



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 06:18 pm BST

PDB ID : 1T1L
Title : Crystal structure of the long-chain fatty acid transporter FadL
Authors : van den Berg, B.; Black, P.N.; Clemons Jr., W.M.; Rapoport, T.A.
Deposited on : 2004-04-16
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

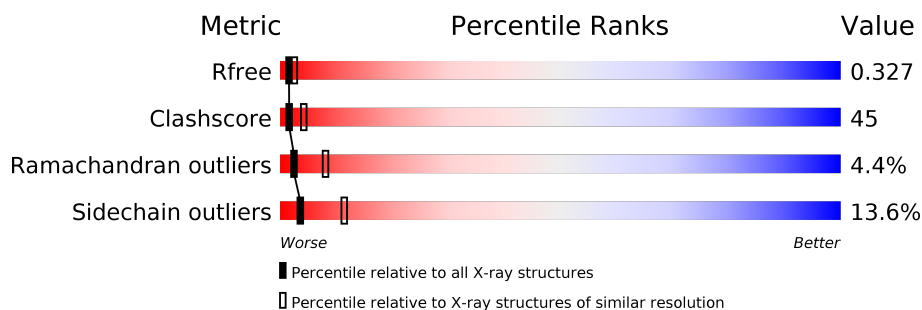
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 respectively. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	427	
1	B	427	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6642 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.

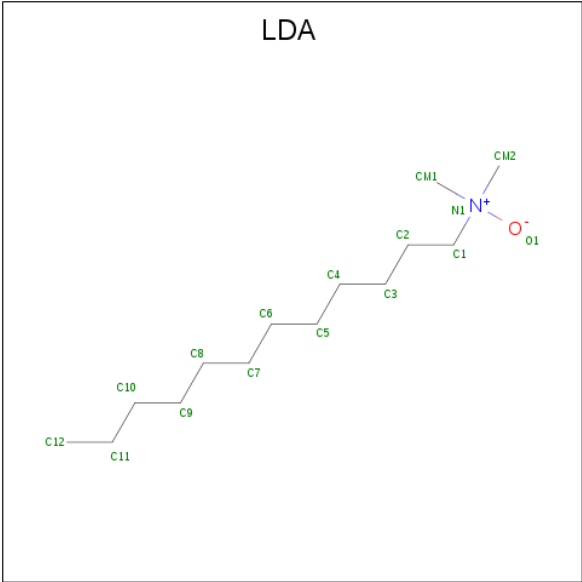
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3252	2057	552	637	6			
1	B	421	Total	C	N	O	S	0	0	0
			3252	2057	552	637	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 LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	54	Total	O	0	0
			54	54		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.02Å 122.02Å 164.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	11.99 – 2.80 49.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.9 (11.99-2.80) 96.8 (49.03-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.298 , 0.331 0.290 , 0.327	Depositor DCC
R_{free} test set	1638 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.447 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6642	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.48	0/3341	0.73	1/4549 (0.0%)
1	B	0.49	0/3341	0.73	2/4549 (0.0%)
All	All	0.49	0/6682	0.73	3/9098 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ILE	N-CA-C	9.41	136.42	111.00
1	B	91	GLN	CA-CB-CG	-6.16	99.85	113.40
1	B	254	ILE	N-CA-C	6.10	127.47	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	3252	0	3033	287	0
1	B	3252	0	3033	285	0
2	A	16	0	31	8	0
2	B	16	0	31	6	0
3	A	52	0	0	17	0
3	B	54	0	0	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6642	0	6128	570	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 45.

