Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 08:34 AM EDT

PDB ID	:	2R4L
Title	:	Crystal structure of the long-chain fatty acid transporter FadL mutant P34A
Authors	:	Hearn, E.M.; Patel, D.R.; Lepore, B.W.; Indic, M.; van den Berg, B.
Deposited on	:	2007-08-31
Resolution	:	3.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

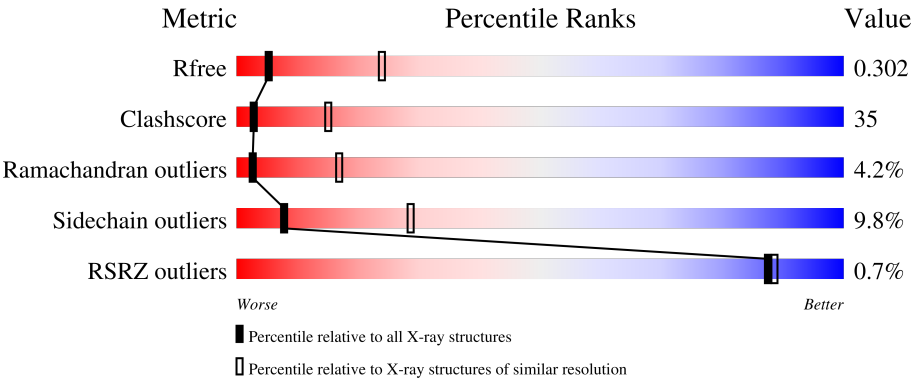
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 of 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 <=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	% 50% 41% 5% .
1	B	427	% 44% 45% 9% .
1	C	427	43% 48% 7% .

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	506	-	-	X	-
2	LDA	B	503	-	-	X	-
2	LDA	C	501	-	-	X	-
2	LDA	C	502	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9740 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	412	Total	C	N	O	S	0	0	0
			3184	2016	539	623	6			
1	B	421	Total	C	N	O	S	0	0	0
			3249	2053	552	638	6			
1	C	416	Total	C	N	O	S	0	0	0
			3211	2032	544	629	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	PRO	engineered mutation	UNP P10384
A	197	THR	ILE	conflict	UNP P10384
A	422	HIS	-	expression tag	UNP P10384
A	423	HIS	-	expression tag	UNP P10384
A	424	HIS	-	expression tag	UNP P10384
A	425	HIS	-	expression tag	UNP P10384
A	426	HIS	-	expression tag	UNP P10384
A	427	HIS	-	expression tag	UNP P10384
B	34	ALA	PRO	engineered mutation	UNP P10384
B	197	THR	ILE	conflict	UNP P10384
B	422	HIS	-	expression tag	UNP P10384
B	423	HIS	-	expression tag	UNP P10384
B	424	HIS	-	expression tag	UNP P10384
B	425	HIS	-	expression tag	UNP P10384
B	426	HIS	-	expression tag	UNP P10384
B	427	HIS	-	expression tag	UNP P10384
C	34	ALA	PRO	engineered mutation	UNP P10384
C	197	THR	ILE	conflict	UNP P10384
C	422	HIS	-	expression tag	UNP P10384
C	423	HIS	-	expression tag	UNP P10384
C	424	HIS	-	expression tag	UNP P10384
C	425	HIS	-	expression tag	UNP P10384
C	426	HIS	-	expression tag	UNP P10384

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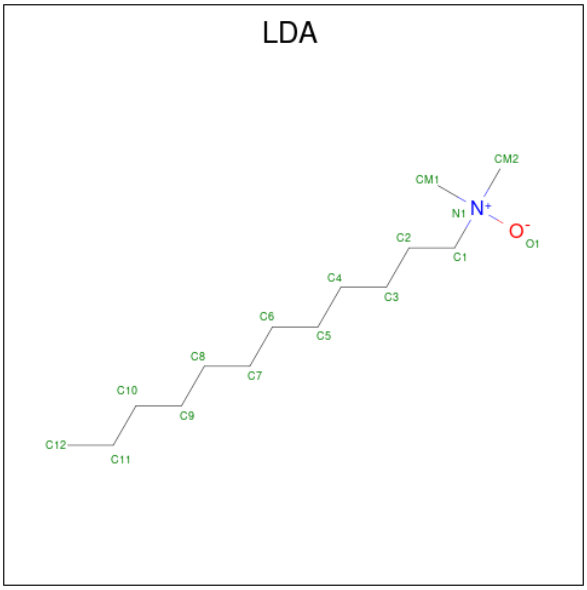
Chain	Residue	Modelled	Actual	Comment	Reference
C	427	HIS	-	expression tag	UNP P10384

