Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:18 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

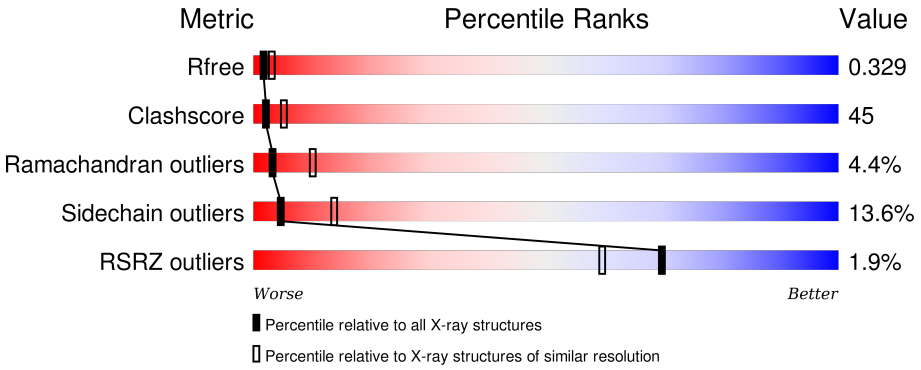
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	427	% 35% 55% 8%
1	B	427	3% 33% 55% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	A	428	-	-	-	X
2	LDA	B	428	-	-	-	X

2 Entry composition (i)

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.

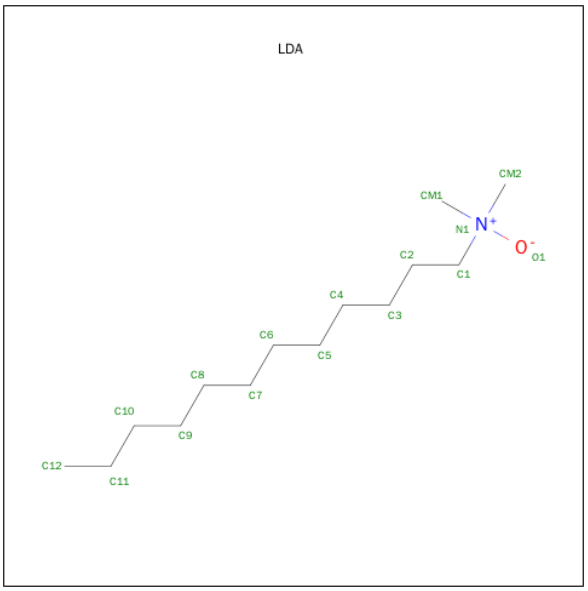
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

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: $C_{14}H_{31}NO$).



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

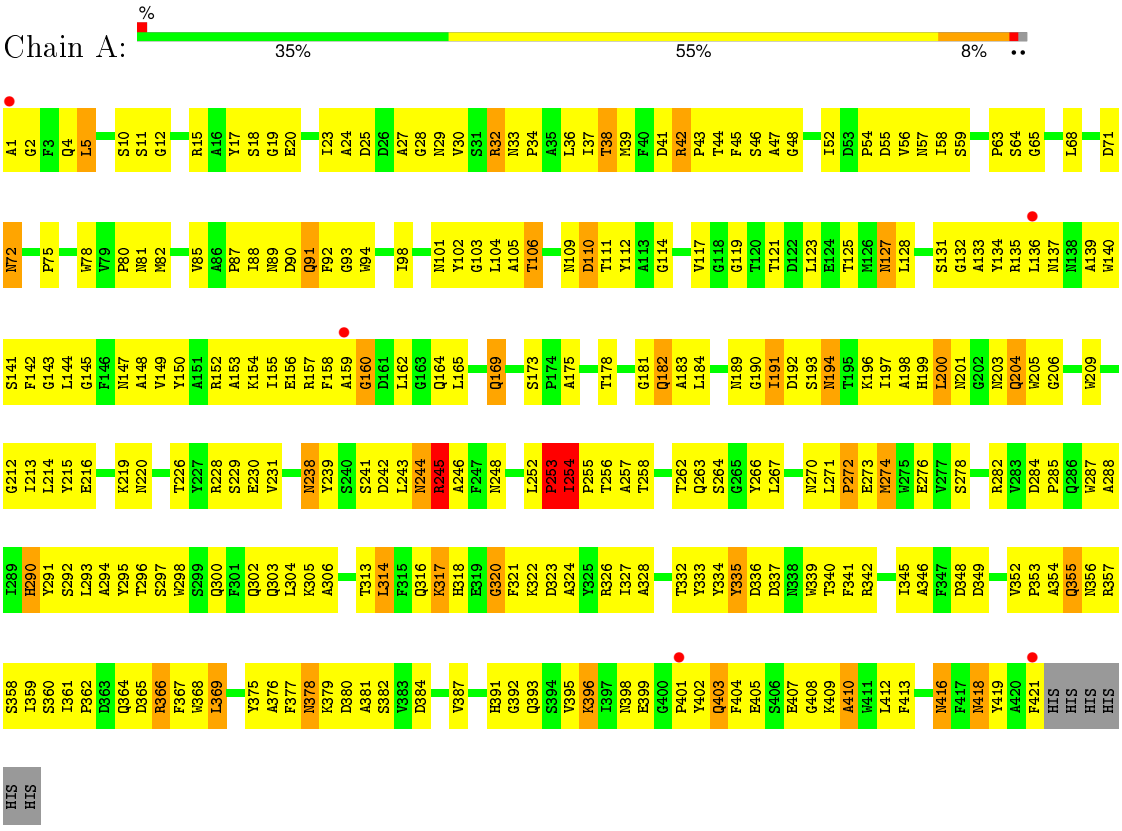
- Molecule 3 is water.