All (570) 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:A:364:GLN:HG2	1:A:408:GLY:HA3	1.37	1.07
1:B:254:ILE:HD12	1:B:255:PRO:HD3	1.40	1.02
1:B:364:GLN:HG3	1:B:392:GLY:HA3	1.42	1.01
1:A:333:TYR:HB3	1:A:341:PHE:HB2	1.40	0.99
1:B:288:ALA:HB3	1:B:332:THR:HB	1.44	0.99
1:A:245:ARG:HB2	1:A:245:ARG:HH11	1.28	0.99
1:B:180:GLN:HG3	1:B:184:LEU:HD13	1.46	0.97
1:A:98:ILE:HG12	1:A:128:LEU:HD23	1.49	0.94
1:A:110:ASP:OD2	1:A:111:THR:HG23	1.68	0.91
1:B:98:ILE:HG12	1:B:128:LEU:HD23	1.49	0.91
1:B:252:LEU:HD23	1:B:252:LEU:N	1.86	0.91
1:A:303:GLN:HE21	1:A:305:LYS:HB2	1.37	0.89
1:A:364:GLN:HG3	1:A:392:GLY:HA3	1.54	0.88
1:B:110:ASP:OD2	1:B:111:THR:HG23	1.72	0.88
1:B:282:ARG:HG2	1:B:282:ARG:HH11	1.39	0.88
1:B:364:GLN:HG2	1:B:408:GLY:HA3	1.56	0.87
1:A:298:TRP:HB3	1:A:321:PHE:HD1	1.38	0.87
1:A:55:ASP:HB3	1:A:409:LYS:CG	2.05	0.86
1:A:55:ASP:HB3	1:A:409:LYS:HG3	1.55	0.86
1:B:232:LYS:HG2	1:B:270:ASN:ND2	1.91	0.86
1:A:88:ILE:HG22	1:A:89:ASN:OD1	1.76	0.85
1:A:305:LYS:HG3	1:A:316:GLN:HE22	1.41	0.85
1:B:57:ASN:ND2	1:B:72:ASN:H	1.75	0.84
1:B:396:LYS:N	1:B:396:LYS:HE3	1.93	0.84
1:B:127:ASN:HD21	1:B:147:ASN:HB2	1.42	0.84
1:A:364:GLN:HE21	1:A:393:GLN:H	1.25	0.84
1:A:364:GLN:HG2	1:A:408:GLY:CA	2.07	0.84
1:B:230:GLU:HB3	3:B:457:HOH:O	1.78	0.83
1:B:393:GLN:HE21	1:B:395:VAL:HG13	1.43	0.82
1:A:199:HIS:C	1:A:200:LEU:HD23	2.01	0.81
1:B:57:ASN:HD22	1:B:72:ASN:H	1.27	0.81
1:A:58:ILE:HB	3:A:468:HOH:O	1.80	0.81
1:A:57:ASN:ND2	1:A:72:ASN:H	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASN:HD21	1:A:147:ASN:HB2	1.44	0.80
1:B:200:LEU:O	1:B:201:ASN:HB3	1.81	0.79
1:B:34:PRO:HB2	1:B:143:GLY:HA3	1.63	0.79
1:B:273:GLU:HG2	3:B:457:HOH:O	1.83	0.79
1:A:34:PRO:HB2	1:A:143:GLY:HA3	1.63	0.78
1:A:57:ASN:HD22	1:A:72:ASN:H	1.31	0.78
1:A:298:TRP:O	1:A:321:PHE:HB2	1.83	0.78
1:B:88:ILE:HG22	1:B:89:ASN:OD1	1.84	0.77
1:A:117:VAL:HG11	1:A:399:GLU:HG2	1.66	0.77
1:A:43:PRO:HB2	1:A:421:PHE:HB2	1.66	0.77
1:A:346:ALA:HB3	1:A:368:TRP:HB2	1.66	0.77
1:A:254:ILE:O	1:A:256:THR:N	2.19	0.76
1:B:254:ILE:O	1:B:256:THR:N	2.19	0.76
1:B:364:GLN:HG2	1:B:408:GLY:CA	2.15	0.76
1:B:233:ILE:O	1:B:268:THR:HA	1.86	0.75
1:B:123:LEU:HD22	2:B:428:LDA:H61	1.67	0.75
1:B:367:PHE:HB2	1:B:391:HIS:H	1.50	0.74
1:B:231:VAL:HB	1:B:271:LEU:HB2	1.70	0.74
1:A:298:TRP:HB3	1:A:321:PHE:CD1	2.22	0.74
1:B:26:ASP:HB2	1:B:418:ASN:HD22	1.52	0.73
1:A:244:ASN:HD22	1:A:245:ARG:N	1.86	0.73
1:B:12:GLY:HA2	1:B:15:ARG:NH1	2.03	0.73
1:B:282:ARG:NH1	1:B:282:ARG:HG2	2.01	0.73
1:B:254:ILE:CD1	1:B:255:PRO:HD3	2.18	0.73
1:A:184:LEU:HD23	1:A:184:LEU:O	1.88	0.72
1:B:61:THR:HB	3:B:439:HOH:O	1.89	0.72
1:A:12:GLY:HA2	1:A:15:ARG:NH1	2.04	0.72
1:B:159:ALA:O	1:B:193:SER:HA	1.88	0.72
1:B:324:ALA:HA	1:B:349:ASP:OD2	1.90	0.72
1:A:248:ASN:HD21	1:A:257:ALA:H	1.35	0.71
1:B:383:VAL:HG22	1:B:384:ASP:N	2.05	0.71
1:A:292:SER:O	1:A:327:ILE:HD12	1.90	0.71
1:A:127:ASN:HD22	1:A:128:LEU:N	1.88	0.70
1:A:291:TYR:HA	1:A:328:ALA:O	1.93	0.69
1:B:127:ASN:HD22	1:B:128:LEU:N	1.90	0.69
1:A:228:ARG:HB3	1:A:274:MET:HB2	1.73	0.69
1:B:297:SER:HA	1:B:323:ASP:OD1	1.93	0.68
1:B:26:ASP:HB2	1:B:418:ASN:ND2	2.09	0.68
1:A:68:LEU:HD11	1:A:402:TYR:HB3	1.75	0.68
1:B:280:TYR:HE1	1:B:288:ALA:HB1	1.58	0.68
1:B:40:PHE:HA	3:B:471:HOH:O	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:O	1:A:206:GLY:N	2.26	0.68
1:B:367:PHE:CG	1:B:391:HIS:HB3	2.29	0.68
1:A:117:VAL:HG23	1:A:359:ILE:HD11	1.76	0.68
1:B:231:VAL:HB	1:B:271:LEU:HD12	1.75	0.68
1:A:244:ASN:HD22	1:A:245:ARG:H	1.40	0.68
1:B:339:TRP:CZ3	1:B:375:TYR:HB2	2.30	0.67
1:B:367:PHE:HB2	1:B:391:HIS:N	2.09	0.67
1:A:364:GLN:HE21	1:A:393:GLN:N	1.92	0.67
1:A:153:ALA:HB1	2:A:428:LDA:H102	1.77	0.67
1:A:409:LYS:O	1:A:410:ALA:HB2	1.95	0.67
1:B:317:LYS:HD3	1:B:318:HIS:H	1.60	0.66
1:B:2:GLY:HA3	1:B:365:ASP:OD2	1.95	0.66
1:A:192:ASP:OD1	1:A:194:ASN:ND2	2.28	0.66
1:A:43:PRO:HA	1:A:85:VAL:O	1.96	0.66
1:B:19:GLY:HA2	1:B:278:SER:HB2	1.76	0.66
1:A:336:ASP:HB3	1:A:339:TRP:H	1.61	0.66
1:B:266:TYR:O	1:B:306:ALA:HA	1.96	0.66
1:B:357:ARG:HD2	1:B:395:VAL:HG21	1.77	0.65
1:A:282:ARG:NH2	1:A:285:PRO:O	2.29	0.65
1:A:209:TRP:O	1:A:229:SER:HB3	1.96	0.65
1:A:252:LEU:O	1:A:254:ILE:HG23	1.96	0.65
1:A:376:ALA:HA	1:A:382:SER:CB	2.26	0.65
1:A:403:GLN:HE21	1:A:403:GLN:HA	1.62	0.65
1:B:5:LEU:HD22	1:B:32:ARG:HH21	1.62	0.65
1:B:104:LEU:HD22	2:B:428:LDA:H31	1.79	0.64
1:A:5:LEU:HD22	1:A:32:ARG:HH21	1.63	0.64
1:B:279:GLY:HA3	1:B:291:TYR:CE1	2.33	0.64
1:B:117:VAL:HG23	1:B:359:ILE:HD11	1.79	0.64
1:B:199:HIS:O	1:B:239:TYR:HA	1.97	0.64
1:A:297:SER:HB2	1:A:300:GLN:OE1	1.97	0.64
1:B:360:SER:O	1:B:362:PRO:HD3	1.96	0.64
1:B:38:THR:HG21	1:B:135:ARG:HB2	1.81	0.63
1:B:173:SER:O	1:B:175:ALA:N	2.31	0.63
1:B:241:SER:HB2	3:B:449:HOH:O	1.97	0.63
1:A:231:VAL:HB	1:A:271:LEU:HB2	1.80	0.63
1:A:220:ASN:HD21	1:A:282:ARG:HD3	1.63	0.63
1:B:302:GLN:O	1:B:320:GLY:N	2.27	0.63
1:A:38:THR:HG21	1:A:135:ARG:HB2	1.81	0.63
1:A:117:VAL:HB	1:A:399:GLU:OE1	1.98	0.63
