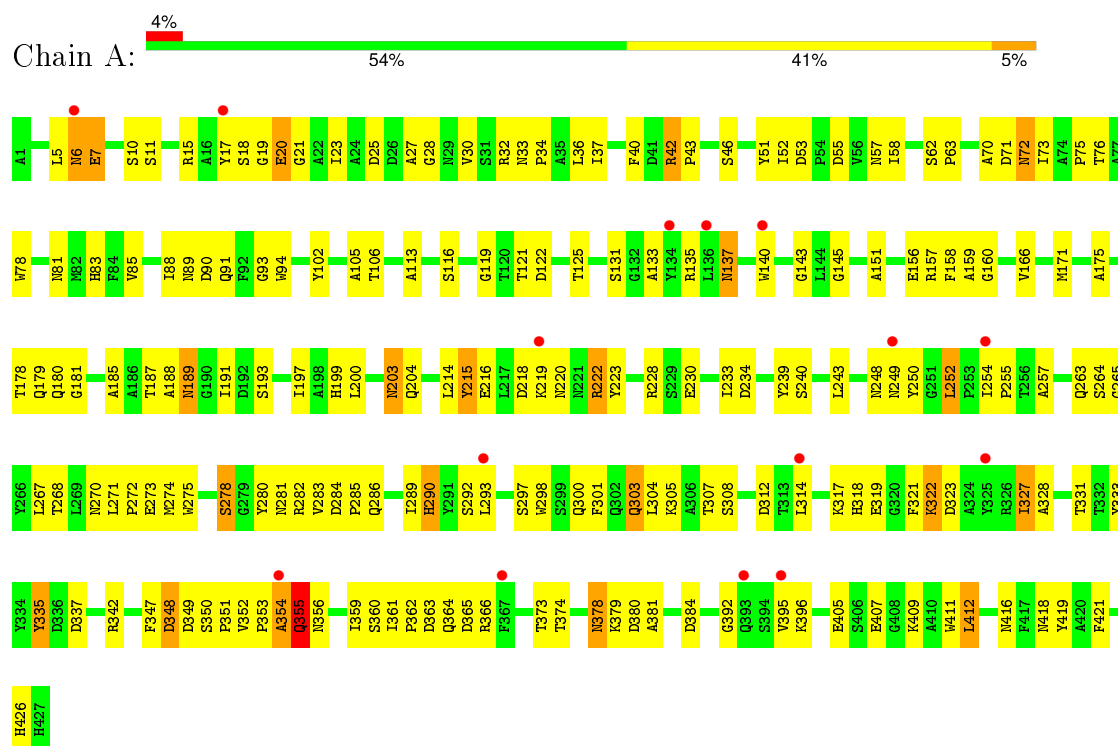
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		
5	B	64	Total	O	0	0
			64	64		

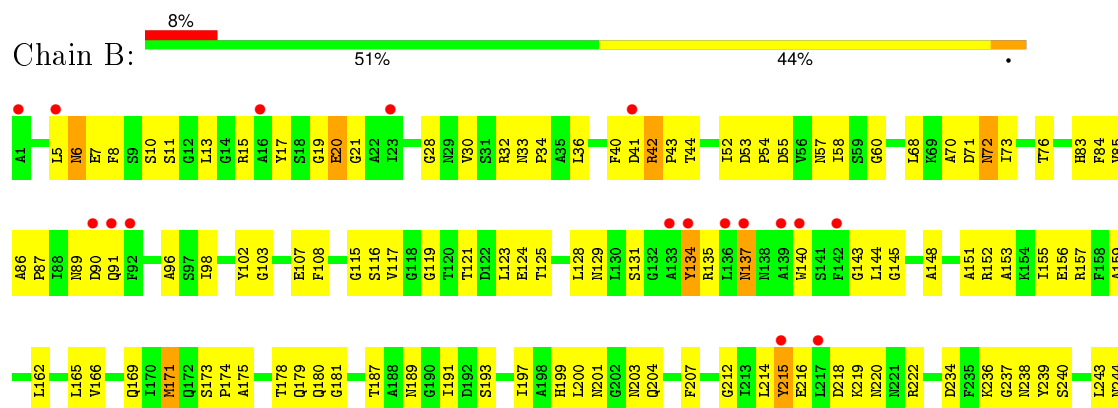
### 3 Residue-property plots [i](#)

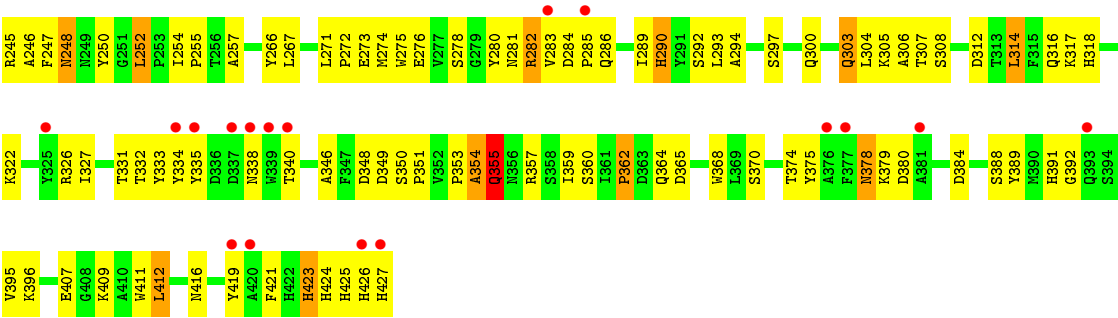
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



#### • Molecule 1: Long-chain fatty acid transport protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.38Å 68.66Å 106.02Å 90.00° 96.37° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 35.12 – 2.49	Depositor EDS
% Data completeness (in resolution range)	91.9 (10.00-2.60) 87.3 (35.12-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.70 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.257 , 0.301 0.256 , 0.299	Depositor DCC
$R_{free}$ test set	2033 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 46492 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup> Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, C8E, CU

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	0/3408	0.66	0/4639
1	B	0.42	0/3408	0.67	1/4639 (0.0%)
All	All	0.44	0/6816	0.67	1/9278 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	ASN	N-CA-C	7.27	130.63	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3313	0	3075	203	0
1	B	3313	0	3075	217	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	32	0	62	7	0
3	B	32	0	62	16	0
4	A	21	0	34	7	0
4	B	42	0	68	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	86	0	0	12	0
5	B	64	0	0	13	0
All	All	6909	0	6376	415	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 32.