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



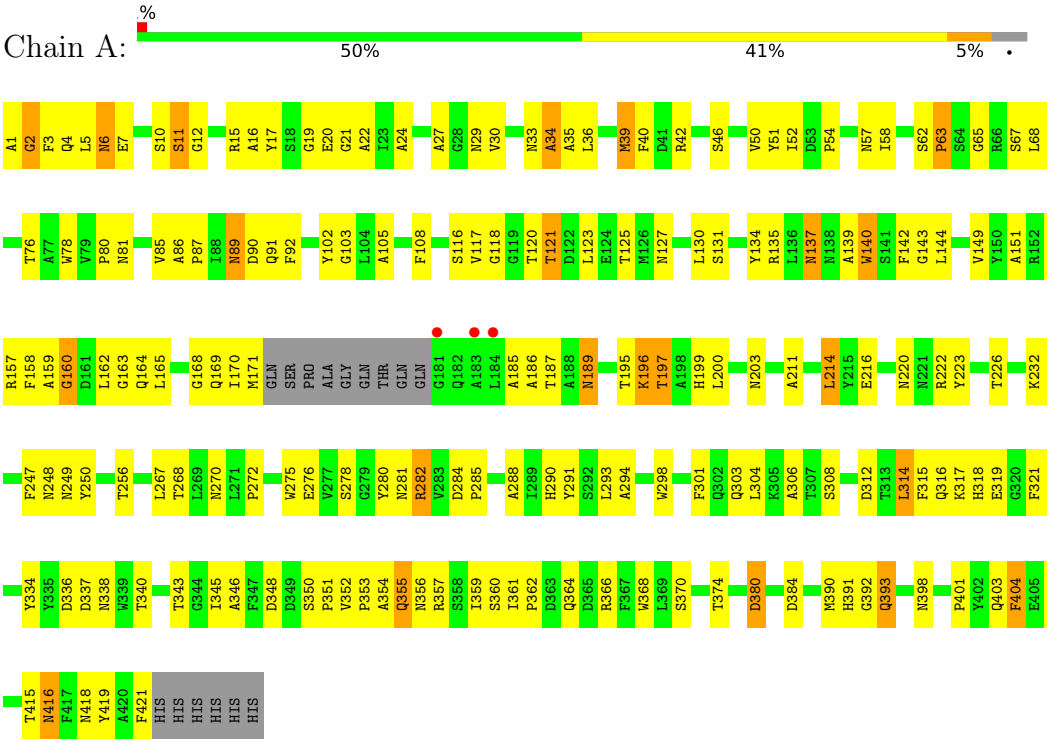
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		

3 Residue-property plots (i)

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

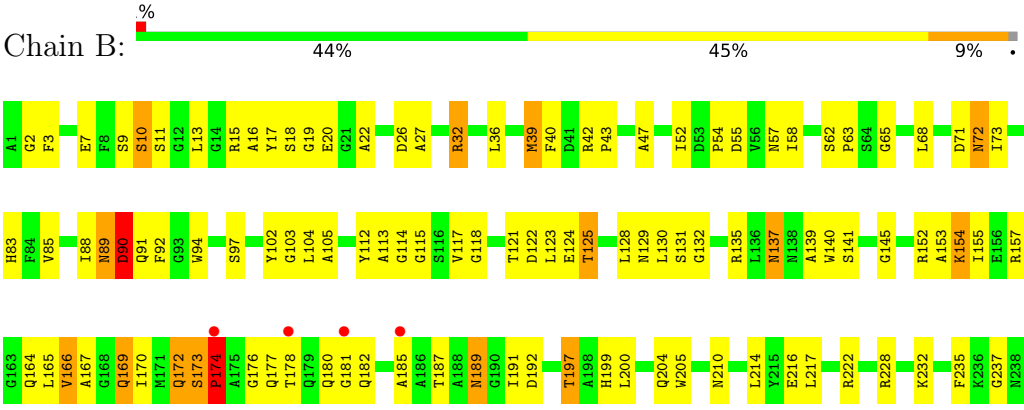
• Molecule 1: Long-chain fatty acid transport protein

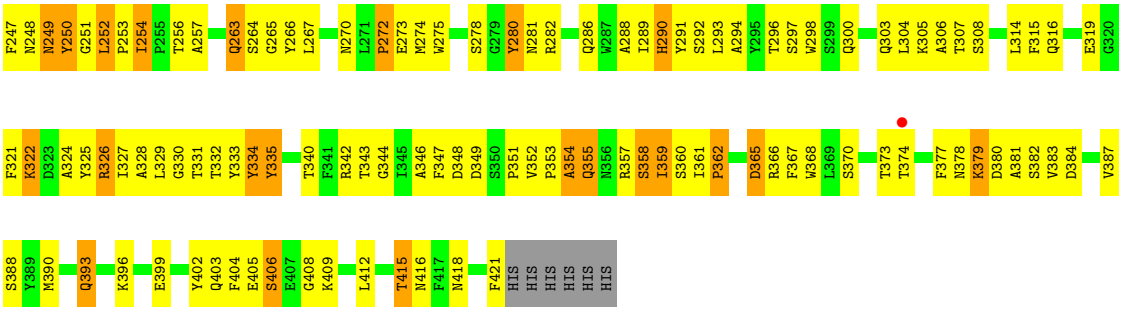
Chain A:



• Molecule 1: Long-chain fatty acid transport protein

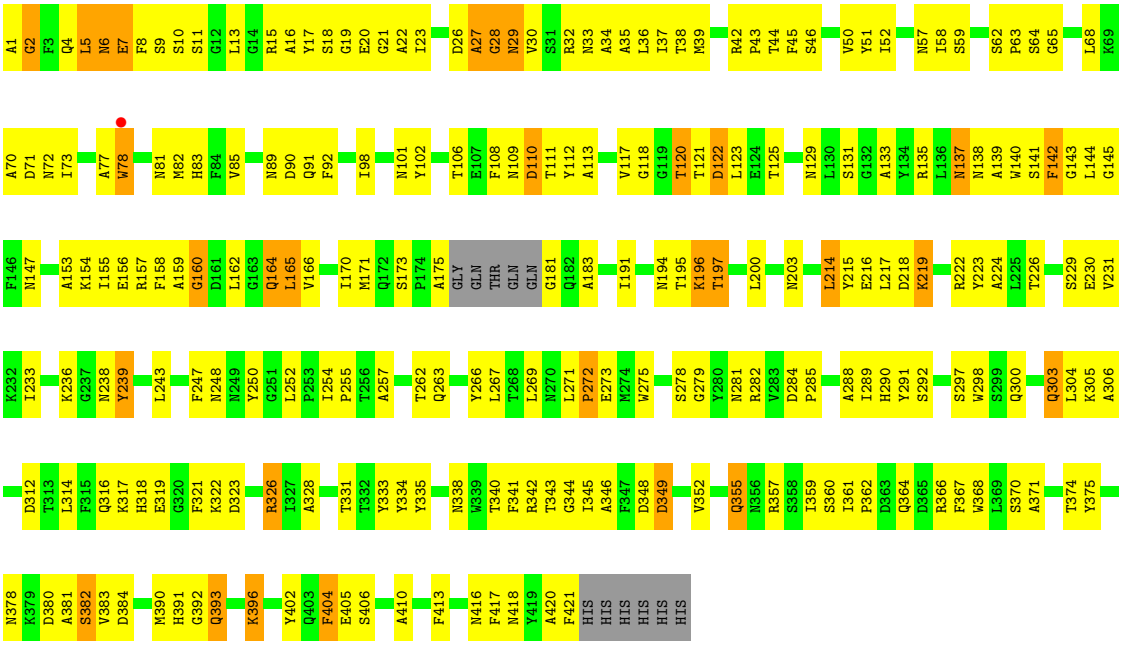
Chain B:





• Molecule 1: Long-chain fatty acid transport protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	112.80Å 167.04Å 197.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.30 48.40 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (10.00-3.30) 94.8 (48.40-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.302 0.240 , 0.302	Depositor DCC
R_{free} test set	2721 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 28.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	9740	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.49	0/3270	0.74	0/4450
1	B	0.47	0/3337	0.71	0/4543
1	C	0.47	0/3298	0.74	0/4489
All	All	0.48	0/9905	0.73	0/13482

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	TYR	Sidechain
1	C	239	TYR	Sidechain

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	3184	0	2967	194	0
1	B	3249	0	3027	222	0
1	C	3211	0	2992	254	0
2	A	32	0	62	18	0
2	B	32	0	62	11	0
2	C	32	0	62	19	0
All	All	9740	0	9172	668	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 35.