1:B:393:GLN:HE21	1:B:395:VAL:CG1	2.12	0.63
1:A:245:ARG:HB2	1:A:245:ARG:NH1	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:THR:HG22	1:B:150:TYR:O	1.98	0.62
1:A:156:GLU:HA	1:A:198:ALA:O	1.99	0.62
1:B:52:ILE:HG23	1:B:412:LEU:HD22	1.81	0.62
1:A:377:PHE:CD1	1:A:382:SER:HA	2.35	0.62
1:B:43:PRO:HA	1:B:85:VAL:O	2.00	0.62
1:B:303:GLN:NE2	1:B:316:GLN:HE22	1.97	0.62
1:B:364:GLN:CG	1:B:392:GLY:HA3	2.25	0.62
1:B:277:VAL:O	1:B:292:SER:HA	2.00	0.62
1:B:346:ALA:HB3	1:B:368:TRP:HB2	1.82	0.62
1:A:324:ALA:HB1	1:A:349:ASP:O	1.99	0.61
1:B:155:ILE:HG13	2:B:428:LDA:H111	1.81	0.61
1:B:55:ASP:HB3	1:B:409:LYS:HG3	1.83	0.61
1:B:395:VAL:C	1:B:396:LYS:HE3	2.21	0.61
1:A:157:ARG:O	1:A:197:ILE:HG12	2.01	0.61
1:A:244:ASN:ND2	1:A:245:ARG:N	2.50	0.60
1:B:68:LEU:HD21	1:B:402:TYR:CD2	2.37	0.60
1:A:11:SER:HB2	1:A:15:ARG:NH2	2.16	0.60
1:A:91:GLN:O	1:A:134:TYR:HA	2.02	0.60
1:B:30:VAL:HG23	3:B:473:HOH:O	2.00	0.60
1:A:242:ASP:OD2	1:B:111:THR:HG21	2.01	0.60
1:A:175:ALA:O	1:A:181:GLY:HA3	2.02	0.60
1:A:64:SER:HB3	1:A:165:LEU:HG	1.84	0.60
1:A:393:GLN:HB3	1:A:395:VAL:HG13	1.82	0.60
1:A:245:ARG:HH11	1:A:245:ARG:CB	2.10	0.59
1:A:303:GLN:NE2	1:A:305:LYS:HB2	2.12	0.59
1:A:313:THR:HG21	1:A:316:GLN:HB2	1.84	0.59
1:A:364:GLN:HG3	1:A:393:GLN:H	1.67	0.59
1:B:34:PRO:O	1:B:37:ILE:HG13	2.02	0.59
1:B:90:ASP:O	1:B:90:ASP:OD1	2.19	0.59
1:A:125:THR:HG22	1:A:150:TYR:O	2.02	0.59
1:A:189:ASN:HB3	3:A:472:HOH:O	2.02	0.59
1:A:52:ILE:HG12	1:A:412:LEU:CD1	2.32	0.59
1:A:136:LEU:HD22	1:A:142:PHE:CE1	2.37	0.59
1:B:232:LYS:HG2	1:B:270:ASN:HD21	1.63	0.59
1:A:157:ARG:C	1:A:197:ILE:HG12	2.22	0.59
1:A:282:ARG:NH1	1:A:334:TYR:CE1	2.70	0.59
1:A:364:GLN:CG	1:A:392:GLY:HA3	2.28	0.59
1:A:360:SER:O	1:A:362:PRO:HD3	2.02	0.59
1:B:308:SER:HB3	1:B:314:LEU:CD1	2.32	0.59
1:A:403:GLN:NE2	1:A:403:GLN:HA	2.18	0.59
1:B:411:TRP:HB3	1:B:413:PHE:CZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:N	1:A:206:GLY:O	2.31	0.58
1:A:144:LEU:HD12	1:A:145:GLY:N	2.19	0.58
1:B:396:LYS:HG3	1:B:405:GLU:OE1	2.02	0.58
1:A:184:LEU:HB2	3:A:444:HOH:O	2.02	0.58
1:B:383:VAL:CG2	1:B:384:ASP:N	2.65	0.58
1:A:254:ILE:O	1:A:255:PRO:C	2.39	0.58
1:A:4:GLN:OE1	1:A:348:ASP:HB3	2.03	0.58
1:A:139:ALA:O	1:A:215:TYR:HA	2.04	0.58
1:B:131:SER:HB3	1:B:145:GLY:HA3	1.84	0.58
1:B:183:ALA:C	1:B:185:ALA:H	2.06	0.58
1:B:393:GLN:NE2	1:B:395:VAL:CG1	2.67	0.58
1:A:297:SER:HA	1:A:323:ASP:OD1	2.04	0.57
1:A:103:GLY:N	2:A:428:LDA:HM23	2.19	0.57
1:A:243:LEU:HD12	3:A:458:HOH:O	2.03	0.57
1:A:57:ASN:HD22	1:A:72:ASN:N	2.02	0.57
1:A:68:LEU:CD1	1:A:402:TYR:HB3	2.35	0.57
1:B:54:PRO:HD2	1:B:75:PRO:O	2.04	0.57
1:B:339:TRP:HZ3	1:B:375:TYR:HB2	1.68	0.57
1:A:37:ILE:HB	1:A:133:ALA:HB3	1.86	0.57
1:B:333:TYR:HB3	1:B:341:PHE:HB2	1.85	0.57
1:B:136:LEU:HD22	1:B:142:PHE:CE1	2.40	0.57
1:A:18:SER:O	1:A:23:ILE:HD11	2.05	0.57
1:A:376:ALA:HA	1:A:382:SER:HB3	1.87	0.57
1:A:157:ARG:HB3	1:A:197:ILE:HD11	1.86	0.56
1:A:106:THR:HG21	1:A:360:SER:HA	1.86	0.56
1:A:54:PRO:HD2	1:A:75:PRO:O	2.04	0.56
1:A:387:VAL:HG22	1:A:413:PHE:HD2	1.70	0.56
1:B:288:ALA:O	1:B:289:ILE:HG13	2.04	0.56
1:A:159:ALA:O	1:A:193:SER:HA	2.04	0.56
1:A:381:ALA:HB2	1:A:419:TYR:HD1	1.70	0.56
1:B:18:SER:O	1:B:23:ILE:HD11	2.05	0.56
1:B:343:THR:HG22	1:B:344:GLY:N	2.21	0.56
1:A:284:ASP:HB3	1:A:287:TRP:H	1.69	0.56
1:B:11:SER:HB2	1:B:15:ARG:NH2	2.20	0.56
1:B:37:ILE:HB	1:B:133:ALA:HB3	1.87	0.56
1:A:34:PRO:HB2	1:A:143:GLY:CA	2.34	0.56
1:A:364:GLN:HG2	1:A:408:GLY:N	2.21	0.56
1:A:393:GLN:NE2	3:A:442:HOH:O	2.38	0.56
1:A:102:TYR:HB3	2:A:428:LDA:HM21	1.87	0.56
1:B:144:LEU:HD12	1:B:145:GLY:N	2.21	0.56
1:B:91:GLN:O	1:B:134:TYR:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:SER:HB3	1:B:165:LEU:HG	1.88	0.56
1:B:157:ARG:O	1:B:197:ILE:HG12	2.06	0.55
1:B:317:LYS:HD3	1:B:318:HIS:N	2.21	0.55
1:A:253:PRO:HB2	3:A:480:HOH:O	2.06	0.55
1:A:33:ASN:HB3	1:A:36:LEU:HD12	1.89	0.55
1:A:377:PHE:CE1	1:A:382:SER:HA	2.40	0.55
1:B:308:SER:HB3	1:B:314:LEU:HD13	1.89	0.55
1:A:220:ASN:ND2	1:A:282:ARG:HD3	2.21	0.55
1:B:33:ASN:HB3	1:B:36:LEU:HD12	1.88	0.55
1:A:136:LEU:HD22	1:A:142:PHE:HE1	1.71	0.55
1:B:178:THR:O	1:B:182:GLN:HG3	2.07	0.55
1:B:86:ALA:HB1	3:B:466:HOH:O	2.06	0.55
1:A:354:ALA:O	1:A:357:ARG:HG3	2.07	0.55
1:A:203:ASN:C	1:A:204:GLN:NE2	2.60	0.55
1:A:41:ASP:OD1	1:A:42:ARG:HD3	2.07	0.55
1:B:12:GLY:CA	1:B:15:ARG:NH1	2.70	0.55
1:A:123:LEU:HD22	2:A:428:LDA:H51	1.89	0.54
1:A:131:SER:HB3	1:A:145:GLY:HA3	1.88	0.54
1:A:378:ASN:HD22	1:A:378:ASN:N	2.04	0.54
1:B:376:ALA:HB3	3:B:475:HOH:O	2.06	0.54
1:A:340:THR:HG22	1:A:341:PHE:N	2.22	0.54
1:B:37:ILE:C	1:B:39:MET:H	2.10	0.54
1:A:270:ASN:O	1:A:272:PRO:HD3	2.07	0.54
1:A:34:PRO:O	1:A:37:ILE:HG13	2.07	0.54
1:B:342:ARG:HD2	3:B:462:HOH:O	2.07	0.54
1:B:106:THR:HG21	1:B:360:SER:HA	1.89	0.54
1:A:57:ASN:HD22	1:A:71:ASP:HA	1.71	0.54
1:A:90:ASP:OD1	1:A:90:ASP:O	2.24	0.54
1:A:282:ARG:HA	1:A:288:ALA:CB	2.38	0.54
1:B:366:ARG:HB3	1:B:367:PHE:HD1	1.73	0.54
1:B:57:ASN:HD22	1:B:72:ASN:N	1.99	0.54