All (415) 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:254:ILE:HD12	1:B:255:PRO:HD2	1.31	1.12
1:B:89:ASN:ND2	1:B:90:ASP:H	1.60	0.99
1:A:248:ASN:HD21	1:A:257:ALA:H	1.05	0.97
1:A:89:ASN:ND2	1:A:90:ASP:H	1.65	0.94
1:A:252:LEU:HB2	1:A:254:ILE:HG22	1.49	0.93
1:B:293:LEU:HD13	1:B:327:ILE:HD13	1.52	0.92
1:A:178:THR:HG22	1:A:180:GLN:H	1.33	0.92
1:B:289:ILE:HG13	1:B:331:THR:HG22	1.52	0.91
1:B:250:TYR:HB2	1:B:252:LEU:HD11	1.50	0.90
1:A:34:PRO:HB2	1:A:143:GLY:HA3	1.52	0.90
1:B:252:LEU:HB2	1:B:254:ILE:HG22	1.51	0.89
1:B:303:GLN:HE22	1:B:305:LYS:HB2	1.36	0.88
1:A:364:GLN:HG2	3:A:432:LDA:HM23	1.54	0.88
1:A:6:ASN:HB2	1:A:32:ARG:HH12	1.40	0.85
1:A:254:ILE:HD12	1:A:255:PRO:HD2	1.58	0.84
1:B:252:LEU:HD12	1:B:252:LEU:H	1.41	0.84
1:A:57:ASN:ND2	1:A:72:ASN:H	1.76	0.84
1:A:102:TYR:O	1:A:125:THR:HB	1.77	0.84
1:B:237:GLY:HA2	5:B:471:HOH:O	1.77	0.83
1:A:274:MET:HG2	5:A:472:HOH:O	1.78	0.83
1:B:254:ILE:HD12	1:B:255:PRO:CD	2.08	0.82
1:A:252:LEU:HD12	1:A:252:LEU:H	1.44	0.81
1:A:250:TYR:HB2	1:A:252:LEU:HD11	1.61	0.81
1:A:140:TRP:HB2	1:A:214:LEU:O	1.82	0.80
1:B:346:ALA:HB3	1:B:368:TRP:HB2	1.64	0.79
1:A:304:LEU:HD22	3:A:431:LDA:HM13	1.66	0.78
1:A:140:TRP:HA	5:A:441:HOH:O	1.84	0.78
1:A:293:LEU:HD13	1:A:327:ILE:HG12	1.64	0.78
1:A:57:ASN:HD22	1:A:71:ASP:HA	1.49	0.78
1:B:364:GLN:HE21	1:B:392:GLY:HA3	1.49	0.77
1:B:191:ILE:H	1:B:191:ILE:HD12	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HG3	1:A:421:PHE:O	1.85	0.76
1:A:364:GLN:HE21	1:A:392:GLY:HA3	1.49	0.75
1:A:289:ILE:HG13	1:A:331:THR:HG22	1.68	0.75
1:B:280:TYR:C	1:B:281:ASN:HD22	1.90	0.75
1:B:42:ARG:HG3	1:B:421:PHE:O	1.88	0.74
1:B:396:LYS:N	1:B:396:LYS:HD2	2.02	0.74
1:B:153:ALA:HB1	3:B:431:LDA:H82	1.70	0.73
1:B:89:ASN:ND2	1:B:90:ASP:N	2.35	0.73
1:A:248:ASN:ND2	1:A:257:ALA:H	1.86	0.73
1:B:248:ASN:HD21	1:B:257:ALA:H	1.36	0.72
1:B:140:TRP:HB2	1:B:214:LEU:O	1.88	0.72
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.54	0.72
1:A:248:ASN:HD21	1:A:257:ALA:N	1.86	0.71
1:B:178:THR:HG22	1:B:180:GLN:H	1.55	0.70
1:B:252:LEU:HD12	1:B:252:LEU:N	2.06	0.70
1:B:244:ASN:ND2	4:B:434:C8E:H201	2.06	0.70
1:A:281:ASN:HB2	1:A:289:ILE:HG22	1.72	0.70
1:B:152:ARG:HD3	5:B:461:HOH:O	1.91	0.70
1:A:292:SER:O	1:A:327:ILE:HD13	1.91	0.70
1:A:11:SER:HB2	1:A:15:ARG:NH2	2.07	0.70
1:A:396:LYS:HD2	1:A:396:LYS:N	2.06	0.70
1:A:137:ASN:HD21	1:A:140:TRP:H	1.39	0.69
1:A:230:GLU:HB2	1:A:300:GLN:HE22	1.58	0.69
1:A:353:PRO:O	1:A:355:GLN:N	2.26	0.69
1:A:55:ASP:HB3	1:A:409:LYS:HG2	1.73	0.69
1:A:81:ASN:HD21	1:A:416:ASN:HD21	1.41	0.68
1:B:278:SER:HB3	1:B:292:SER:HB3	1.74	0.68
1:A:303:GLN:HE22	1:A:305:LYS:HB2	1.58	0.68
1:B:21:GLY:HA2	1:B:36:LEU:HD11	1.75	0.68
1:B:200:LEU:HB3	3:B:431:LDA:H122	1.74	0.67
1:A:131:SER:HB3	1:A:145:GLY:HA2	1.76	0.67
1:A:278:SER:HB3	1:A:292:SER:HB3	1.75	0.67
1:B:34:PRO:HB2	1:B:143:GLY:HA3	1.76	0.67
1:A:263:GLN:HG2	1:A:264:SER:H	1.58	0.67
1:A:137:ASN:ND2	1:A:140:TRP:H	1.92	0.67
1:B:255:PRO:HD3	4:B:433:C8E:H141	1.77	0.67
1:A:89:ASN:ND2	1:A:90:ASP:N	2.40	0.66
1:B:292:SER:O	1:B:327:ILE:HD12	1.95	0.66
1:B:119:GLY:HA3	1:B:156:GLU:O	1.97	0.65
1:A:252:LEU:HB2	1:A:254:ILE:CG2	2.26	0.65
1:A:6:ASN:HD22	1:A:6:ASN:H	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HD23	1:B:165:LEU:HD12	1.78	0.65
1:B:11:SER:HB2	1:B:15:ARG:NH2	2.12	0.65
1:A:187:THR:O	1:A:191:ILE:HD12	1.97	0.65
1:B:55:ASP:HB3	1:B:409:LYS:HG2	1.78	0.65
1:A:348:ASP:N	1:A:348:ASP:OD2	2.29	0.64
1:A:250:TYR:HB2	1:A:252:LEU:CD1	2.27	0.64
1:B:254:ILE:CD1	1:B:255:PRO:HD2	2.19	0.63
1:A:131:SER:HB3	1:A:145:GLY:CA	2.29	0.62
1:A:135:ARG:HD2	5:A:507:HOH:O	1.98	0.62
1:B:380:ASP:O	1:B:419:TYR:HA	1.98	0.62
1:A:7:GLU:HA	1:A:17:TYR:OH	2.00	0.62
1:A:34:PRO:HB2	1:A:143:GLY:CA	2.27	0.61
1:B:304:LEU:HD13	3:B:431:LDA:H11	1.80	0.61
1:A:121:THR:OG1	1:A:157:ARG:NH2	2.32	0.61
1:B:191:ILE:N	1:B:191:ILE:HD12	2.16	0.61
1:A:199:HIS:C	1:A:200:LEU:HD12	2.21	0.61
1:B:42:ARG:NH1	1:B:42:ARG:HG3	2.16	0.61
1:A:317:LYS:HD3	1:A:318:HIS:N	2.16	0.60
1:B:353:PRO:O	1:B:355:GLN:N	2.34	0.60
1:B:162:LEU:O	1:B:166:VAL:HG23	2.01	0.60
1:B:137:ASN:N	1:B:137:ASN:HD22	2.00	0.60
1:B:121:THR:HG21	3:B:431:LDA:H21	1.84	0.60
1:B:354:ALA:O	1:B:355:GLN:HB3	2.01	0.59
1:A:380:ASP:O	1:A:419:TYR:HA	2.02	0.59
1:B:11:SER:HB2	1:B:15:ARG:HH21	1.65	0.59
1:A:333:TYR:HH	1:A:335:TYR:HD1	1.50	0.59
1:B:252:LEU:HB2	1:B:254:ILE:CG2	2.28	0.59
1:B:41:ASP:HB2	5:B:435:HOH:O	2.01	0.59
1:B:15:ARG:HD3	1:B:290:HIS:CD2	2.37	0.59
1:B:166:VAL:HG11	4:B:433:C8E:H42	1.84	0.59
1:A:283:VAL:O	1:A:283:VAL:HG12	2.03	0.59
1:B:57:ASN:ND2	1:B:72:ASN:H	2.01	0.59