All (668) 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:C:34:ALA:O	1:C:143:GLY:HA3	1.46	1.15
1:C:361:ILE:HD11	2:C:501:LDA:H22	1.22	1.10
1:C:58:ILE:HB	1:C:70:ALA:HB3	1.39	1.05
1:B:346:ALA:HB3	1:B:368:TRP:HB2	1.40	1.03
1:B:252:LEU:HB3	1:B:254:ILE:HG12	1.41	1.00
1:B:382:SER:HB3	1:B:418:ASN:HB2	1.45	0.96
1:C:64:SER:HB3	1:C:165:LEU:HD21	1.49	0.94
1:C:10:SER:H	1:C:416:ASN:HD22	1.18	0.92
1:A:293:LEU:HD13	1:A:327:ILE:HG12	1.49	0.92
1:A:10:SER:OG	1:A:416:ASN:HB2	1.70	0.91
1:C:21:GLY:HA2	1:C:36:LEU:HD11	1.50	0.90
1:C:10:SER:H	1:C:416:ASN:ND2	1.68	0.90
1:A:21:GLY:H	1:A:29:ASN:HD22	1.17	0.89
1:A:117:VAL:HG23	1:A:359:ILE:HD11	1.55	0.88
1:B:293:LEU:HD13	1:B:327:ILE:CD1	2.04	0.87
1:C:368:TRP:HZ2	2:C:502:LDA:HM23	1.39	0.87
1:C:303:GLN:HE22	1:C:316:GLN:HE21	1.22	0.87
1:B:63:PRO:HA	1:C:138:ASN:OD1	1.74	0.87
1:B:293:LEU:HD13	1:B:327:ILE:HD11	1.58	0.86
1:C:278:SER:HB3	1:C:292:SER:HB3	1.56	0.85
1:A:319:GLU:OE2	2:A:506:LDA:HM22	1.76	0.85
1:C:346:ALA:HB3	1:C:368:TRP:HB2	1.58	0.84
1:A:102:TYR:O	1:A:125:THR:HB	1.78	0.83
1:C:390:MET:HE1	2:C:502:LDA:HM22	1.61	0.83
1:A:354:ALA:O	1:A:355:GLN:HB2	1.78	0.82
1:A:343:THR:HG23	1:A:370:SER:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD23	1:A:268:THR:N	1.95	0.81
1:C:390:MET:HG3	1:C:410:ALA:HB3	1.60	0.81
1:B:319:GLU:OE1	2:B:503:LDA:HM21	1.82	0.80
1:C:361:ILE:HD11	2:C:501:LDA:C2	2.10	0.80
1:C:38:THR:HG21	1:C:141:SER:OG	1.81	0.79
1:C:110:ASP:O	1:C:194:ASN:HB3	1.82	0.79
1:C:21:GLY:H	1:C:29:ASN:HD22	1.27	0.79
1:C:131:SER:HB3	1:C:145:GLY:HA3	1.63	0.79
1:C:27:ALA:HB2	1:C:44:THR:HG22	1.63	0.79
1:A:89:ASN:ND2	1:A:90:ASP:H	1.81	0.79
1:B:306:ALA:HB3	1:B:315:PHE:HB3	1.63	0.78
1:A:196:LYS:HB2	1:A:242:ASP:OD2	1.84	0.78
1:A:164:GLN:HG3	1:A:189:ASN:ND2	1.99	0.78
1:B:102:TYR:O	1:B:125:THR:HB	1.85	0.77
1:C:281:ASN:HB2	1:C:289:ILE:HG23	1.66	0.76
1:A:4:GLN:C	1:A:5:LEU:HD12	2.06	0.76
1:A:153:ALA:CB	2:A:506:LDA:H91	2.16	0.76
1:C:157:ARG:HH12	2:C:501:LDA:HM22	1.51	0.75
1:B:62:SER:HB2	1:B:68:LEU:HD21	1.67	0.75
1:B:131:SER:HB3	1:B:145:GLY:HA2	1.69	0.75
1:A:200:LEU:HB3	2:A:506:LDA:H123	1.67	0.74
1:A:303:GLN:HE22	1:A:316:GLN:HE21	1.33	0.74
1:B:199:HIS:C	1:B:200:LEU:HD12	2.08	0.74
1:A:168:GLY:O	1:A:171:MET:HG2	1.88	0.74
1:C:137:ASN:HD21	1:C:140:TRP:H	1.34	0.73
1:A:276:GLU:HG3	1:A:294:ALA:HB2	1.70	0.73
1:C:137:ASN:HD21	1:C:140:TRP:N	1.86	0.73
1:C:164:GLN:O	1:C:166:VAL:N	2.20	0.73
1:C:131:SER:HB3	1:C:145:GLY:CA	2.18	0.73
1:C:278:SER:HB3	1:C:292:SER:CB	2.19	0.72
1:B:154:LYS:HA	1:B:200:LEU:O	1.88	0.72
1:C:137:ASN:HD22	1:C:137:ASN:C	1.92	0.72
1:C:281:ASN:ND2	1:C:291:TYR:HE2	1.88	0.72
1:B:19:GLY:H	1:B:292:SER:HB3	1.55	0.72
1:C:338:ASN:HB3	1:C:375:TYR:HE1	1.55	0.72
1:B:273:GLU:H	1:B:300:GLN:NE2	1.88	0.72