1:B:192:ASP:OD2	1:B:195:THR:OG1	2.26	0.54
1:A:19:GLY:HA2	1:A:278:SER:HB2	1.90	0.53
1:B:68:LEU:HD11	1:B:402:TYR:HB3	1.90	0.53
1:B:384:ASP:O	1:B:415:THR:HA	2.09	0.53
1:A:364:GLN:NE2	1:A:393:GLN:H	2.01	0.53
1:B:324:ALA:HB1	1:B:349:ASP:O	2.09	0.53
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.73	0.53
1:B:159:ALA:O	1:B:160:GLY:O	2.27	0.53
1:B:57:ASN:HD22	1:B:71:ASP:HA	1.73	0.53
1:A:317:LYS:HD3	1:A:318:HIS:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ILE:HG13	2:A:428:LDA:H101	1.90	0.53
1:B:380:ASP:O	1:B:419:TYR:HA	2.09	0.53
1:B:254:ILE:HD12	1:B:255:PRO:CD	2.26	0.53
1:A:200:LEU:HD22	1:A:239:TYR:HD1	1.74	0.53
1:A:23:ILE:HB	1:A:29:ASN:HD21	1.74	0.53
1:A:253:PRO:O	1:A:255:PRO:HD2	2.09	0.53
1:B:112:TYR:CE2	1:B:114:GLY:HA3	2.45	0.52
1:B:143:GLY:O	1:B:211:ALA:HB1	2.08	0.52
1:A:293:LEU:HD13	1:A:327:ILE:HD13	1.90	0.52
1:A:398:ASN:OD1	1:A:403:GLN:NE2	2.42	0.52
1:A:37:ILE:C	1:A:39:MET:H	2.11	0.52
1:B:220:ASN:O	1:B:282:ARG:HB3	2.08	0.52
1:B:364:GLN:HG3	1:B:392:GLY:CA	2.30	0.52
1:A:101:ASN:ND2	1:A:127:ASN:HB2	2.25	0.52
1:A:220:ASN:ND2	1:A:282:ARG:HB3	2.25	0.52
1:B:291:TYR:HB3	1:B:329:LEU:HD23	1.91	0.52
1:B:299:SER:HA	1:B:321:PHE:O	2.09	0.52
1:B:322:LYS:NZ	1:B:352:VAL:N	2.57	0.52
1:A:18:SER:OG	1:A:290:HIS:HD2	1.91	0.52
1:A:346:ALA:O	1:A:368:TRP:N	2.37	0.52
1:B:153:ALA:HB1	2:B:428:LDA:H112	1.91	0.52
1:B:222:ARG:NH1	1:B:222:ARG:HG2	2.25	0.52
1:A:266:TYR:O	1:A:306:ALA:HA	2.10	0.52
1:B:201:ASN:O	1:B:237:GLY:HA3	2.10	0.52
1:B:94:TRP:HA	1:B:132:GLY:HA2	1.92	0.52
1:A:52:ILE:HG12	1:A:412:LEU:HD13	1.92	0.52
1:B:375:TYR:HB3	1:B:383:VAL:CG1	2.39	0.52
1:B:75:PRO:HD2	1:B:105:ALA:O	2.10	0.52
1:A:98:ILE:CG1	1:A:128:LEU:HD23	2.34	0.52
1:A:12:GLY:CA	1:A:15:ARG:NH1	2.71	0.52
1:B:198:ALA:HA	3:B:449:HOH:O	2.09	0.51
1:B:23:ILE:HB	1:B:29:ASN:HD21	1.74	0.51
1:A:340:THR:HG21	1:A:342:ARG:HH21	1.75	0.51
1:A:393:GLN:O	1:A:407:GLU:HA	2.10	0.51
1:B:342:ARG:NH2	1:B:374:THR:OG1	2.43	0.51
1:B:117:VAL:HG11	1:B:399:GLU:HG2	1.92	0.51
1:A:112:TYR:CE2	1:A:114:GLY:HA3	2.45	0.51
1:B:218:ASP:OD1	1:B:221:ASN:N	2.44	0.51
1:A:220:ASN:OD1	1:A:282:ARG:HD3	2.10	0.51
1:A:364:GLN:CG	1:A:408:GLY:HA3	2.24	0.51
1:B:157:ARG:C	1:B:197:ILE:HG12	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD23	1:A:200:LEU:N	2.25	0.51
1:A:267:LEU:HD13	2:A:428:LDA:H112	1.93	0.51
1:B:139:ALA:O	1:B:215:TYR:HA	2.10	0.51
1:B:162:LEU:HB2	3:B:444:HOH:O	2.10	0.51
1:B:232:LYS:HG2	1:B:270:ASN:HD22	1.71	0.51
1:A:403:GLN:CA	1:A:403:GLN:HE21	2.24	0.51
1:B:293:LEU:HA	1:B:326:ARG:O	2.11	0.51
1:B:218:ASP:CG	1:B:219:LYS:N	2.65	0.51
1:A:245:ARG:HH12	1:A:258:THR:C	2.14	0.50
1:A:30:VAL:HG23	3:A:460:HOH:O	2.10	0.50
1:A:48:GLY:O	1:A:80:PRO:HA	2.11	0.50
1:A:94:TRP:HA	1:A:132:GLY:HA2	1.93	0.50
1:B:89:ASN:HB2	1:B:91:GLN:HG2	1.94	0.50
1:A:127:ASN:C	1:A:127:ASN:HD22	2.12	0.50
1:B:366:ARG:NH2	1:B:393:GLN:OE1	2.44	0.50
1:B:48:GLY:O	1:B:80:PRO:HA	2.12	0.50
1:A:178:THR:C	1:A:182:GLN:NE2	2.65	0.50
1:B:297:SER:O	1:B:299:SER:N	2.44	0.50
1:B:303:GLN:HE21	1:B:305:LYS:HB2	1.77	0.50
1:B:34:PRO:HG2	1:B:211:ALA:HA	1.93	0.50
1:A:340:THR:O	1:A:341:PHE:CD2	2.65	0.49
1:B:266:TYR:HE1	1:B:309:THR:HG22	1.77	0.49
1:B:281:ASN:ND2	1:B:291:TYR:OH	2.45	0.49
1:B:345:ILE:CG2	1:B:346:ALA:N	2.75	0.49
1:B:360:SER:C	1:B:362:PRO:HD3	2.33	0.49
1:A:203:ASN:H	1:A:204:GLN:HE22	1.58	0.49
1:A:23:ILE:HB	1:A:29:ASN:ND2	2.27	0.49
1:B:158:PHE:O	1:B:197:ILE:HD13	2.12	0.49
1:B:364:GLN:HG2	1:B:408:GLY:N	2.27	0.49
1:A:276:GLU:OE1	1:A:294:ALA:HB2	2.12	0.49
1:A:238:ASN:N	1:A:238:ASN:ND2	2.60	0.49
1:B:23:ILE:HB	1:B:29:ASN:ND2	2.28	0.49
1:B:315:PHE:HE2	1:B:317:LYS:HB2	1.77	0.49
1:B:34:PRO:HB2	1:B:143:GLY:CA	2.38	0.49
1:B:41:ASP:OD1	1:B:42:ARG:HD3	2.12	0.49
1:A:272:PRO:HB3	1:A:296:THR:HG22	1.95	0.49
1:B:104:LEU:HD11	1:B:361:ILE:HG12	1.93	0.49
1:B:41:ASP:O	1:B:87:PRO:HG3	2.12	0.49
1:A:381:ALA:HB2	1:A:419:TYR:CD1	2.47	0.49
1:B:136:LEU:HD22	1:B:142:PHE:HE1	1.77	0.49
1:B:288:ALA:HB2	1:B:334:TYR:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:SER:HB2	1:A:416:ASN:HB2	1.95	0.49
1:B:70:ALA:HA	3:B:432:HOH:O	2.13	0.49
1:A:104:LEU:HB3	2:A:428:LDA:O1	2.13	0.49
1:B:109:ASN:O	1:B:111:THR:N	2.46	0.49
1:B:305:LYS:HE3	1:B:316:GLN:HE22	1.78	0.48
1:A:34:PRO:HD2	1:A:212:GLY:HA3	1.94	0.48
1:A:353:PRO:HB2	1:A:355:GLN:NE2	2.27	0.48
1:B:219:LYS:HE2	1:B:219:LYS:HB2	1.56	0.48
1:B:20:GLU:HB3	1:B:32:ARG:HG2	1.95	0.48
1:A:158:PHE:O	1:A:197:ILE:HD13	2.13	0.48
1:A:20:GLU:HB3	1:A:32:ARG:HG2	1.96	0.48
1:A:2:GLY:HA3	1:A:365:ASP:OD2	2.14	0.48
1:B:180:GLN:CG	1:B:184:LEU:HD22	2.44	0.48
1:A:149:VAL:HG21	1:A:231:VAL:HG21	1.95	0.48
1:B:135:ARG:NH1	1:B:137:ASN:O	2.42	0.48
1:B:303:GLN:HE22	1:B:305:LYS:HE3	1.79	0.48
1:A:407:GLU:HG3	1:A:408:GLY:N	2.28	0.48
1:B:276:GLU:HA	1:B:294:ALA:HA	1.96	0.48
1:A:291:TYR:CD2	1:A:291:TYR:N	2.82	0.48
1:A:409:LYS:NZ	3:A:451:HOH:O	2.45	0.48
1:B:16:ALA:HA	3:B:453:HOH:O	2.14	0.48
1:B:3:PHE:CD1	2:B:428:LDA:HM21	2.49	0.48
1:A:109:ASN:O	1:A:111:THR:N	2.46	0.48