1:B:215:TYR:HD2	1:B:216:GLU:N	2.00	0.59
1:B:131:SER:HB2	1:B:144:LEU:O	2.02	0.59
1:B:58:ILE:HB	1:B:70:ALA:HB3	1.85	0.59
1:A:18:SER:HB3	1:A:328:ALA:HB1	1.84	0.59
1:B:102:TYR:O	1:B:125:THR:HB	2.02	0.59
1:A:178:THR:HG22	1:A:180:GLN:N	2.12	0.58
1:B:273:GLU:HG2	1:B:297:SER:OG	2.03	0.58
1:A:6:ASN:H	1:A:6:ASN:ND2	2.01	0.58
3:A:431:LDA:HM21	5:A:519:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASN:CB	1:A:32:ARG:HH12	2.13	0.58
1:B:247:PHE:HE2	4:B:433:C8E:H52	1.68	0.58
1:A:137:ASN:C	1:A:137:ASN:HD22	2.04	0.58
1:B:193:SER:HB2	5:B:474:HOH:O	2.02	0.58
1:A:254:ILE:HB	4:A:433:C8E:H81	1.84	0.58
1:B:273:GLU:H	1:B:300:GLN:HE22	1.51	0.58
1:B:254:ILE:HG13	1:B:255:PRO:O	2.03	0.58
1:B:255:PRO:HG3	4:B:433:C8E:H171	1.86	0.57
1:B:293:LEU:CD1	1:B:327:ILE:HD13	2.29	0.57
1:A:85:VAL:HG13	5:A:436:HOH:O	2.05	0.57
1:A:21:GLY:HA2	1:A:36:LEU:HD11	1.86	0.57
1:A:15:ARG:HD2	1:A:20:GLU:OE1	2.05	0.57
1:B:248:ASN:HD21	1:B:257:ALA:N	2.03	0.56
1:A:284:ASP:OD1	1:A:285:PRO:HD2	2.05	0.56
1:A:230:GLU:HB2	1:A:300:GLN:NE2	2.19	0.56
1:A:58:ILE:HB	1:A:70:ALA:HB3	1.85	0.56
1:A:89:ASN:HD22	1:A:90:ASP:H	1.48	0.56
1:A:254:ILE:HD12	1:A:255:PRO:CD	2.33	0.56
1:A:250:TYR:HA	1:B:173:SER:HB2	1.88	0.56
1:A:51:TYR:HD1	1:A:78:TRP:CD1	2.24	0.56
1:B:374:THR:HG23	1:B:384:ASP:OD2	2.06	0.55
1:A:361:ILE:HD11	3:A:431:LDA:H11	1.87	0.55
1:A:15:ARG:HD3	1:A:290:HIS:CD2	2.42	0.55
1:B:175:ALA:O	1:B:181:GLY:HA3	2.06	0.55
1:B:349:ASP:HA	1:B:365:ASP:OD1	2.07	0.55
1:A:116:SER:HB2	4:A:433:C8E:H51	1.88	0.55
1:A:252:LEU:N	1:A:252:LEU:HD12	2.18	0.55
1:B:73:ILE:HD11	1:B:362:PRO:HG2	1.88	0.55
1:A:243:LEU:HD12	1:A:254:ILE:HD11	1.89	0.54
1:A:140:TRP:HB3	1:A:215:TYR:HA	1.89	0.54
1:B:351:PRO:O	1:B:353:PRO:HD3	2.06	0.54
1:B:378:ASN:OD1	1:B:380:ASP:HB2	2.07	0.54
1:A:156:GLU:OE1	1:A:199:HIS:ND1	2.34	0.54
1:A:52:ILE:HG12	1:A:412:LEU:HD13	1.90	0.54
1:B:250:TYR:HB2	1:B:252:LEU:CD1	2.29	0.54
1:B:140:TRP:HB3	1:B:215:TYR:HA	1.90	0.54
1:B:28:GLY:HA2	1:B:83:HIS:CG	2.43	0.54
1:B:395:VAL:C	1:B:396:LYS:HD2	2.28	0.54
1:B:135:ARG:HG3	1:B:137:ASN:O	2.07	0.54
1:A:255:PRO:HD3	4:A:433:C8E:H61	1.90	0.54
1:A:191:ILE:HD12	1:A:191:ILE:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:HA	1:A:191:ILE:HD13	1.89	0.54
1:B:307:THR:HG22	1:B:308:SER:O	2.07	0.54
1:B:57:ASN:HD22	1:B:71:ASP:HA	1.73	0.53
1:B:54:PRO:HB3	3:B:432:LDA:HM11	1.91	0.53
1:B:378:ASN:C	1:B:380:ASP:H	2.12	0.53
1:A:166:VAL:HG21	4:A:433:C8E:H142	1.91	0.53
1:B:304:LEU:HD11	3:B:431:LDA:H32	1.91	0.53
1:A:351:PRO:O	1:A:353:PRO:HD3	2.09	0.53
1:A:116:SER:HA	1:A:158:PHE:O	2.08	0.52
1:A:215:TYR:HD2	1:A:216:GLU:N	2.08	0.52
1:A:411:TRP:C	1:A:412:LEU:HD22	2.30	0.52
1:A:53:ASP:HA	1:A:76:THR:HG22	1.90	0.52
1:A:23:ILE:HG12	1:A:280:TYR:CD1	2.45	0.52
1:B:426:HIS:CG	1:B:427:HIS:H	2.27	0.52
1:A:52:ILE:HG12	1:A:412:LEU:CD1	2.40	0.52
1:A:273:GLU:HG2	1:A:297:SER:OG	2.10	0.52
1:A:378:ASN:C	1:A:380:ASP:H	2.12	0.52
1:B:236:LYS:HG3	5:B:487:HOH:O	2.08	0.52
1:A:250:TYR:HE1	1:B:175:ALA:HB2	1.74	0.52
1:B:41:ASP:O	1:B:87:PRO:HG2	2.09	0.52
1:A:51:TYR:CD1	1:A:78:TRP:NE1	2.77	0.52
1:B:201:ASN:OD1	1:B:238:ASN:HB2	2.09	0.52
1:B:171:MET:HA	1:B:171:MET:CE	2.40	0.52
1:A:303:GLN:HE21	1:A:304:LEU:N	2.08	0.52
1:A:254:ILE:HA	4:A:433:C8E:H61	1.91	0.52
1:B:236:LYS:HE2	5:B:457:HOH:O	2.09	0.52
1:B:137:ASN:N	1:B:137:ASN:ND2	2.58	0.51
1:A:396:LYS:HE3	1:A:405:GLU:OE2	2.11	0.51
1:A:30:VAL:HG21	1:A:85:VAL:HG22	1.92	0.51
1:B:274:MET:HE3	5:B:452:HOH:O	2.10	0.51
1:B:21:GLY:CA	1:B:36:LEU:HD11	2.41	0.51
1:A:204:GLN:HG2	1:A:234:ASP:O	2.10	0.51
1:B:155:ILE:HG13	3:B:431:LDA:H81	1.93	0.51
1:A:197:ILE:HD11	1:A:243:LEU:HD11	1.93	0.51
1:A:359:ILE:O	1:A:362:PRO:HG3	2.10	0.51
1:A:6:ASN:HD22	1:A:6:ASN:N	2.04	0.51
1:A:252:LEU:CD1	1:A:252:LEU:H	2.21	0.50
1:B:19:GLY:O	1:B:278:SER:HB2	2.12	0.50
1:A:131:SER:HB2	5:A:469:HOH:O	2.10	0.50
1:A:6:ASN:N	1:A:6:ASN:ND2	2.56	0.50
1:B:41:ASP:C	1:B:87:PRO:HG2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLU:OE1	1:B:199:HIS:ND1	2.45	0.50
1:B:89:ASN:HD22	1:B:90:ASP:H	1.52	0.50
1:A:254:ILE:HG13	1:A:255:PRO:O	2.10	0.50
1:A:57:ASN:ND2	1:A:72:ASN:N	2.54	0.50
1:B:155:ILE:CD1	3:B:431:LDA:H81	2.41	0.50
1:B:246:ALA:CB	4:B:434:C8E:H171	2.41	0.50
1:A:362:PRO:O	3:A:432:LDA:HM22	2.12	0.50
1:A:395:VAL:C	1:A:396:LYS:HD2	2.32	0.50
1:B:216:GLU:HB3	1:B:222:ARG:HB3	1.94	0.50
1:A:7:GLU:HA	1:A:17:TYR:CZ	2.47	0.50
1:B:338:ASN:HB3	1:B:375:TYR:HE1	1.76	0.50
1:B:378:ASN:O	1:B:380:ASP:N	2.45	0.49
1:B:89:ASN:HD22	1:B:426:HIS:HE1	1.59	0.49
1:A:322:LYS:HD2	1:A:323:ASP:O	2.12	0.49