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

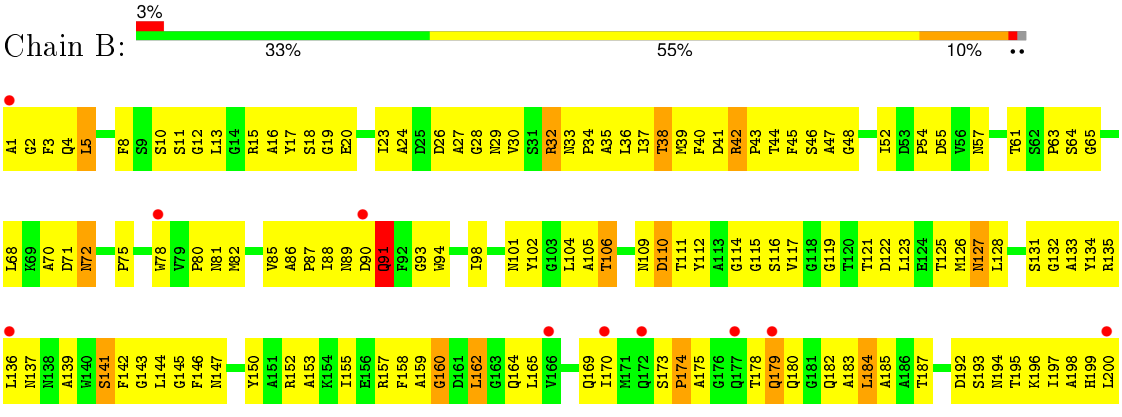
3 Residue-property plots (i)

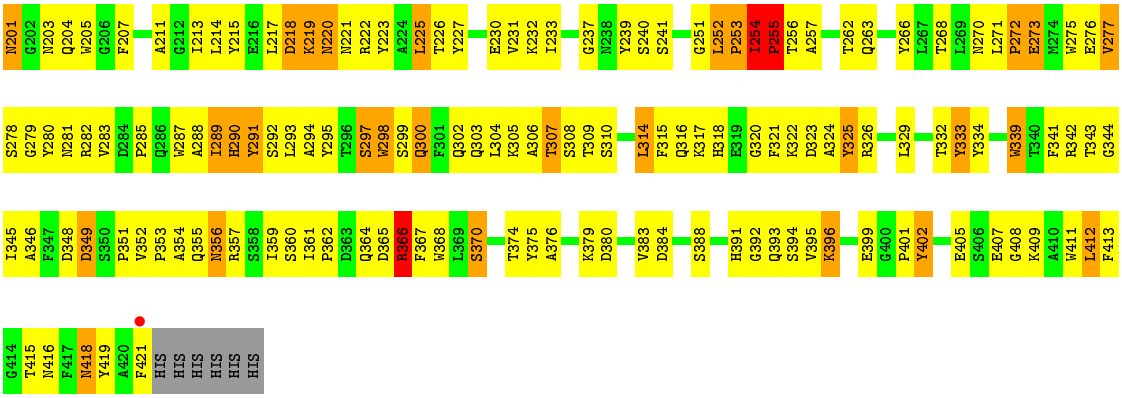
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Long-chain fatty acid transport protein