1:B:42:ARG:HD2	1:B:421:PHE:O	1.91	0.71
1:C:102:TYR:O	1:C:125:THR:HB	1.89	0.71
1:C:254:ILE:HG13	1:C:255:PRO:HD2	1.72	0.71
1:B:65:GLY:C	1:C:91:GLN:HE21	1.94	0.71
1:B:396:LYS:H	1:B:396:LYS:HD2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LYS:HD2	1:B:396:LYS:N	2.06	0.70
1:B:393:GLN:HA	1:B:393:GLN:HE21	1.55	0.70
1:A:17:TYR:HA	1:A:20:GLU:OE1	1.90	0.70
1:A:5:LEU:HA	2:A:505:LDA:HM13	1.72	0.70
1:C:5:LEU:HD22	1:C:6:ASN:H	1.57	0.70
1:A:364:GLN:HG3	1:A:393:GLN:O	1.91	0.69
1:B:346:ALA:HB3	1:B:368:TRP:CB	2.20	0.69
1:C:20:GLU:OE2	1:C:20:GLU:HA	1.92	0.69
1:A:232:LYS:HE2	1:A:270:ASN:ND2	2.07	0.69
1:B:303:GLN:HE22	1:B:316:GLN:NE2	1.90	0.69
1:C:21:GLY:CA	1:C:36:LEU:HD11	2.20	0.69
1:A:352:VAL:HG11	1:A:357:ARG:HA	1.75	0.69
1:A:415:THR:HG22	1:A:416:ASN:H	1.57	0.68
1:B:178:THR:HG22	1:B:180:GLN:H	1.56	0.68
1:C:374:THR:HG23	1:C:384:ASP:OD2	1.94	0.68
1:B:378:ASN:O	1:B:379:LYS:HB2	1.94	0.68
1:C:52:ILE:HG21	2:C:502:LDA:H52	1.76	0.68
1:C:393:GLN:HE21	1:C:393:GLN:HA	1.58	0.68
1:C:27:ALA:O	1:C:30:VAL:HG22	1.94	0.67
1:C:7:GLU:HG2	1:C:50:VAL:HG11	1.76	0.67
1:B:131:SER:HB3	1:B:145:GLY:CA	2.24	0.67
1:C:303:GLN:HE22	1:C:316:GLN:NE2	1.92	0.66
1:B:135:ARG:HG3	1:B:137:ASN:O	1.95	0.66
1:C:338:ASN:HB3	1:C:375:TYR:CE1	2.31	0.66
1:C:281:ASN:HB2	1:C:289:ILE:CG2	2.26	0.66
1:A:33:ASN:HB2	1:A:226:THR:HG21	1.78	0.66
1:B:199:HIS:O	1:B:200:LEU:HD12	1.96	0.66
1:B:17:TYR:HA	1:B:20:GLU:OE1	1.96	0.65
1:B:272:PRO:HA	1:B:300:GLN:HE21	1.59	0.65
1:A:89:ASN:HD22	1:A:90:ASP:H	1.44	0.65
1:B:306:ALA:O	1:B:314:LEU:HB2	1.97	0.65
1:C:7:GLU:HA	1:C:17:TYR:OH	1.96	0.65
1:A:326:ARG:HG3	1:A:348:ASP:HB3	1.76	0.65
1:B:10:SER:HB3	1:B:416:ASN:ND2	2.12	0.65
1:B:68:LEU:HD13	1:B:404:PHE:CE2	2.32	0.65
1:C:305:LYS:HD2	1:C:316:GLN:NE2	2.12	0.65
1:B:137:ASN:HD21	1:B:140:TRP:H	1.44	0.65
1:B:170:ILE:HG21	1:B:185:ALA:HB2	1.79	0.65
1:C:346:ALA:HB3	1:C:368:TRP:CB	2.28	0.64
1:A:67:SER:C	1:A:68:LEU:HD23	2.18	0.64
1:C:173:SER:O	1:C:175:ALA:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASP:O	1:C:194:ASN:CB	2.45	0.64
1:B:237:GLY:O	1:B:265:GLY:N	2.30	0.63
1:C:157:ARG:HB2	1:C:197:THR:HG22	1.80	0.63
1:C:380:ASP:HA	1:C:420:ALA:HB3	1.81	0.63
1:A:7:GLU:OE1	1:A:7:GLU:N	2.32	0.63
1:A:284:ASP:OD1	1:A:285:PRO:HD2	1.98	0.63
1:C:6:ASN:O	1:C:7:GLU:HB2	1.98	0.63
1:B:52:ILE:O	1:B:54:PRO:HD3	1.99	0.62
1:B:293:LEU:HD13	1:B:327:ILE:HD13	1.80	0.62
1:A:360:SER:C	1:A:362:PRO:HD3	2.20	0.62
1:C:238:ASN:HD22	1:C:262:THR:HG21	1.63	0.62
1:C:396:LYS:H	1:C:396:LYS:HD2	1.65	0.62
1:C:137:ASN:C	1:C:137:ASN:ND2	2.52	0.62
1:C:321:PHE:CE2	1:C:352:VAL:HG22	2.34	0.62
1:A:303:GLN:HE22	1:A:316:GLN:NE2	1.95	0.62
1:B:137:ASN:ND2	1:B:139:ALA:H	1.96	0.62
1:A:42:ARG:HD2	1:A:421:PHE:O	1.99	0.62