1:B:7:GLU:HA	1:B:17:TYR:OH	2.13	0.49
1:B:89:ASN:C	1:B:91:GLN:H	2.15	0.49
1:A:33:ASN:HB3	1:A:36:LEU:CD1	2.42	0.49
1:A:301:PHE:CZ	1:A:304:LEU:HD11	2.48	0.49
1:B:199:HIS:C	1:B:200:LEU:HD12	2.31	0.49
1:A:73:ILE:HD11	1:A:362:PRO:HG2	1.94	0.49
1:A:90:ASP:OD2	1:A:426:HIS:CE1	2.66	0.49
1:B:317:LYS:HG3	3:B:431:LDA:HM23	1.93	0.49
1:B:370:SER:HB3	1:B:388:SER:OG	2.12	0.49
1:A:349:ASP:HA	1:A:365:ASP:OD1	2.12	0.49
1:A:342:ARG:HD2	5:A:475:HOH:O	2.12	0.49
1:A:15:ARG:NH2	5:A:450:HOH:O	2.45	0.49
1:B:245:ARG:HG2	5:B:491:HOH:O	2.12	0.49
1:A:28:GLY:HA2	1:A:83:HIS:CG	2.47	0.49
1:A:94:TRP:C	5:A:436:HOH:O	2.52	0.48
1:A:239:TYR:CG	1:A:240:SER:N	2.81	0.48
1:B:254:ILE:HB	4:B:433:C8E:H112	1.95	0.48
1:B:215:TYR:CD2	1:B:216:GLU:N	2.80	0.48
1:A:19:GLY:O	1:A:20:GLU:C	2.51	0.48
1:A:284:ASP:CG	1:A:285:PRO:HD2	2.34	0.48
1:A:319:GLU:OE1	3:A:431:LDA:HM11	2.13	0.48
1:B:155:ILE:HD11	3:B:431:LDA:H81	1.94	0.48
1:B:289:ILE:HG23	1:B:289:ILE:O	2.14	0.48
1:A:228:ARG:HB3	1:A:274:MET:HB3	1.96	0.48
1:A:267:LEU:HD11	1:A:304:LEU:HB3	1.95	0.48
1:A:105:ALA:HA	1:A:121:THR:O	2.13	0.48
1:B:283:VAL:O	1:B:283:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLY:O	1:B:20:GLU:C	2.51	0.48
1:B:53:ASP:HA	1:B:76:THR:HG22	1.94	0.48
1:B:6:ASN:CB	1:B:32:ARG:HH12	2.27	0.48
1:B:334:TYR:HA	1:B:340:THR:HG23	1.96	0.48
1:B:102:TYR:CZ	1:B:272:PRO:HD2	2.50	0.47
1:B:274:MET:CE	5:B:452:HOH:O	2.61	0.47
1:B:243:LEU:HA	5:B:475:HOH:O	2.14	0.47
1:B:338:ASN:HB3	1:B:375:TYR:CE1	2.49	0.47
1:A:249:ASN:CB	1:B:174:PRO:HD3	2.44	0.47
1:A:249:ASN:HB2	1:B:174:PRO:CG	2.45	0.47
1:A:191:ILE:HD12	1:A:191:ILE:H	1.78	0.47
1:A:378:ASN:O	1:A:380:ASP:N	2.48	0.47
1:A:222:ARG:C	1:A:223:TYR:CD1	2.88	0.47
1:B:155:ILE:HD11	3:B:431:LDA:H61	1.97	0.47
1:B:239:TYR:CG	1:B:240:SER:N	2.81	0.47
1:B:89:ASN:CG	1:B:90:ASP:N	2.68	0.47
1:B:282:ARG:HG3	1:B:282:ARG:HH11	1.78	0.47
1:B:317:LYS:HD3	1:B:318:HIS:N	2.29	0.47
1:B:218:ASP:OD1	1:B:220:ASN:N	2.46	0.47
1:B:360:SER:HB2	5:B:437:HOH:O	2.14	0.46
1:B:236:LYS:HD3	1:B:266:TYR:CE2	2.50	0.46
1:B:303:GLN:HE22	1:B:305:LYS:CB	2.17	0.46
1:A:42:ARG:HB2	1:A:43:PRO:HD2	1.97	0.46
1:B:273:GLU:H	1:B:300:GLN:NE2	2.13	0.46
1:B:159:ALA:O	1:B:193:SER:O	2.33	0.46
1:B:308:SER:HB3	1:B:314:LEU:HD11	1.97	0.46
1:A:42:ARG:HB2	1:A:43:PRO:CD	2.45	0.46
1:B:52:ILE:HG12	1:B:412:LEU:CD1	2.46	0.46
1:A:178:THR:HG22	1:A:179:GLN:N	2.31	0.46
1:A:228:ARG:HB3	1:A:274:MET:CB	2.45	0.46
1:B:28:GLY:HA2	1:B:83:HIS:CD2	2.51	0.46
1:A:254:ILE:CD1	4:A:433:C8E:H81	2.45	0.46
1:B:19:GLY:O	1:B:278:SER:CB	2.64	0.46
1:A:187:THR:O	1:A:191:ILE:CD1	2.62	0.46
1:B:103:GLY:HA2	1:B:123:LEU:O	2.15	0.46
1:B:364:GLN:HE21	1:B:392:GLY:CA	2.24	0.46
1:B:52:ILE:HG12	1:B:412:LEU:HD13	1.97	0.46
1:B:43:PRO:HA	1:B:85:VAL:O	2.16	0.46
1:A:265:GLY:HA2	1:A:307:THR:O	2.16	0.46
1:A:137:ASN:C	1:A:137:ASN:ND2	2.69	0.46
1:B:6:ASN:HB2	1:B:32:ARG:HH12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLY:HA2	1:A:83:HIS:CD2	2.51	0.45
1:B:10:SER:O	1:B:13:LEU:HB3	2.15	0.45
1:A:243:LEU:O	1:A:257:ALA:HB1	2.15	0.45
1:B:8:PHE:CE2	1:B:32:ARG:HD3	2.51	0.45
1:A:218:ASP:OD1	1:A:220:ASN:N	2.49	0.45
1:B:6:ASN:N	1:B:6:ASN:ND2	2.64	0.45
1:B:411:TRP:C	1:B:412:LEU:HD22	2.37	0.45
1:B:326:ARG:HG3	1:B:348:ASP:HB3	1.99	0.45
1:B:140:TRP:HE3	1:B:215:TYR:CD2	2.34	0.45
1:B:30:VAL:HG21	1:B:85:VAL:HG22	1.97	0.45
1:B:44:THR:O	1:B:84:PHE:HA	2.16	0.45
1:B:204:GLN:HG2	1:B:234:ASP:O	2.17	0.45
1:B:276:GLU:HG3	1:B:294:ALA:HB2	1.98	0.45
1:A:243:LEU:HD12	1:A:254:ILE:CD1	2.45	0.45
1:A:298:TRP:HB2	1:A:322:LYS:O	2.16	0.45
1:A:374:THR:HG23	1:A:384:ASP:OD2	2.16	0.45
1:A:249:ASN:HB2	1:B:174:PRO:HD3	1.98	0.45
1:B:267:LEU:HD23	1:B:267:LEU:C	2.37	0.45
1:A:140:TRP:HE3	1:A:215:TYR:CD2	2.35	0.45
1:A:51:TYR:HD1	1:A:78:TRP:NE1	2.14	0.44
1:B:252:LEU:CD1	1:B:252:LEU:H	2.20	0.44
1:A:42:ARG:NH1	1:A:421:PHE:O	2.49	0.44
1:A:364:GLN:NE2	1:A:392:GLY:HA3	2.24	0.44
1:A:301:PHE:HD2	1:A:321:PHE:CD1	2.35	0.44
1:A:412:LEU:CD2	1:A:412:LEU:N	2.80	0.44
1:B:42:ARG:NH1	1:B:421:PHE:O	2.51	0.44
1:A:88:ILE:HG13	1:A:93:GLY:HA2	1.98	0.44
1:A:272:PRO:HG2	1:A:298:TRP:CE3	2.53	0.44
1:A:322:LYS:C	1:A:322:LYS:HD2	2.38	0.44
1:A:204:GLN:HB3	1:A:233:ILE:CG2	2.47	0.44
1:B:42:ARG:HD2	1:B:423:HIS:ND1	2.33	0.44
1:A:37:ILE:HB	1:A:133:ALA:CB	2.47	0.44
1:B:286:GLN:O	1:B:333:TYR:HA	2.17	0.44
1:B:271:LEU:HA	1:B:272:PRO:HD3	1.82	0.43
1:A:250:TYR:CE1	1:B:175:ALA:HB2	2.53	0.43
1:B:155:ILE:HD13	3:B:431:LDA:HM13	2.00	0.43
1:B:131:SER:HB3	1:B:145:GLY:CA	2.48	0.43
1:B:304:LEU:HD13	3:B:431:LDA:HM21	2.00	0.43
1:B:243:LEU:O	1:B:257:ALA:HB1	2.18	0.43