- Molecule 1: Long-chain fatty acid transport protein




N201 G202 N203 Q204 W205 G206 F207 A211 G212 I213 L214 Y215 E216 L217 D218 K219 N220 N221 R222 Y223 A224 L225 T226 Y227 E230 V231 K232 I233 G237 W238 Y239 S240 S241 G251 L252 P253 I254 P255 T256 A257 T262 Q263 Y266 L267 T268 L269 N270 L271 P272 E273 W274 W275 E276 V277
S278 G279 Y280 N281 R282 V283 D284 P285 Q286 W287 A288 I289 H290 Y291 S292 L293 A294 Y295 T296 S297 W298 S299 Q300 F301 Q302 Q303 L304 K305 A306 T307 S308 T309 S310 L314 F315 Q316 K317 H318 E319 G320 F321 K322 D323 A324 Y325 R326 L329 T332 Y333 Y334 W339 T340 F341 R342 T343 G344
I345 A346 F347 D348 D349 S350 P351 V352 P353 A354 Q355 N356 R357 S358 I359 S360 I361 P362 D363 Q364 D365 R366 F367 W368 L369 S370 T374 Y375 A376 K379 D380 V383 D384 S388 H391 G392 Q393 S394 V395 K396 E399 G400 P401 Y402 E405 S406 E407 G408 K409 A410 W411 L412 F413
G414 T415 N416 F417 N418 Y419 A420 F421 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.96 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.298 , 0.331 0.298 , 0.329	Depositor DCC
R_{free} test set	1638 reflections (4.98%)	DCC
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
Estimated twinning fraction	0.447 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	0 of 39365 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.48	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(^{o})	Ideal(^{o})
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