1:A:375:TYR:HE2	1:A:377:PHE:CD2	2.32	0.48
1:A:387:VAL:HG22	1:A:413:PHE:CD2	2.47	0.48
1:A:384:ASP:N	1:A:416:ASN:O	2.38	0.48
1:B:101:ASN:ND2	1:B:127:ASN:HB2	2.28	0.48
1:B:104:LEU:HD23	1:B:104:LEU:H	1.79	0.48
1:B:33:ASN:HB3	1:B:36:LEU:CD1	2.44	0.48
1:A:305:LYS:CG	1:A:316:GLN:HE22	2.20	0.48
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.77	0.47
1:B:122:ASP:HB3	3:B:470:HOH:O	2.12	0.47
1:B:266:TYR:CE1	1:B:309:THR:HG22	2.48	0.47
1:A:75:PRO:HD2	1:A:105:ALA:O	2.13	0.47
1:A:5:LEU:HD23	3:A:463:HOH:O	2.14	0.47
1:B:383:VAL:CG2	1:B:384:ASP:H	2.28	0.47
1:B:321:PHE:HA	1:B:353:PRO:HD3	1.97	0.47
1:B:401:PRO:HG2	1:B:402:TYR:CE1	2.50	0.47
1:B:139:ALA:C	3:B:451:HOH:O	2.53	0.47
1:A:159:ALA:O	1:A:160:GLY:O	2.32	0.47
1:A:353:PRO:HB2	1:A:355:GLN:HE22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LYS:O	1:A:410:ALA:CB	2.61	0.47
1:B:142:PHE:CD2	1:B:213:ILE:HG12	2.50	0.47
1:B:146:PHE:CE2	1:B:207:PHE:HD1	2.33	0.47
1:B:304:LEU:HB2	1:B:317:LYS:HB3	1.96	0.47
1:B:89:ASN:ND2	3:B:445:HOH:O	2.48	0.47
1:A:367:PHE:CE1	1:A:391:HIS:HB3	2.50	0.47
1:B:37:ILE:HB	1:B:133:ALA:CB	2.45	0.47
1:A:244:ASN:N	3:A:457:HOH:O	2.39	0.47
1:B:196:LYS:HD2	1:B:199:HIS:HB2	1.97	0.47
1:A:345:ILE:HG12	1:A:369:LEU:HD12	1.96	0.47
1:B:127:ASN:HD22	1:B:127:ASN:C	2.14	0.47
1:A:348:ASP:N	1:A:348:ASP:OD2	2.47	0.46
1:A:345:ILE:HA	1:A:368:TRP:O	2.16	0.46
1:B:180:GLN:NE2	1:B:184:LEU:CD2	2.78	0.46
1:B:345:ILE:HG22	1:B:346:ALA:N	2.30	0.46
1:A:140:TRP:CZ2	1:A:215:TYR:HD2	2.32	0.46
1:B:157:ARG:HG3	1:B:157:ARG:HH11	1.79	0.46
1:B:15:ARG:NH1	1:B:20:GLU:OE2	2.48	0.46
1:B:13:LEU:O	1:B:370:SER:OG	2.33	0.46
1:B:146:PHE:CZ	1:B:207:PHE:HD1	2.33	0.46
1:A:241:SER:HB3	1:A:258:THR:H	1.81	0.46
1:A:33:ASN:HB3	1:A:36:LEU:CD1	2.46	0.46
1:B:180:GLN:HE21	1:B:184:LEU:CD1	2.28	0.46
1:B:104:LEU:HD21	2:B:428:LDA:H52	1.97	0.46
1:B:152:ARG:NH1	1:B:203:ASN:HD21	2.14	0.46
1:B:307:THR:HA	1:B:314:LEU:H	1.80	0.46
1:B:45:PHE:C	1:B:45:PHE:CD1	2.89	0.46
1:A:395:VAL:O	1:A:395:VAL:HG23	2.16	0.46
1:B:343:THR:CG2	1:B:344:GLY:N	2.78	0.46
1:A:88:ILE:HB	1:A:92:PHE:O	2.16	0.46
1:B:63:PRO:C	1:B:65:GLY:H	2.19	0.46
1:A:169:GLN:O	1:A:173:SER:HB3	2.16	0.46
1:A:263:GLN:HB3	1:A:264:SER:H	1.48	0.46
1:A:45:PHE:CD1	1:A:45:PHE:C	2.88	0.46
1:A:157:ARG:HH11	1:A:157:ARG:HG3	1.79	0.45
1:A:352:VAL:HG12	1:A:353:PRO:O	2.16	0.45
1:A:340:THR:CG2	1:A:341:PHE:N	2.79	0.45
1:A:396:LYS:HE3	1:A:396:LYS:N	2.31	0.45
1:A:90:ASP:H	1:A:91:GLN:HG2	1.82	0.45
1:B:152:ARG:NH1	1:B:203:ASN:ND2	2.63	0.45
1:B:297:SER:C	1:B:299:SER:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLN:NE2	1:B:395:VAL:HG13	2.18	0.45
1:A:15:ARG:NH1	1:A:20:GLU:OE2	2.49	0.45
1:A:142:PHE:CD2	1:A:213:ILE:HG12	2.52	0.45
1:A:378:ASN:O	1:A:380:ASP:N	2.49	0.45
1:B:38:THR:CG2	1:B:135:ARG:HB2	2.46	0.45
1:B:187:THR:HA	3:B:468:HOH:O	2.16	0.45
1:B:10:SER:CB	1:B:416:ASN:HD22	2.28	0.45
1:A:321:PHE:CE2	1:A:352:VAL:HG22	2.51	0.45
1:B:355:GLN:C	1:B:356:ASN:OD1	2.55	0.45
1:A:302:GLN:OE1	1:A:320:GLY:HA2	2.17	0.45
1:B:32:ARG:HA	1:B:32:ARG:HD2	1.60	0.45
1:A:38:THR:CG2	1:A:135:ARG:HB2	2.46	0.45
1:A:197:ILE:O	3:A:458:HOH:O	2.21	0.45
1:A:148:ALA:HA	1:A:206:GLY:O	2.17	0.45
1:B:180:GLN:NE2	1:B:184:LEU:HD21	2.32	0.45
1:A:194:ASN:ND2	1:B:194:ASN:ND2	2.65	0.45
1:B:230:GLU:HA	1:B:272:PRO:O	2.16	0.45
1:B:342:ARG:HD3	3:B:465:HOH:O	2.17	0.45
1:B:37:ILE:HG21	1:B:93:GLY:O	2.16	0.45
1:A:17:TYR:HB2	1:A:326:ARG:HH22	1.82	0.44
1:B:241:SER:OG	1:B:257:ALA:HA	2.16	0.44
1:B:102:TYR:CD1	1:B:271:LEU:HD22	2.52	0.44
1:B:339:TRP:HA	1:B:339:TRP:CE3	2.52	0.44
1:B:4:GLN:OE1	1:B:348:ASP:HB3	2.17	0.44
1:A:244:ASN:O	1:A:246:ALA:N	2.51	0.44
1:A:267:LEU:C	1:A:267:LEU:HD23	2.38	0.44
1:A:59:SER:O	1:A:405:GLU:N	2.50	0.44
1:A:63:PRO:C	1:A:65:GLY:H	2.20	0.44
1:A:32:ARG:HA	1:A:32:ARG:HD2	1.59	0.44
1:B:281:ASN:O	1:B:282:ARG:C	2.55	0.44
1:A:200:LEU:HD22	1:A:239:TYR:CD1	2.53	0.44
1:A:276:GLU:HA	1:A:294:ALA:HA	1.99	0.44
1:A:335:TYR:CD2	1:A:336:ASP:HB2	2.53	0.44
1:A:36:LEU:O	1:A:39:MET:HB2	2.18	0.44
1:A:364:GLN:CB	1:A:392:GLY:HA3	2.47	0.44
1:A:41:ASP:C	1:A:87:PRO:HG3	2.37	0.44
1:B:127:ASN:ND2	1:B:127:ASN:C	2.70	0.44
1:A:378:ASN:ND2	1:A:378:ASN:N	2.66	0.44
1:A:154:LYS:HB3	3:A:448:HOH:O	2.18	0.44
1:A:355:GLN:O	1:A:356:ASN:ND2	2.50	0.44
1:A:376:ALA:HA	1:A:382:SER:HB2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASP:OD2	1:A:334:TYR:OH	2.26	0.44
1:B:160:GLY:N	3:B:444:HOH:O	2.51	0.44
1:B:322:LYS:HE2	3:B:481:HOH:O	2.18	0.44
1:A:239:TYR:HE2	1:A:256:THR:O	2.01	0.44
1:A:402:TYR:HB2	1:A:404:PHE:CE1	2.52	0.44
1:B:225:LEU:HG	1:B:226:THR:N	2.33	0.44
1:B:36:LEU:O	1:B:39:MET:HB2	2.17	0.44
1:B:357:ARG:CD	1:B:395:VAL:HG21	2.47	0.44
1:A:317:LYS:HD3	1:A:318:HIS:H	1.83	0.43
1:A:290:HIS:CE1	1:A:332:THR:OG1	2.71	0.43
1:A:37:ILE:HB	1:A:133:ALA:CB	2.47	0.43
1:B:128:LEU:O	1:B:147:ASN:HA	2.18	0.43
1:B:325:TYR:H	1:B:349:ASP:HB3	1.81	0.43
1:A:204:GLN:N	1:A:204:GLN:NE2	2.66	0.43
1:A:366:ARG:O	1:A:367:PHE:HB3	2.18	0.43