1:B:10:SER:H	1:B:416:ASN:ND2	2.17	0.43
1:B:355:GLN:HB2	1:B:355:GLN:HE21	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:O	1:A:181:GLY:HA3	2.18	0.43
1:A:254:ILE:HD13	4:A:433:C8E:H81	1.99	0.43
1:B:33:ASN:OD1	1:B:212:GLY:HA3	2.18	0.43
1:B:244:ASN:O	1:B:247:PHE:HD1	2.01	0.43
1:A:197:ILE:HD12	1:A:243:LEU:HG	2.00	0.43
1:A:360:SER:C	1:A:362:PRO:HD3	2.39	0.43
1:A:25:ASP:HB2	5:A:450:HOH:O	2.18	0.43
1:A:354:ALA:O	1:A:355:GLN:HB3	2.19	0.43
1:B:424:HIS:O	1:B:426:HIS:N	2.52	0.43
1:B:187:THR:O	1:B:191:ILE:HD12	2.19	0.43
1:B:121:THR:OG1	1:B:157:ARG:NH2	2.51	0.43
1:B:108:PHE:CZ	1:B:359:ILE:HD12	2.53	0.43
1:A:268:THR:HG22	1:A:270:ASN:ND2	2.34	0.43
1:B:60:GLY:C	1:B:68:LEU:HB2	2.39	0.43
1:A:159:ALA:O	1:A:193:SER:O	2.36	0.43
1:A:307:THR:HG22	1:A:308:SER:O	2.19	0.42
1:B:134:TYR:C	1:B:134:TYR:CD2	2.91	0.42
1:A:185:ALA:O	1:A:189:ASN:HB2	2.19	0.42
1:A:363:ASP:HA	3:A:432:LDA:HM22	2.01	0.42
1:A:298:TRP:CD1	1:A:351:PRO:CG	3.01	0.42
1:A:286:GLN:O	1:A:333:TYR:HA	2.19	0.42
1:B:348:ASP:N	1:B:348:ASP:OD2	2.51	0.42
1:B:423:HIS:HE1	5:B:435:HOH:O	2.01	0.42
1:B:178:THR:HG22	1:B:179:GLN:N	2.34	0.42
1:B:389:TYR:CE2	1:B:391:HIS:HB3	2.54	0.42
1:A:293:LEU:CD1	1:A:327:ILE:HG12	2.43	0.42
1:A:10:SER:HB2	1:A:416:ASN:HB2	2.02	0.42
1:A:113:ALA:O	1:A:160:GLY:HA3	2.20	0.42
1:B:255:PRO:CG	4:B:433:C8E:H171	2.48	0.42
1:B:246:ALA:HB3	4:B:434:C8E:H171	2.01	0.42
1:B:40:PHE:N	1:B:40:PHE:CD1	2.88	0.42
1:A:11:SER:HA	5:A:475:HOH:O	2.20	0.42
1:B:290:HIS:N	1:B:290:HIS:ND1	2.67	0.42
1:B:290:HIS:HE1	1:B:332:THR:N	2.18	0.42
1:B:307:THR:CG2	1:B:308:SER:N	2.83	0.42
1:A:89:ASN:C	1:A:91:GLN:H	2.23	0.42
1:B:327:ILE:HA	1:B:327:ILE:HD12	1.90	0.42
1:B:86:ALA:HA	1:B:87:PRO:HD3	1.87	0.42
1:A:75:PRO:HD2	1:A:105:ALA:O	2.20	0.42
1:A:30:VAL:HG11	1:A:85:VAL:CG2	2.50	0.42
1:A:322:LYS:CD	1:A:323:ASP:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ALA:HB2	1:B:357:ARG:NH2	2.35	0.42
1:B:155:ILE:CG1	3:B:431:LDA:H81	2.49	0.41
1:B:58:ILE:HG12	1:B:73:ILE:HD13	2.00	0.41
1:B:266:TYR:N	1:B:307:THR:O	2.49	0.41
1:A:317:LYS:C	1:A:317:LYS:HD3	2.40	0.41
1:A:43:PRO:HB2	1:A:421:PHE:CD2	2.55	0.41
1:A:27:ALA:O	1:A:30:VAL:HG22	2.19	0.41
1:B:124:GLU:HG2	3:B:432:LDA:H102	2.02	0.41
1:B:246:ALA:HB1	4:B:434:C8E:H171	2.03	0.41
1:A:303:GLN:HB2	1:A:317:LYS:O	2.20	0.41
1:B:140:TRP:CB	1:B:214:LEU:O	2.65	0.41
1:A:271:LEU:HA	1:A:272:PRO:HD3	1.88	0.41
1:B:252:LEU:CB	1:B:254:ILE:HG22	2.37	0.41
1:B:289:ILE:CG2	1:B:289:ILE:O	2.68	0.41
1:A:215:TYR:C	1:A:215:TYR:CD2	2.94	0.41
1:B:350:SER:HA	1:B:351:PRO:HD3	1.78	0.41
1:B:98:ILE:HG12	1:B:128:LEU:CD2	2.50	0.41
1:A:73:ILE:HD12	1:A:106:THR:CG2	2.50	0.41
1:A:151:ALA:O	1:A:203:ASN:HA	2.20	0.41
1:B:96:ALA:HA	1:B:129:ASN:O	2.21	0.41
1:A:135:ARG:HG3	1:A:137:ASN:O	2.20	0.41
1:B:304:LEU:HD21	3:B:431:LDA:H52	2.02	0.41
1:A:119:GLY:HA3	1:A:156:GLU:O	2.20	0.41
1:B:151:ALA:O	1:B:203:ASN:HA	2.20	0.41
1:A:381:ALA:HA	1:A:418:ASN:O	2.20	0.41
1:B:173:SER:HB2	1:B:174:PRO:CD	2.51	0.41
1:B:53:ASP:C	1:B:53:ASP:OD2	2.59	0.41
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.82	0.41
1:A:6:ASN:HA	5:A:494:HOH:O	2.20	0.41
1:A:321:PHE:CZ	1:A:352:VAL:HG22	2.55	0.41
1:B:34:PRO:HB2	1:B:143:GLY:CA	2.47	0.41
1:B:378:ASN:C	1:B:380:ASP:N	2.75	0.41
1:B:144:LEU:HD23	1:B:145:GLY:N	2.36	0.41
1:B:6:ASN:H	1:B:6:ASN:ND2	2.19	0.41
1:B:148:ALA:HA	1:B:207:PHE:CD1	2.56	0.41
1:A:333:TYR:OH	1:A:335:TYR:HD1	2.02	0.41
1:B:360:SER:C	1:B:362:PRO:HD3	2.41	0.41
1:B:115:GLY:O	1:B:117:VAL:N	2.54	0.41
1:A:304:LEU:N	1:A:304:LEU:HD12	2.35	0.40
1:B:187:THR:O	1:B:191:ILE:CD1	2.70	0.40
1:B:178:THR:HG22	1:B:180:GLN:N	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:HA	1:A:366:ARG:O	2.22	0.40
1:A:33:ASN:HA	1:A:34:PRO:HD3	1.89	0.40
1:A:267:LEU:C	1:A:267:LEU:HD23	2.41	0.40
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.86	0.40
1:A:298:TRP:CG	1:A:351:PRO:HB3	2.56	0.40
1:A:350:SER:HA	1:A:351:PRO:HD3	1.69	0.40
1:B:272:PRO:HA	1:B:300:GLN:HE21	1.87	0.40
1:B:266:TYR:O	1:B:306:ALA:HA	2.21	0.40
1:B:284:ASP:OD1	1:B:285:PRO:HD2	2.21	0.40
1:A:62:SER:OG	1:A:63:PRO:HD2	2.21	0.40
1:B:169:GLN:HA	1:B:169:GLN:OE1	2.21	0.40
1:A:40:PHE:CD1	1:A:40:PHE:N	2.90	0.40
1:A:216:GLU:HB3	1:A:222:ARG:HB3	2.02	0.40
1:B:129:ASN:ND2	5:B:443:HOH:O	2.50	0.40
1:A:46:SER:OG	1:A:418:ASN:ND2	2.55	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	425/427 (100%)	391 (92%)	28 (7%)	6 (1%)	14	28
1	B	425/427 (100%)	385 (91%)	31 (7%)	9 (2%)	9	16
All	All	850/854 (100%)	776 (91%)	59 (7%)	15 (2%)	11	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ALA
1	A	355	GLN
1	B	355	GLN