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:57:ASN:HD22	1:A:72:ASN:H	1.31	0.78
1:A:34:PRO:HB2	1:A:143:GLY:HA3	1.63	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:43:PRO:HB2	1:A:421:PHE:HB2	1.66	0.77
1:A:117:VAL:HG11	1:A:399:GLU:HG2	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:B:367:PHE:CG	1:B:391:HIS:HB3	2.29	0.68
1:A:149:VAL:O	1:A:206:GLY:N	2.26	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:409:LYS:O	1:A:410:ALA:HB2	1.95	0.67
1:A:153:ALA:HB1	2:A:428:LDA:H102	1.77	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:43:PRO:HA	1:A:85:VAL:O	1.96	0.66
1:A:192:ASP:OD1	1:A:194:ASN:ND2	2.28	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:B:5:LEU:HD22	1:B:32:ARG:HH21	1.62	0.65
1:A:403:GLN:HE21	1:A:403:GLN:HA	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:199:HIS:O	1:B:239:TYR:HA	1.97	0.64
1:B:117:VAL:HG23	1:B:359:ILE:HD11	1.79	0.64
1:B:360:SER:O	1:B:362:PRO:HD3	1.96	0.64
1:A:297:SER:HB2	1:A:300:GLN:OE1	1.97	0.64
1:B:173:SER:O	1:B:175:ALA:N	2.31	0.63
1:B:38:THR:HG21	1:B:135:ARG:HB2	1.81	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:B:393:GLN:HE21	1:B:395:VAL:CG1	2.12	0.63
1:A:117:VAL:HB	1:A:399:GLU:OE1	1.98	0.63
1:A:38:THR:HG21	1:A:135:ARG:HB2	1.81	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:364:GLN:CG	1:B:392:GLY:HA3	2.25	0.62
1:B:303:GLN:NE2	1:B:316:GLN:HE22	1.97	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: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:125:THR:HG22	1:A:150:TYR:O	2.02	0.59
1:B:232:LYS:HG2	1:B:270:ASN:HD21	1.63	0.59
1:A:136:LEU:HD22	1:A:142:PHE:CE1	2.37	0.59
1:A:364:GLN:CG	1:A:392:GLY:HA3	2.28	0.59
1:A:282:ARG:NH1	1:A:334:TYR:CE1	2.70	0.59
1:A:157:ARG:C	1:A:197:ILE:HG12	2.22	0.59
1:B:308:SER:HB3	1:B:314:LEU:CD1	2.32	0.59
1:A:360:SER:O	1:A:362:PRO:HD3	2.02	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:B:396:LYS:HG3	1:B:405:GLU:OE1	2.02	0.58
1:A:144:LEU:HD12	1:A:145:GLY:N	2.19	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:57:ASN:HD22	1:A:72:ASN:N	2.02	0.57
1:A:243:LEU:HD12	3:A:458:HOH:O	2.03	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:376:ALA:HA	1:A:382:SER:HB3	1.87	0.57
1:A:18:SER:O	1:A:23:ILE:HD11	2.05	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:B:288:ALA:O	1:B:289:ILE:HG13	2.04	0.56
1:A:387:VAL:HG22	1:A:413:PHE:HD2	1.70	0.56
1:A:159:ALA:O	1:A:193:SER:HA	2.04	0.56
1:B:18:SER:O	1:B:23:ILE:HD11	2.05	0.56
1:A:381:ALA:HB2	1:A:419:TYR:HD1	1.70	0.56
1:B:343:THR:HG22	1:B:344:GLY:N	2.21	0.56
1:B:11:SER:HB2	1:B:15:ARG:NH2	2.20	0.56
1:A:284:ASP:HB3	1:A:287:TRP:H	1.69	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:91:GLN:O	1:B:134:TYR:HA	2.06	0.56
1:B:144:LEU:HD12	1:B:145:GLY:N	2.21	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:317:LYS:HD3	1:B:318:HIS:N	2.21	0.55
1:B:157:ARG:O	1:B:197:ILE:HG12	2.06	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:B:33:ASN:HB3	1:B:36:LEU:HD12	1.88	0.55
1:A:220:ASN:ND2	1:A:282:ARG:HD3	2.21	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:B:12:GLY:CA	1:B:15:ARG:NH1	2.70	0.55
1:A:41:ASP:OD1	1:A:42:ARG:HD3	2.07	0.55
1:A:203:ASN:C	1:A:204:GLN:NE2	2.60	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:106:THR:HG21	1:B:360:SER:HA	1.89	0.54
1:B:342:ARG:HD2	3:B:462:HOH:O	2.07	0.54
1:A:57:ASN:HD22	1:A:71:ASP:HA	1.71	0.54
1:A:90:ASP:O	1:A:90:ASP:OD1	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:B:384:ASP:O	1:B:415:THR:HA	2.09	0.53
1:B:68:LEU:HD11	1:B:402:TYR:HB3	1.90	0.53
1:A:19:GLY:HA2	1:A:278:SER:HB2	1.90	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:57:ASN:HD22	1:B:71:ASP:HA	1.73	0.53
1:B:159:ALA:O	1:B:160:GLY:O	2.27	0.53