1:A:44:THR:N	1:A:85:VAL:O	2.47	0.43
1:B:116:SER:HB2	3:B:450:HOH:O	2.17	0.43
1:B:47:ALA:HA	1:B:81:ASN:O	2.19	0.43
1:A:127:ASN:ND2	1:A:127:ASN:C	2.70	0.43
1:A:41:ASP:O	1:A:87:PRO:HG3	2.18	0.43
1:A:178:THR:C	1:A:182:GLN:HE21	2.22	0.43
1:A:403:GLN:CA	1:A:403:GLN:NE2	2.82	0.43
1:A:37:ILE:HG21	1:A:93:GLY:O	2.19	0.43
1:B:180:GLN:HE21	1:B:184:LEU:HD11	1.83	0.43
1:B:27:ALA:HB2	1:B:44:THR:HG22	2.01	0.43
1:B:326:ARG:HG3	1:B:348:ASP:OD2	2.17	0.43
1:B:1:ALA:HB3	1:B:368:TRP:CZ2	2.53	0.43
1:B:1:ALA:HB3	1:B:368:TRP:HZ2	1.84	0.43
1:A:152:ARG:HA	1:A:203:ASN:OD1	2.19	0.43
1:B:282:ARG:NH1	1:B:282:ARG:CG	2.72	0.43
1:A:295:TYR:CZ	1:A:323:ASP:HB3	2.54	0.43
1:B:170:ILE:O	1:B:173:SER:O	2.36	0.43
1:B:223:TYR:CD1	1:B:223:TYR:N	2.86	0.43
1:B:204:GLN:HG3	1:B:205:TRP:N	2.32	0.43
1:B:218:ASP:CG	1:B:219:LYS:H	2.21	0.43
1:B:272:PRO:C	3:B:457:HOH:O	2.57	0.43
1:B:303:GLN:NE2	1:B:305:LYS:HE3	2.34	0.43
1:B:295:TYR:OH	1:B:323:ASP:OD2	2.31	0.43
1:A:333:TYR:N	1:A:341:PHE:O	2.49	0.43
1:A:1:ALA:HB3	1:A:368:TRP:CZ2	2.54	0.43
1:B:227:TYR:CE1	1:B:275:TRP:NE1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:HG22	1:A:106:THR:O	2.17	0.42
1:A:336:ASP:HA	3:A:461:HOH:O	2.18	0.42
1:B:225:LEU:HD12	1:B:277:VAL:CG1	2.49	0.42
1:A:360:SER:HB2	1:A:361:ILE:HD12	2.02	0.42
1:A:56:VAL:HG13	1:A:407:GLU:O	2.18	0.42
1:B:251:GLY:C	1:B:252:LEU:HD23	2.39	0.42
1:A:135:ARG:NH1	1:A:137:ASN:O	2.42	0.42
1:A:47:ALA:HA	1:A:81:ASN:O	2.19	0.42
1:B:342:ARG:NH1	3:B:465:HOH:O	2.52	0.42
1:B:8:PHE:CE2	1:B:32:ARG:HD3	2.54	0.42
1:A:238:ASN:N	1:A:238:ASN:HD22	2.18	0.42
1:A:110:ASP:OD2	1:A:111:THR:N	2.52	0.42
1:A:149:VAL:O	1:A:205:TRP:HA	2.19	0.42
1:A:184:LEU:C	1:A:184:LEU:HD23	2.39	0.42
1:A:155:ILE:O	1:A:199:HIS:HA	2.19	0.42
1:A:213:ILE:HG22	1:A:214:LEU:N	2.34	0.42
1:A:4:GLN:NE2	1:A:326:ARG:HB2	2.34	0.42
1:B:5:LEU:CD2	1:B:32:ARG:HH21	2.31	0.42
1:B:141:SER:HB2	1:B:214:LEU:HB3	2.02	0.42
1:A:156:GLU:CD	1:A:196:LYS:HE3	2.40	0.42
1:B:18:SER:O	1:B:290:HIS:HB2	2.20	0.42
1:B:91:GLN:HG2	1:B:91:GLN:H	1.41	0.42
1:B:115:GLY:CA	3:B:464:HOH:O	2.68	0.42
1:B:322:LYS:NZ	1:B:351:PRO:C	2.73	0.42
1:B:54:PRO:CD	1:B:75:PRO:O	2.68	0.42
1:B:41:ASP:C	1:B:87:PRO:HG3	2.40	0.42
1:A:190:GLY:O	1:A:191:ILE:C	2.58	0.42
1:A:215:TYR:CD1	1:A:215:TYR:C	2.93	0.42
1:A:353:PRO:CB	1:A:355:GLN:HE22	2.33	0.42
1:B:281:ASN:O	1:B:283:VAL:HG13	2.19	0.42
1:A:241:SER:OG	1:A:257:ALA:HA	2.20	0.41
1:A:253:PRO:O	1:A:255:PRO:CD	2.68	0.41
1:A:367:PHE:HE2	1:A:369:LEU:HD22	1.85	0.41
1:A:4:GLN:HA	3:A:467:HOH:O	2.20	0.41
1:A:33:ASN:OD1	1:A:212:GLY:HA3	2.20	0.41
1:A:306:ALA:O	1:A:314:LEU:HB2	2.21	0.41
1:B:305:LYS:CE	1:B:316:GLN:NE2	2.83	0.41
1:B:179:GLN:H	1:B:179:GLN:HG2	1.64	0.41
1:B:302:GLN:HA	1:B:320:GLY:HA2	2.02	0.41
1:B:295:TYR:CD1	1:B:325:TYR:CE2	3.08	0.41
1:B:37:ILE:HG21	1:B:93:GLY:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:HB1	2:A:428:LDA:C10	2.49	0.41
1:A:238:ASN:HB2	1:A:262:THR:HG23	2.02	0.41
1:A:345:ILE:HG12	1:A:369:LEU:CD1	2.51	0.41
1:A:46:SER:OG	1:A:418:ASN:ND2	2.53	0.41
1:B:44:THR:N	1:B:85:VAL:O	2.44	0.41
1:A:155:ILE:HD11	1:A:304:LEU:HD21	2.01	0.41
1:B:282:ARG:HD2	1:B:287:TRP:O	2.21	0.41
1:B:375:TYR:O	1:B:383:VAL:HG12	2.20	0.41
1:A:342:ARG:HE	1:A:342:ARG:HB3	1.74	0.41
1:B:230:GLU:HG2	1:B:230:GLU:H	1.55	0.41
1:B:218:ASP:OD2	1:B:220:ASN:CB	2.69	0.41
1:B:220:ASN:OD1	1:B:282:ARG:HG2	2.21	0.41
1:B:346:ALA:HB3	1:B:368:TRP:CB	2.49	0.41
1:A:183:ALA:HA	3:A:469:HOH:O	2.20	0.41
1:A:27:ALA:HB2	1:A:44:THR:HG22	2.03	0.41
1:B:200:LEU:O	1:B:201:ASN:CB	2.58	0.41
1:A:209:TRP:H	1:A:229:SER:HB3	1.86	0.41
1:A:254:ILE:H	1:A:254:ILE:HG13	1.65	0.41
1:A:273:GLU:HG2	1:A:297:SER:OG	2.21	0.41
1:A:33:ASN:HA	1:A:34:PRO:HD3	1.89	0.41
1:B:322:LYS:HE2	3:B:441:HOH:O	2.20	0.41
1:B:45:PHE:HD1	1:B:46:SER:N	2.19	0.41
1:A:298:TRP:O	1:A:321:PHE:CB	2.62	0.41
1:A:5:LEU:CD2	1:A:32:ARG:HH21	2.33	0.41
1:A:45:PHE:HD1	1:A:46:SER:N	2.19	0.41
1:B:306:ALA:HB3	1:B:315:PHE:HB3	2.03	0.41
1:B:10:SER:H	1:B:416:ASN:ND2	2.19	0.41
1:B:106:THR:O	1:B:106:THR:HG22	2.20	0.41
1:B:364:GLN:HE21	1:B:393:GLN:N	2.19	0.41
1:B:411:TRP:HB3	1:B:413:PHE:CE1	2.55	0.41
1:A:317:LYS:NZ	3:A:445:HOH:O	2.53	0.40
1:B:388:SER:HB2	3:B:453:HOH:O	2.21	0.40
1:B:12:GLY:HA3	1:B:17:TYR:CE2	2.56	0.40
1:A:375:TYR:HE2	1:A:377:PHE:CE2	2.39	0.40
1:B:158:PHE:C	1:B:197:ILE:HG23	2.41	0.40
1:B:109:ASN:C	1:B:111:THR:N	2.75	0.40
1:B:98:ILE:CG1	1:B:128:LEU:HD23	2.34	0.40
1:B:288:ALA:HB2	1:B:334:TYR:CE1	2.57	0.40
1:A:358:SER:HB2	3:A:462:HOH:O	2.21	0.40
1:A:37:ILE:HG21	1:A:93:GLY:C	2.41	0.40
1:A:384:ASP:OD2	1:A:418:ASN:OD1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ALA:C	1:B:185:ALA:N	2.74	0.40
1:B:282:ARG:NH2	1:B:285:PRO:O	2.52	0.40
1:B:298:TRP:C	1:B:300:GLN:H	2.21	0.40
1:B:308:SER:HB3	1:B:314:LEU:HD11	2.01	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	419/427 (98%)	346 (83%)	57 (14%)	16 (4%)	3	10
1	B	419/427 (98%)	340 (81%)	58 (14%)	21 (5%)	2	6
All	All	838/854 (98%)	686 (82%)	115 (14%)	37 (4%)	2	8