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Mol	Chain	Res	Type
1	B	425	HIS
1	A	20	GLU
1	A	335	TYR
1	B	20	GLU
1	B	335	TYR
1	B	354	ALA
1	B	378	ASN
1	A	378	ASN
1	B	116	SER
1	B	379	LYS
1	A	379	LYS
1	B	362	PRO

### 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	337/337 (100%)	307 (91%)	30 (9%)	12	23
1	B	337/337 (100%)	312 (93%)	25 (7%)	17	34
All	All	674/674 (100%)	619 (92%)	55 (8%)	14	27

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	ASN
1	A	7	GLU
1	A	42	ARG
1	A	72	ASN
1	A	122	ASP
1	A	137	ASN
1	A	171	MET
1	A	189	ASN
1	A	203	ASN
1	A	215	TYR

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Mol	Chain	Res	Type
1	A	219	LYS
1	A	222	ARG
1	A	252	LEU
1	A	275	TRP
1	A	278	SER
1	A	282	ARG
1	A	290	HIS
1	A	303	GLN
1	A	312	ASP
1	A	314	LEU
1	A	322	LYS
1	A	327	ILE
1	A	337	ASP
1	A	348	ASP
1	A	355	GLN
1	A	356	ASN
1	A	373	THR
1	A	407	GLU
1	A	412	LEU
1	B	5	LEU
1	B	6	ASN
1	B	42	ARG
1	B	72	ASN
1	B	107	GLU
1	B	134	TYR
1	B	137	ASN
1	B	171	MET
1	B	189	ASN
1	B	197	ILE
1	B	215	TYR
1	B	219	LYS
1	B	252	LEU
1	B	275	TRP
1	B	282	ARG
1	B	290	HIS
1	B	303	GLN
1	B	312	ASP
1	B	314	LEU
1	B	316	GLN
1	B	322	LYS
1	B	355	GLN
1	B	407	GLU