1:A:415:THR:HG22	1:A:416:ASN:N	2.13	0.62
1:B:32:ARG:HG2	1:B:32:ARG:HH11	1.65	0.62
1:C:10:SER:N	1:C:416:ASN:HD22	1.94	0.61
1:C:106:THR:HG21	1:C:360:SER:HA	1.81	0.61
1:C:272:PRO:HA	1:C:300:GLN:HE21	1.66	0.61
1:C:303:GLN:NE2	1:C:316:GLN:HE21	1.94	0.61
1:C:159:ALA:O	1:C:160:GLY:C	2.38	0.61
1:A:92:PHE:CE2	1:A:134:TYR:HB2	2.36	0.60
1:A:398:ASN:OD1	1:A:403:GLN:HG3	2.00	0.60
1:A:360:SER:O	1:A:362:PRO:HD3	2.02	0.60
1:B:228:ARG:HB3	1:B:274:MET:HB3	1.84	0.60
1:C:352:VAL:HG11	1:C:357:ARG:HA	1.84	0.60
1:B:57:ASN:HD22	1:B:71:ASP:HA	1.67	0.60
1:C:26:ASP:HB2	1:C:418:ASN:ND2	2.17	0.59
1:A:308:SER:HB3	1:A:314:LEU:HD11	1.83	0.59
1:C:19:GLY:H	1:C:292:SER:CB	2.15	0.59
1:C:51:TYR:N	1:C:413:PHE:O	2.21	0.59
1:A:304:LEU:HD11	2:A:506:LDA:H32	1.85	0.59
1:A:345:ILE:HA	1:A:368:TRP:O	2.02	0.59
1:B:358:SER:HB2	1:B:399:GLU:CD	2.22	0.59
1:A:243:LEU:HD22	1:A:247:PHE:CE1	2.38	0.59
1:B:10:SER:CB	1:B:416:ASN:HD22	2.16	0.59
1:C:18:SER:OG	1:C:290:HIS:HD2	1.85	0.59
1:A:12:GLY:HA2	1:A:15:ARG:CZ	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:O	1:B:91:GLN:N	2.35	0.59
1:C:38:THR:HG21	1:C:141:SER:HG	1.68	0.59
1:B:281:ASN:HB2	1:B:289:ILE:HG23	1.84	0.58
1:A:319:GLU:HB3	1:A:321:PHE:CE2	2.37	0.58
1:B:396:LYS:HG3	1:B:405:GLU:OE2	2.04	0.58
1:C:155:ILE:HD11	2:C:501:LDA:H62	1.86	0.58
1:B:347:PHE:HE1	1:B:365:ASP:HB3	1.69	0.58
1:C:120:THR:HG23	1:C:122:ASP:OD1	2.03	0.58
1:C:236:LYS:HE3	1:C:266:TYR:OH	2.04	0.58
1:C:378:ASN:OD1	1:C:380:ASP:N	2.35	0.58
1:A:293:LEU:CD1	1:A:327:ILE:HG12	2.29	0.58
1:B:273:GLU:N	1:B:300:GLN:NE2	2.51	0.58
1:A:355:GLN:C	1:A:356:ASN:HD22	2.06	0.58
1:B:55:ASP:HB3	1:B:409:LYS:HG2	1.85	0.58
1:A:62:SER:O	1:A:65:GLY:N	2.33	0.58
1:C:29:ASN:HB3	1:C:36:LEU:CD1	2.34	0.58
1:A:39:MET:HE1	1:A:216:GLU:OE1	2.03	0.58
1:B:157:ARG:HB2	1:B:197:THR:HG22	1.85	0.58
1:B:170:ILE:HD12	1:B:185:ALA:HB2	1.84	0.58
1:C:191:ILE:HD11	1:C:247:PHE:CZ	2.38	0.58
1:A:58:ILE:HB	1:A:70:ALA:HB3	1.86	0.58
1:B:27:ALA:HA	1:B:40:PHE:CZ	2.39	0.58
1:C:239:TYR:CD2	1:C:314:LEU:HD23	2.39	0.58
1:C:223:TYR:HA	1:C:279:GLY:HA2	1.85	0.57
1:A:135:ARG:NH2	1:A:216:GLU:OE2	2.37	0.57
1:A:195:THR:O	1:A:197:THR:N	2.36	0.57
1:C:35:ALA:C	1:C:37:ILE:H	2.07	0.57
1:C:368:TRP:HZ2	2:C:502:LDA:CM2	2.16	0.57
1:B:81:ASN:HD21	1:B:416:ASN:HD21	1.52	0.57
1:B:402:TYR:HB2	1:B:404:PHE:CE1	2.39	0.57
1:C:267:LEU:HD12	1:C:306:ALA:HB2	1.86	0.57
1:A:33:ASN:C	1:A:35:ALA:H	2.08	0.57
1:A:304:LEU:HD12	2:A:506:LDA:HM21	1.86	0.57
1:A:155:ILE:HD11	2:A:506:LDA:H81	1.86	0.57
1:B:26:ASP:O	1:B:40:PHE:HZ	1.88	0.57
1:A:354:ALA:HA	1:A:357:ARG:CG	2.35	0.57
1:A:7:GLU:HG2	1:A:50:VAL:HG11	1.87	0.57
1:A:19:GLY:O	1:A:22:ALA:HB3	2.05	0.57
1:A:27:ALA:HB1	1:A:85:VAL:HG23	1.87	0.57
1:B:324:ALA:HB2	1:B:351:PRO:HG3	1.87	0.57