1:A:155:ILE:HG13	2:A:428:LDA:H101	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HD3	1:A:318:HIS:N	2.24	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:253:PRO:O	1:A:255:PRO:HD2	2.09	0.53
1:A:23:ILE:HB	1:A:29:ASN:HD21	1.74	0.53
1:B:143:GLY:O	1:B:211:ALA:HB1	2.08	0.52
1:B:112:TYR:CE2	1:B:114:GLY:HA3	2.45	0.52
1:B:364:GLN:HG3	1:B:392:GLY:CA	2.30	0.52
1:B:220:ASN:O	1:B:282:ARG:HB3	2.08	0.52
1:A:37:ILE:C	1:A:39:MET:H	2.11	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:101:ASN:ND2	1:A:127:ASN:HB2	2.25	0.52
1:B:291:TYR:HB3	1:B:329:LEU:HD23	1.91	0.52
1:A:220:ASN:ND2	1:A:282:ARG:HB3	2.25	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: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:A:18:SER:OG	1:A:290:HIS:HD2	1.91	0.52
1:B:222:ARG:NH1	1:B:222:ARG:HG2	2.25	0.52
1:B:201:ASN:O	1:B:237:GLY:HA3	2.10	0.52
1:A:266:TYR:O	1:A:306:ALA:HA	2.10	0.52
1:B:94:TRP:HA	1:B:132:GLY:HA2	1.92	0.52
1:B:375:TYR:HB3	1:B:383:VAL:CG1	2.39	0.52
1:A:52:ILE:HG12	1:A:412:LEU:HD13	1.92	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:393:GLN:O	1:A:407:GLU:HA	2.10	0.51
1:A:340:THR:HG21	1:A:342:ARG:HH21	1.75	0.51
1:B:117:VAL:HG11	1:B:399:GLU:HG2	1.92	0.51
1:B:342:ARG:NH2	1:B:374:THR:OG1	2.43	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:364:GLN:CG	1:A:408:GLY:HA3	2.24	0.51
1:A:220:ASN:OD1	1:A:282:ARG:HD3	2.10	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:N	1:A:200:LEU:HD23	2.25	0.51
1:A:267:LEU:HD13	2:A:428:LDA:H112	1.93	0.51
1:B:162:LEU:HB2	3:B:444:HOH:O	2.10	0.51
1:B:139:ALA:O	1:B:215:TYR:HA	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:B:89:ASN:HB2	1:B:91:GLN:HG2	1.94	0.50
1:A:94:TRP:HA	1:A:132:GLY:HA2	1.93	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:34:PRO:HG2	1:B:211:ALA:HA	1.93	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:A:340:THR:O	1:A:341:PHE:CD2	2.65	0.49
1:B:281:ASN:ND2	1:B:291:TYR:OH	2.45	0.49
1:B:266:TYR:HE1	1:B:309:THR:HG22	1.77	0.49
1:B:360:SER:C	1:B:362:PRO:HD3	2.33	0.49
1:B:345:ILE:CG2	1:B:346:ALA:N	2.75	0.49
1:B:364:GLN:HG2	1:B:408:GLY:N	2.27	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:A:203:ASN:H	1:A:204:GLN:HE22	1.58	0.49
1:A:276:GLU:OE1	1:A:294:ALA:HB2	2.12	0.49
1:B:315:PHE:HE2	1:B:317:LYS:HB2	1.77	0.49
1:B:23:ILE:HB	1:B:29:ASN:ND2	2.28	0.49
1:A:238:ASN:N	1:A:238:ASN:ND2	2.60	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:B:104:LEU:HD11	1:B:361:ILE:HG12	1.93	0.49
1:A:272:PRO:HB3	1:A:296:THR:HG22	1.95	0.49
1:B:41:ASP:O	1:B:87:PRO:HG3	2.12	0.49
1:B:288:ALA:HB2	1:B:334:TYR:HE1	1.77	0.49
1:B:136:LEU:HD22	1:B:142:PHE:HE1	1.77	0.49
1:A:381:ALA:HB2	1:A:419:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ALA:HA	3:B:432:HOH:O	2.13	0.49
1:A:10:SER:HB2	1:A:416:ASN:HB2	1.95	0.49
1:B:109:ASN:O	1:B:111:THR:N	2.46	0.49
1:A:104:LEU:HB3	2:A:428:LDA:O1	2.13	0.49
1:B:305:LYS:HE3	1:B:316:GLN:HE22	1.78	0.48
1:B:219:LYS:HE2	1:B:219:LYS:HB2	1.56	0.48
1:A:353:PRO:HB2	1:A:355:GLN:NE2	2.27	0.48
1:A:34:PRO:HD2	1:A:212:GLY:HA3	1.94	0.48
1:B:20:GLU:HB3	1:B:32:ARG:HG2	1.95	0.48
1:B:180:GLN:CG	1:B:184:LEU:HD22	2.44	0.48
1:A:20:GLU:HB3	1:A:32:ARG:HG2	1.96	0.48
1:A:158:PHE:O	1:A:197:ILE:HD13	2.13	0.48
1:A:2:GLY:HA3	1:A:365:ASP:OD2	2.14	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:409:LYS:NZ	3:A:451:HOH:O	2.45	0.48
1:B:3:PHE:CD1	2:B:428:LDA:HM21	2.49	0.48
1:A:291:TYR:CD2	1:A:291:TYR:N	2.82	0.48
1:B:16:ALA:HA	3:B:453:HOH:O	2.14	0.48
1:A:109:ASN:O	1:A:111:THR:N	2.46	0.48
1:B:101:ASN:ND2	1:B:127:ASN:HB2	2.28	0.48
1:B:33:ASN:HB3	1:B:36:LEU:CD1	2.44	0.48
1:B:104:LEU:HD23	1:B:104:LEU:H	1.79	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: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:266:TYR:CE1	1:B:309:THR:HG22	2.48	0.47