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Mol	Chain	Res	Type
1	B	412	LEU
1	B	423	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	57	ASN
1	A	72	ASN
1	A	81	ASN
1	A	83	HIS
1	A	89	ASN
1	A	109	ASN
1	A	129	ASN
1	A	137	ASN
1	A	189	ASN
1	A	248	ASN
1	A	270	ASN
1	A	281	ASN
1	A	290	HIS
1	A	300	GLN
1	A	303	GLN
1	A	316	GLN
1	A	355	GLN
1	A	356	ASN
1	A	364	GLN
1	A	418	ASN
1	A	423	HIS
1	B	4	GLN
1	B	6	ASN
1	B	57	ASN
1	B	72	ASN
1	B	83	HIS
1	B	89	ASN
1	B	129	ASN
1	B	137	ASN
1	B	182	GLN
1	B	189	ASN
1	B	248	ASN
1	B	270	ASN
1	B	281	ASN
1	B	290	HIS

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Mol	Chain	Res	Type
1	B	300	GLN
1	B	303	GLN
1	B	316	GLN
1	B	355	GLN
1	B	356	ASN
1	B	364	GLN
1	B	416	ASN
1	B	418	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](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z  > 2$
3	LDA	A	431	-	15,15,15	3.71	2 (13%)	16,17,17	2.39	5 (31%)
3	LDA	A	432	-	15,15,15	3.73	2 (13%)	16,17,17	2.33	5 (31%)
4	C8E	A	433	-	20,20,20	1.10	1 (5%)	19,19,19	2.34	7 (36%)
3	LDA	B	431	-	15,15,15	4.12	2 (13%)	16,17,17	2.44	5 (31%)
3	LDA	B	432	-	15,15,15	3.60	2 (13%)	16,17,17	2.36	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	C8E	B	433	-	20,20,20	0.85	0	19,19,19	2.15	6 (31%)
4	C8E	B	434	-	20,20,20	0.89	0	19,19,19	2.12	6 (31%)

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
3	LDA	A	431	-	-	0/13/13/13	0/0/0/0
3	LDA	A	432	-	-	0/13/13/13	0/0/0/0
4	C8E	A	433	-	-	0/18/18/18	0/0/0/0
3	LDA	B	431	-	-	0/13/13/13	0/0/0/0
3	LDA	B	432	-	-	0/13/13/13	0/0/0/0
4	C8E	B	433	-	-	0/18/18/18	0/0/0/0
4	C8E	B	434	-	-	0/18/18/18	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	431	LDA	O1-N1	-14.95	1.25	1.39
3	A	431	LDA	O1-N1	-13.64	1.26	1.39
3	A	432	LDA	O1-N1	-13.58	1.26	1.39
3	B	432	LDA	O1-N1	-13.22	1.27	1.39
3	B	431	LDA	CM2-N1	-4.84	1.42	1.49
3	A	432	LDA	CM2-N1	-4.29	1.42	1.49
3	A	431	LDA	CM2-N1	-3.96	1.43	1.49
3	B	432	LDA	CM2-N1	-3.87	1.43	1.49
4	A	433	C8E	C14-C13	2.10	1.59	1.48