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	ILE
1	A	272	PRO
1	A	379	LYS
1	B	174	PRO
1	B	253	PRO
1	B	254	ILE
1	A	110	ASP
1	A	160	GLY
1	A	191	ILE
1	A	335	TYR
1	B	110	ASP
1	B	160	GLY
1	B	201	ASN
1	B	272	PRO

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Mol	Chain	Res	Type
1	B	298	TRP
1	B	354	ALA
1	A	245	ARG
1	A	410	ALA
1	B	297	SER
1	B	379	LYS
1	A	38	THR
1	B	24	ALA
1	B	38	THR
1	B	220	ASN
1	B	394	SER
1	A	24	ALA
1	A	253	PRO
1	A	320	GLY
1	B	35	ALA
1	B	184	LEU
1	B	255	PRO
1	B	366	ARG
1	A	119	GLY
1	B	119	GLY
1	A	28	GLY
1	A	401	PRO
1	B	28	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	331/337 (98%)	290 (88%)	41 (12%)	4	14
1	B	331/337 (98%)	282 (85%)	49 (15%)	3	9
All	All	662/674 (98%)	572 (86%)	90 (14%)	3	11

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	32	ARG
1	A	42	ARG
1	A	72	ASN
1	A	78	TRP
1	A	82	MET
1	A	91	GLN
1	A	106	THR
1	A	121	THR
1	A	127	ASN
1	A	141	SER
1	A	162	LEU
1	A	164	GLN
1	A	169	GLN
1	A	182	GLN
1	A	194	ASN
1	A	200	LEU
1	A	201	ASN
1	A	204	GLN
1	A	216	GLU
1	A	219	LYS
1	A	226	THR
1	A	230	GLU
1	A	238	ASN
1	A	244	ASN
1	A	245	ARG
1	A	253	PRO
1	A	274	MET
1	A	290	HIS
1	A	314	LEU
1	A	317	LYS
1	A	322	LYS
1	A	337	ASP
1	A	355	GLN
1	A	366	ARG
1	A	369	LEU
1	A	378	ASN
1	A	396	LYS
1	A	403	GLN
1	A	416	ASN
1	A	418	ASN
1	B	5	LEU
1	B	32	ARG