1:B:122:ASP:HB3	3:B:470:HOH:O	2.12	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:A:353:PRO:HB2	1:A:355:GLN:HE22	1.79	0.47
1:A:409:LYS:O	1:A:410:ALA:CB	2.61	0.47
1:B:89:ASN:ND2	3:B:445:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LEU:HB2	1:B:317:LYS:HB3	1.96	0.47
1:B:142:PHE:CD2	1:B:213:ILE:HG12	2.50	0.47
1:A:159:ALA:O	1:A:160:GLY:O	2.32	0.47
1:B:139:ALA:C	3:B:451:HOH:O	2.53	0.47
1:B:146:PHE:CE2	1:B:207:PHE:HD1	2.33	0.47
1:B:37:ILE:HB	1:B:133:ALA:CB	2.45	0.47
1:A:367:PHE:CE1	1:A:391:HIS:HB3	2.50	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:B:127:ASN:HD22	1:B:127:ASN:C	2.14	0.47
1:A:345:ILE:HG12	1:A:369:LEU:HD12	1.96	0.47
1:B:180:GLN:NE2	1:B:184:LEU:CD2	2.78	0.46
1:A:345:ILE:HA	1:A:368:TRP:O	2.16	0.46
1:A:348:ASP:N	1:A:348:ASP:OD2	2.47	0.46
1:B:345:ILE:HG22	1:B:346:ALA:N	2.30	0.46
1:B:15:ARG:NH1	1:B:20:GLU:OE2	2.48	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: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:B:180:GLN:HE21	1:B:184:LEU:CD1	2.28	0.46
1:A:33:ASN:HB3	1:A:36:LEU:CD1	2.46	0.46
1:B:104:LEU:HD21	2:B:428:LDA:H52	1.97	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:B:152:ARG:NH1	1:B:203:ASN:HD21	2.14	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:45:PHE:C	1:A:45:PHE:CD1	2.88	0.46
1:A:263:GLN:HB3	1:A:264:SER:H	1.48	0.46
1:A:169:GLN:O	1:A:173:SER:HB3	2.16	0.46
1:A:352:VAL:HG12	1:A:353:PRO:O	2.16	0.45
1:A:157:ARG:HH11	1:A:157:ARG:HG3	1.79	0.45
1:B:393:GLN:NE2	1:B:395:VAL:HG13	2.18	0.45
1:A:340:THR:CG2	1:A:341:PHE:N	2.79	0.45
1:B:297:SER:C	1:B:299:SER:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LYS:HE3	1:A:396:LYS:N	2.31	0.45
1:A:15:ARG:NH1	1:A:20:GLU:OE2	2.49	0.45
1:B:38:THR:CG2	1:B:135:ARG:HB2	2.46	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: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:B:32:ARG:HA	1:B:32:ARG:HD2	1.60	0.45
1:A:302:GLN:OE1	1:A:320:GLY:HA2	2.17	0.45
1:B:180:GLN:NE2	1:B:184:LEU:HD21	2.32	0.45
1:B:230:GLU:HA	1:B:272:PRO:O	2.16	0.45
1:A:148:ALA:HA	1:A:206:GLY:O	2.17	0.45
1:A:194:ASN:ND2	1:B:194:ASN:ND2	2.65	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: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:B:102:TYR:CD1	1:B:271:LEU:HD22	2.52	0.44
1:B:339:TRP:CE3	1:B:339:TRP:HA	2.52	0.44
1:B:241:SER:OG	1:B:257:ALA:HA	2.16	0.44
1:A:17:TYR:HB2	1:A:326:ARG:HH22	1.82	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:63:PRO:C	1:A:65:GLY:H	2.20	0.44
1:A:59:SER:O	1:A:405:GLU:N	2.50	0.44
1:B:281:ASN:O	1:B:282:ARG:C	2.55	0.44
1:A:32:ARG:HA	1:A:32:ARG:HD2	1.59	0.44
1:A:364:GLN:CB	1:A:392:GLY:HA3	2.47	0.44
1:B:127:ASN:ND2	1:B:127:ASN:C	2.70	0.44
1:A:200:LEU:HD22	1:A:239:TYR:CD1	2.53	0.44
1:A:36:LEU:O	1:A:39:MET:HB2	2.18	0.44
1:A:335:TYR:CD2	1:A:336:ASP:HB2	2.53	0.44
1:A:41:ASP:C	1:A:87:PRO:HG3	2.37	0.44
1:A:276:GLU:HA	1:A:294:ALA:HA	1.99	0.44
1:A:378:ASN:ND2	1:A:378:ASN:N	2.66	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
1:A:154:LYS:HB3	3:A:448:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLY:N	3:B:444:HOH:O	2.51	0.44
1:A:25:ASP:OD2	1:A:334:TYR:OH	2.26	0.44
1:B:322:LYS:HE2	3:B:481:HOH:O	2.18	0.44
1:B:357:ARG:CD	1:B:395:VAL:HG21	2.47	0.44
1:A:239:TYR:HE2	1:A:256:THR:O	2.01	0.44
1:B:36:LEU:O	1:B:39:MET:HB2	2.17	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:128:LEU:O	1:B:147:ASN:HA	2.18	0.43
1:A:37:ILE:HB	1:A:133:ALA:CB	2.47	0.43
1:B:325:TYR:H	1:B:349:ASP:HB3	1.81	0.43
1:A:290:HIS:CE1	1:A:332:THR:OG1	2.71	0.43
1:A:317:LYS:HD3	1:A:318:HIS:H	1.83	0.43
1:A:44:THR:N	1:A:85:VAL:O	2.47	0.43
1:A:366:ARG:O	1:A:367:PHE:HB3	2.18	0.43
1:A:204:GLN:N	1:A:204:GLN:NE2	2.66	0.43
1:B:47:ALA:HA	1:B:81:ASN:O	2.19	0.43
1:B:116:SER:HB2	3:B:450:HOH:O	2.17	0.43