1:C:281:ASN:ND2	1:C:291:TYR:CE2	2.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ALA:HB1	1:B:85:VAL:HG23	1.86	0.56
1:A:153:ALA:HB1	2:A:506:LDA:H91	1.85	0.56
1:A:153:ALA:HB3	2:A:506:LDA:H91	1.86	0.56
1:A:391:HIS:ND1	1:A:392:GLY:N	2.53	0.56
1:A:411:TRP:C	1:A:412:LEU:HD12	2.26	0.56
1:B:57:ASN:ND2	1:B:71:ASP:HA	2.20	0.56
1:B:88:ILE:HB	1:B:92:PHE:O	2.05	0.56
1:C:137:ASN:ND2	1:C:139:ALA:N	2.53	0.56
1:C:273:GLU:H	1:C:300:GLN:NE2	2.03	0.56
1:B:104:LEU:HG	1:B:105:ALA:N	2.20	0.56
1:A:21:GLY:H	1:A:29:ASN:ND2	1.96	0.56
1:B:272:PRO:HG2	1:B:298:TRP:CE3	2.41	0.56
1:B:346:ALA:CB	1:B:368:TRP:HB2	2.27	0.56
1:C:36:LEU:HD23	1:C:214:LEU:HD13	1.88	0.56
1:C:266:TYR:O	1:C:306:ALA:HA	2.05	0.56
1:B:304:LEU:HD13	2:B:503:LDA:H12	1.88	0.56
1:B:390:MET:SD	2:B:504:LDA:CM2	2.94	0.56
1:C:254:ILE:HG23	1:C:255:PRO:O	2.06	0.56
1:C:250:TYR:C	1:C:252:LEU:H	2.09	0.55
1:B:367:PHE:O	1:B:390:MET:HA	2.05	0.55
1:C:191:ILE:HD11	1:C:247:PHE:HZ	1.72	0.55
1:A:11:SER:HB2	1:A:384:ASP:OD1	2.06	0.55
1:B:170:ILE:CD1	1:B:185:ALA:HB2	2.37	0.55
1:C:166:VAL:O	1:C:170:ILE:HG13	2.07	0.55
1:C:281:ASN:HD22	1:C:291:TYR:HE2	1.54	0.55
1:C:21:GLY:O	1:C:36:LEU:HD21	2.06	0.55
1:C:360:SER:OG	2:C:501:LDA:HM21	2.07	0.55
1:C:367:PHE:O	1:C:390:MET:HA	2.06	0.55
1:A:12:GLY:HA2	1:A:15:ARG:NH1	2.21	0.55
1:B:159:ALA:O	1:B:160:GLY:C	2.44	0.55
1:C:368:TRP:CZ2	2:C:502:LDA:HM23	2.31	0.55
1:A:89:ASN:ND2	1:A:90:ASP:N	2.52	0.55
1:B:280:TYR:C	1:B:280:TYR:CD2	2.79	0.55
1:C:223:TYR:CD2	1:C:279:GLY:HA3	2.41	0.55
1:C:304:LEU:HD11	2:C:501:LDA:H32	1.89	0.55
1:A:5:LEU:HD13	1:A:103:GLY:N	2.21	0.55
1:A:57:ASN:ND2	1:A:71:ASP:HA	2.22	0.55
1:A:336:ASP:O	1:A:338:ASN:N	2.40	0.55
1:C:10:SER:CB	1:C:416:ASN:HD22	2.20	0.55
1:C:142:PHE:N	1:C:142:PHE:CD1	2.74	0.55
1:B:13:LEU:HA	1:B:17:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:THR:HG23	1:B:384:ASP:OD2	2.07	0.55
1:B:216:GLU:HA	1:B:222:ARG:HA	1.88	0.55
1:C:343:THR:HG23	1:C:370:SER:O	2.07	0.54
1:A:312:ASP:O	1:A:314:LEU:HD13	2.08	0.54
1:B:83:HIS:HA	1:B:97:SER:HB3	1.90	0.54
1:B:358:SER:HB2	1:B:399:GLU:OE1	2.07	0.54
1:B:304:LEU:CD1	2:B:503:LDA:H11	2.38	0.54
1:B:384:ASP:O	1:B:415:THR:HA	2.08	0.54
1:A:90:ASP:O	1:A:91:GLN:HG2	2.07	0.54
1:B:374:THR:HG23	1:B:383:VAL:O	2.08	0.54
1:B:153:ALA:HB3	2:B:503:LDA:H102	1.89	0.54
1:B:58:ILE:CD1	1:B:406:SER:HB2	2.38	0.54
1:A:364:GLN:N	1:A:364:GLN:OE1	2.39	0.54
1:A:67:SER:O	1:A:68:LEU:HD23	2.08	0.54
1:A:361:ILE:HG13	2:A:506:LDA:H22	1.90	0.54
1:B:329:LEU:HD12	1:B:330:GLY:H	1.72	0.54
1:B:16:ALA:O	1:B:326:ARG:NH2	2.41	0.54
1:B:303:GLN:HE22	1:B:316:GLN:HE21	1.51	0.54
1:C:326:ARG:HG3	1:C:326:ARG:HH11	1.73	0.54
1:A:419:TYR:HE2	1:A:421:PHE:CE1	2.26	0.53
1:B:65:GLY:C	1:C:91:GLN:NE2	2.62	0.53