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Mol	Chain	Res	Type
1	B	42	ARG
1	B	72	ASN
1	B	78	TRP
1	B	82	MET
1	B	91	GLN
1	B	106	THR
1	B	121	THR
1	B	126	MET
1	B	127	ASN
1	B	141	SER
1	B	162	LEU
1	B	164	GLN
1	B	169	GLN
1	B	174	PRO
1	B	179	GLN
1	B	217	LEU
1	B	218	ASP
1	B	219	LYS
1	B	225	LEU
1	B	240	SER
1	B	252	LEU
1	B	253	PRO
1	B	255	PRO
1	B	262	THR
1	B	263	GLN
1	B	273	GLU
1	B	277	VAL
1	B	289	ILE
1	B	290	HIS
1	B	291	TYR
1	B	300	GLN
1	B	307	THR
1	B	310	SER
1	B	314	LEU
1	B	325	TYR
1	B	333	TYR
1	B	339	TRP
1	B	349	ASP
1	B	356	ASN
1	B	366	ARG
1	B	370	SER
1	B	396	LYS

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Mol	Chain	Res	Type
1	B	402	TYR
1	B	407	GLU
1	B	412	LEU
1	B	418	ASN
1	B	421	PHE

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	57	ASN
1	A	72	ASN
1	A	81	ASN
1	A	101	ASN
1	A	127	ASN
1	A	164	GLN
1	A	182	GLN
1	A	189	ASN
1	A	194	ASN
1	A	204	GLN
1	A	244	ASN
1	A	248	ASN
1	A	270	ASN
1	A	290	HIS
1	A	303	GLN
1	A	316	GLN
1	A	355	GLN
1	A	356	ASN
1	A	364	GLN
1	A	378	ASN
1	A	398	ASN
1	A	403	GLN
1	A	416	ASN
1	A	418	ASN
1	B	57	ASN
1	B	72	ASN
1	B	81	ASN
1	B	101	ASN
1	B	127	ASN
1	B	129	ASN
1	B	147	ASN
1	B	164	GLN
1	B	180	GLN

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Mol	Chain	Res	Type
1	B	194	ASN
1	B	203	ASN
1	B	270	ASN
1	B	281	ASN
1	B	290	HIS
1	B	303	GLN
1	B	316	GLN
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 ⓘ

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	B	428	-	12,15,15	2.16	1 (8%)	14,17,17	1.67	4 (28%)
2	LDA	A	428	-	12,15,15	2.04	1 (8%)	14,17,17	1.63	3 (21%)

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	B	428	-	-	4/13/13/13	-
2	LDA	A	428	-	-	5/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	428	LDA	O1-N1	-7.22	1.25	1.42
2	A	428	LDA	O1-N1	-6.76	1.26	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	428	LDA	CM1-N1-C1	-3.97	101.89	110.23
2	A	428	LDA	CM1-N1-C1	-3.68	102.51	110.23
2	A	428	LDA	O1-N1-C1	2.49	115.38	109.27
2	B	428	LDA	O1-N1-C1	2.24	114.76	109.27
2	B	428	LDA	C9-C8-C7	-2.16	103.47	114.42
2	B	428	LDA	CM2-N1-C1	2.13	114.71	110.23
2	A	428	LDA	C9-C8-C7	-2.12	103.68	114.42

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	428	LDA	N1-C1-C2-C3
2	A	428	LDA	N1-C1-C2-C3
2	B	428	LDA	C1-C2-C3-C4
2	A	428	LDA	C6-C7-C8-C9
2	B	428	LDA	C3-C4-C5-C6
2	A	428	LDA	C1-C2-C3-C4
2	B	428	LDA	C2-C1-N1-CM2
2	A	428	LDA	C2-C1-N1-CM2
2	A	428	LDA	C11-C10-C9-C8

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	428	LDA	6	0
2	A	428	LDA	8	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.