1:A:127:ASN:C	1:A:127:ASN:ND2	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:B:180:GLN:HE21	1:B:184:LEU:HD11	1.83	0.43
1:A:37:ILE:HG21	1:A:93:GLY:O	2.19	0.43
1:A:403:GLN:CA	1:A:403:GLN:NE2	2.82	0.43
1:B:27:ALA:HB2	1:B:44:THR:HG22	2.01	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:B:326:ARG:HG3	1:B:348:ASP:OD2	2.17	0.43
1:B:282:ARG:NH1	1:B:282:ARG:CG	2.72	0.43
1:A:152:ARG:HA	1:A:203:ASN:OD1	2.19	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: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:295:TYR:OH	1:B:323:ASP:OD2	2.31	0.43
1:B:303:GLN:NE2	1:B:305:LYS:HE3	2.34	0.43
1:B:204:GLN:HG3	1:B:205:TRP:N	2.32	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: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:106:THR:O	1:A:106:THR:HG22	2.17	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:360:SER:HB2	1:A:361:ILE:HD12	2.02	0.42
1:B:8:PHE:CE2	1:B:32:ARG:HD3	2.54	0.42
1:A:135:ARG:NH1	1:A:137:ASN:O	2.42	0.42
1:B:342:ARG:NH1	3:B:465:HOH:O	2.52	0.42
1:A:47:ALA:HA	1:A:81:ASN:O	2.19	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:155:ILE:O	1:A:199:HIS:HA	2.19	0.42
1:B:5:LEU:CD2	1:B:32:ARG:HH21	2.31	0.42
1:A:184:LEU:C	1:A:184:LEU:HD23	2.39	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:141:SER:HB2	1:B:214:LEU:HB3	2.02	0.42
1:B:91:GLN:HG2	1:B:91:GLN:H	1.41	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:54:PRO:CD	1:B:75:PRO:O	2.68	0.42
1:B:322:LYS:NZ	1:B:351:PRO:C	2.73	0.42
1:B:41:ASP:C	1:B:87:PRO:HG3	2.40	0.42
1:B:115:GLY:CA	3:B:464:HOH:O	2.68	0.42
1:B:281:ASN:O	1:B:283:VAL:HG13	2.19	0.42
1:A:353:PRO:CB	1:A:355:GLN:HE22	2.33	0.42
1:A:215:TYR:CD1	1:A:215:TYR:C	2.93	0.42
1:A:190:GLY:O	1:A:191:ILE:C	2.58	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:B:305:LYS:CE	1:B:316:GLN:NE2	2.83	0.41
1:A:306:ALA:O	1:A:314:LEU:HB2	2.21	0.41
1:B:37:ILE:HG21	1:B:93:GLY:C	2.40	0.41
1:B:295:TYR:CD1	1:B:325:TYR:CE2	3.08	0.41
1:B:302:GLN:HA	1:B:320:GLY:HA2	2.02	0.41
1:B:179:GLN:H	1:B:179:GLN:HG2	1.64	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:345:ILE:HG12	1:A:369:LEU:CD1	2.51	0.41
1:B:44:THR:N	1:B:85:VAL:O	2.44	0.41
1:A:238:ASN:HB2	1:A:262:THR:HG23	2.02	0.41
1:A:46:SER:OG	1:A:418:ASN:ND2	2.53	0.41
1:B:282:ARG:HD2	1:B:287:TRP:O	2.21	0.41
1:A:155:ILE:HD11	1:A:304:LEU:HD21	2.01	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:H	1:B:230:GLU:HG2	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:B:200:LEU:O	1:B:201:ASN:CB	2.58	0.41
1:A:27:ALA:HB2	1:A:44:THR:HG22	2.03	0.41
1:A:183:ALA:HA	3:A:469:HOH:O	2.20	0.41
1:A:298:TRP:O	1:A:321:PHE:CB	2.62	0.41
1:A:254:ILE:HG13	1:A:254:ILE:H	1.65	0.41
1:A:33:ASN:HA	1:A:34:PRO:HD3	1.89	0.41
1:A:5:LEU:CD2	1:A:32:ARG:HH21	2.33	0.41
1:B:306:ALA:HB3	1:B:315:PHE:HB3	2.03	0.41
1:A:209:TRP:H	1:A:229:SER:HB3	1.86	0.41
1:A:273:GLU:HG2	1:A:297:SER:OG	2.21	0.41
1:B:322:LYS:HE2	3:B:441:HOH:O	2.20	0.41
1:A:45:PHE:HD1	1:A:46:SER:N	2.19	0.41
1:B:45:PHE:HD1	1:B:46:SER:N	2.19	0.41
1:B:10:SER:H	1:B:416:ASN:ND2	2.19	0.41
1:B:364:GLN:HE21	1:B:393:GLN:N	2.19	0.41
1:B:106:THR:HG22	1:B:106:THR:O	2.20	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:288:ALA:HB2	1:B:334:TYR:CE1	2.57	0.40
1:B:98:ILE:CG1	1:B:128:LEU:HD23	2.34	0.40
1:B:109:ASN:C	1:B:111:THR:N	2.75	0.40
1:B:282:ARG:NH2	1:B:285:PRO:O	2.52	0.40
1:A:37:ILE:HG21	1:A:93:GLY:C	2.41	0.40
1:B:308:SER:HB3	1:B:314:LEU:HD11	2.01	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:A:384:ASP:OD2	1:A:418:ASN:OD1	2.39	0.40
1:B:298:TRP:C	1:B:300:GLN:H	2.21	0.40
1:A:358:SER:HB2	3:A:462:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	419/427 (98%)	346 (83%)	57 (14%)	16 (4%)	4 13
1	B	419/427 (98%)	340 (81%)	58 (14%)	21 (5%)	3 8
All	All	838/854 (98%)	686 (82%)	115 (14%)	37 (4%)	3 10