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	431	LDA	CM2-N1-CM1	-6.77	101.19	108.83
3	B	432	LDA	CM2-N1-CM1	-6.41	101.60	108.83
3	A	431	LDA	CM2-N1-CM1	-6.26	101.77	108.83
3	A	432	LDA	CM2-N1-CM1	-6.00	102.06	108.83
4	B	433	C8E	C7-C6-C5	-2.77	100.20	114.53
4	B	434	C8E	C7-C6-C5	-2.64	100.89	114.53
4	A	433	C8E	C7-C6-C5	-2.58	101.21	114.53
3	A	432	LDA	CM1-N1-C1	-2.54	101.58	109.77
3	B	432	LDA	C9-C8-C7	-2.44	101.91	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	432	LDA	CM1-N1-C1	-2.39	102.06	109.77
3	A	431	LDA	CM1-N1-C1	-2.36	102.16	109.77
3	B	431	LDA	CM1-N1-C1	-2.34	102.23	109.77
3	A	431	LDA	C9-C8-C7	-2.16	103.39	114.53
3	A	432	LDA	C9-C8-C7	-2.14	103.48	114.53
3	B	431	LDA	C6-C5-C4	-2.07	103.83	114.53
4	A	433	C8E	C10-O9-C8	2.14	122.49	113.31
4	B	434	C8E	O18-C19-C20	2.54	122.12	110.43
4	B	433	C8E	O18-C17-C16	2.81	122.84	110.36
4	B	433	C8E	O18-C19-C20	2.84	123.49	110.43
4	A	433	C8E	O18-C19-C20	2.89	123.73	110.43
4	B	434	C8E	O18-C17-C16	3.00	123.70	110.36
3	A	432	LDA	O1-N1-CM2	3.05	113.13	109.05
4	A	433	C8E	O18-C17-C16	3.21	124.63	110.36
3	B	431	LDA	O1-N1-CM2	3.36	113.55	109.05
4	B	434	C8E	O12-C13-C14	3.51	125.95	110.36
3	B	432	LDA	O1-N1-C1	3.53	114.24	110.27
3	B	432	LDA	O1-N1-CM2	3.58	113.84	109.05
3	A	431	LDA	O1-N1-CM2	3.58	113.85	109.05
4	B	433	C8E	O12-C13-C14	3.66	126.64	110.36
4	A	433	C8E	O12-C13-C14	3.83	127.38	110.36
4	B	433	C8E	O9-C8-C7	4.13	126.43	109.87
3	A	431	LDA	O1-N1-C1	4.16	114.95	110.27
4	B	434	C8E	O9-C8-C7	4.16	126.55	109.87
3	B	431	LDA	O1-N1-C1	4.20	115.00	110.27
3	A	432	LDA	O1-N1-C1	4.53	115.37	110.27
4	B	433	C8E	O15-C14-C13	4.81	131.73	110.36
4	A	433	C8E	O9-C8-C7	4.88	129.44	109.87
4	B	434	C8E	O15-C14-C13	4.94	132.33	110.36
4	A	433	C8E	O15-C14-C13	4.97	132.44	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	431	LDA	4	0
3	A	432	LDA	3	0
4	A	433	C8E	7	0
3	B	431	LDA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	432	LDA	2	0
4	B	433	C8E	6	0
4	B	434	C8E	4	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<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	427/427 (100%)	0.12	15 (3%)	48 40	30, 66, 97, 131	0
1	B	427/427 (100%)	0.28	34 (7%)	15 10	30, 72, 117, 163	0
All	All	854/854 (100%)	0.20	49 (5%)	27 20	30, 68, 109, 163	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	HIS	6.7
1	B	217	LEU	6.5
1	B	136	LEU	5.4
1	B	338	ASN	5.3
1	B	91	GLN	4.8
1	B	140	TRP	4.3
1	B	90	ASP	4.3
1	B	134	TYR	3.9
1	B	339	TRP	3.9
1	B	381	ALA	3.8
1	A	325	TYR	3.7
1	B	335	TYR	3.5
1	A	249	ASN	3.4
1	B	285	PRO	3.4
1	B	283	VAL	3.2
1	B	376	ALA	3.0
1	A	314	LEU	2.9
1	B	426	HIS	2.9
1	B	393	GLN	2.8
1	B	340	THR	2.7
1	B	337	ASP	2.7
1	A	6	ASN	2.7
1	A	17	TYR	2.7
1	A	367	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	395	VAL	2.6
1	A	254	ILE	2.5
1	B	420	ALA	2.5
1	A	219	LYS	2.5
1	B	325	TYR	2.4
1	B	142	PHE	2.4
1	A	140	TRP	2.4
1	B	5	LEU	2.2
1	B	1	ALA	2.2
1	A	393	GLN	2.2
1	A	354	ALA	2.2
1	B	419	TYR	2.2
1	A	134	TYR	2.2
1	B	137	ASN	2.2
1	B	215	TYR	2.1
1	B	139	ALA	2.1
1	B	334	TYR	2.1
1	B	23	ILE	2.1
1	B	92	PHE	2.1
1	B	377	PHE	2.0
1	A	136	LEU	2.0
1	A	293	LEU	2.0
1	B	16	ALA	2.0
1	B	133	ALA	2.0
1	B	41	ASP	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	C8E	A	433	21/21	0.45	0.60	6.70	73,82,92,92	0
3	LDA	A	432	16/16	0.62	0.53	5.89	56,74,93,93	0
3	LDA	B	431	16/16	0.68	0.50	5.87	87,90,93,94	0
4	C8E	B	434	21/21	0.77	0.32	3.50	73,82,92,93	0
4	C8E	B	433	21/21	0.74	0.35	3.26	50,67,72,74	0
3	LDA	A	431	16/16	0.78	0.33	3.24	55,64,85,87	0
3	LDA	B	432	16/16	0.83	0.36	2.14	72,77,86,87	0
2	CU	B	429	1/1	0.98	0.12	-1.13	78,78,78,78	0
2	CU	A	429	1/1	0.99	0.08	-2.57	67,67,67,67	0
2	CU	A	428	1/1	0.95	0.05	-	90,90,90,90	0
2	CU	B	430	1/1	0.93	0.15	-	120,120,120,120	0
2	CU	A	430	1/1	0.94	0.05	-	84,84,84,84	0
2	CU	B	428	1/1	0.96	0.04	-	92,92,92,92	0

## 6.5 Other polymers

There are no such residues in this entry.