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	331/337 (98%)	290 (88%)	41 (12%)	6 17
1	B	331/337 (98%)	282 (85%)	49 (15%)	4 11
All	All	662/674 (98%)	572 (86%)	90 (14%)	5 14

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	A	428	-	15,15,15	3.85	2 (13%)	16,17,17	2.47	5 (31%)
2	LDA	B	428	-	15,15,15	4.10	2 (13%)	16,17,17	2.21	5 (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
2	LDA	A	428	-	-	0/13/13/13	0/0/0/0
2	LDA	B	428	-	-	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	B	428	LDA	O1-N1	-15.01	1.25	1.39
2	A	428	LDA	O1-N1	-13.90	1.26	1.39
2	A	428	LDA	CM2-N1	-4.81	1.42	1.49
2	B	428	LDA	CM2-N1	-4.78	1.42	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	428	LDA	CM2-N1-CM1	-6.63	101.35	108.83
2	B	428	LDA	CM2-N1-CM1	-5.83	102.25	108.83
2	B	428	LDA	CM1-N1-C1	-2.45	101.89	109.77
2	A	428	LDA	CM1-N1-C1	-2.25	102.51	109.77
2	B	428	LDA	C9-C8-C7	-2.14	103.47	114.53
2	A	428	LDA	C9-C8-C7	-2.10	103.68	114.53
2	B	428	LDA	O1-N1-CM2	2.78	112.76	109.05
2	A	428	LDA	O1-N1-CM2	3.61	113.88	109.05
2	B	428	LDA	O1-N1-C1	3.99	114.76	110.27
2	A	428	LDA	O1-N1-C1	4.53	115.38	110.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

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

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	421/427 (98%)	0.33	5 (1%)	81	73	24, 41, 52, 63	0
1	B	421/427 (98%)	0.35	11 (2%)	59	47	26, 43, 59, 91	0
All	All	842/854 (98%)	0.34	16 (1%)	70	59	24, 41, 56, 91	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	3.7
1	B	179	GLN	3.3
1	B	177	GLN	3.2
1	B	421	PHE	3.0
1	A	1	ALA	2.9
1	B	170	ILE	2.7
1	B	136	LEU	2.5
1	A	421	PHE	2.3
1	A	401	PRO	2.3
1	B	172	GLN	2.2
1	A	136	LEU	2.1
1	B	78	TRP	2.1
1	B	166	VAL	2.0
1	B	200	LEU	2.0
1	B	90	ASP	2.0
1	A	159	ALA	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	LDA	A	428	16/16	0.91	0.46	5.14	56,60,72,73	0
2	LDA	B	428	16/16	0.87	0.35	2.21	53,57,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.