1:C:273:GLU:HG2	1:C:300:GLN:OE1	2.09	0.53
1:C:10:SER:N	1:C:416:ASN:ND2	2.49	0.53
1:C:254:ILE:HG13	1:C:255:PRO:CD	2.36	0.53
1:A:170:ILE:HG22	1:A:170:ILE:O	2.09	0.53
1:A:155:ILE:CD1	2:A:506:LDA:H81	2.38	0.53
1:B:352:VAL:HG11	1:B:357:ARG:HA	1.91	0.53
1:A:151:ALA:CB	1:A:233:ILE:HD13	2.39	0.53
1:A:199:HIS:C	1:A:200:LEU:HD12	2.29	0.53
1:C:238:ASN:HB3	1:C:262:THR:HG23	1.90	0.53
1:C:319:GLU:OE1	2:C:501:LDA:HM13	2.08	0.53
1:C:342:ARG:NH1	1:C:374:THR:OG1	2.38	0.53
1:A:140:TRP:HA	1:A:214:LEU:O	2.09	0.53
1:A:33:ASN:O	1:A:35:ALA:N	2.38	0.52
1:A:137:ASN:HD21	1:A:140:TRP:HD1	1.56	0.52
1:B:294:ALA:HB3	1:B:326:ARG:HB3	1.91	0.52
1:C:238:ASN:HB3	1:C:262:THR:CG2	2.39	0.52
1:C:272:PRO:HA	1:C:300:GLN:NE2	2.24	0.52
1:C:390:MET:O	1:C:410:ALA:N	2.43	0.52
1:A:108:PHE:HB2	1:A:118:GLY:O	2.08	0.52
1:B:243:LEU:HD22	1:B:247:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:SER:C	1:B:362:PRO:HD3	2.30	0.52
1:C:18:SER:HA	1:C:292:SER:OG	2.09	0.52
1:A:276:GLU:HG3	1:A:294:ALA:CB	2.38	0.52
1:A:281:ASN:O	1:A:288:ALA:HA	2.09	0.52
1:A:359:ILE:O	1:A:362:PRO:HG3	2.08	0.52
1:B:176:GLY:O	1:B:182:GLN:HG3	2.08	0.52
1:B:303:GLN:NE2	1:B:316:GLN:HE21	2.07	0.52
1:A:361:ILE:HD11	2:A:506:LDA:H31	1.92	0.52
1:B:308:SER:HB3	1:B:314:LEU:HD11	1.92	0.52
1:A:2:GLY:H	1:A:351:PRO:CG	2.23	0.52
1:B:94:TRP:HA	1:B:132:GLY:HA2	1.92	0.52
1:C:297:SER:HA	1:C:323:ASP:OD2	2.09	0.52
1:B:47:ALA:HA	1:B:81:ASN:O	2.09	0.52
1:A:5:LEU:CD1	1:A:103:GLY:N	2.73	0.52
1:B:19:GLY:HA2	1:B:278:SER:HB2	1.92	0.52
1:C:15:ARG:NH1	1:C:20:GLU:OE1	2.43	0.52
1:B:326:ARG:HB2	1:B:348:ASP:HB2	1.92	0.52
1:A:69:LYS:HE2	1:A:71:ASP:OD2	2.10	0.51
1:B:319:GLU:HB3	1:B:321:PHE:CE2	2.44	0.51
1:A:58:ILE:HD13	1:A:406:SER:HB2	1.92	0.51
1:A:19:GLY:HA3	1:A:290:HIS:HB2	1.93	0.51
1:A:267:LEU:HD23	1:A:267:LEU:C	2.31	0.51
1:A:355:GLN:C	1:A:356:ASN:ND2	2.63	0.51
1:B:173:SER:CB	1:B:174:PRO:HD2	2.38	0.51
1:A:5:LEU:HA	2:A:505:LDA:CM1	2.38	0.51
1:B:173:SER:HB2	1:B:174:PRO:HD2	1.91	0.51
1:C:9:SER:OG	1:C:11:SER:HB3	2.11	0.51
1:C:16:ALA:HB1	1:C:346:ALA:HB2	1.92	0.51
1:C:20:GLU:HB2	1:C:32:ARG:HD3	1.93	0.51
1:C:89:ASN:OD1	1:C:92:PHE:HB2	2.10	0.51
1:B:166:VAL:HG12	1:B:166:VAL:O	2.10	0.51
1:B:204:GLN:OE1	1:B:205:TRP:N	2.34	0.51
1:A:140:TRP:CD1	1:A:140:TRP:N	2.78	0.51
1:B:172:GLN:O	1:B:173:SER:HB3	2.11	0.51
1:B:248:ASN:OD1	1:B:257:ALA:HB3	2.11	0.51
1:B:326:ARG:HD2	1:B:348:ASP:HB3	1.92	0.51
1:C:1:ALA:O	1:C:2:GLY:C	2.47	0.51
1:C:29:ASN:HB3	1:C:36:LEU:HD13	1.93	0.51
1:C:390:MET:CE	2:C:502:LDA:HM22	2.39	0.51
1:A:2:GLY:H	1:A:351:PRO:HG2	1.76	0.50
1:C:16:ALA:HB1	1:C:346:ALA:CB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LEU:HD12	1:B:330:GLY:N	2.26	0.50
1:B:252:LEU:HB3	1:B:254:ILE:CG1	2.29	0.50
1:C:396:LYS:H	1:C:396:LYS:CD	2.24	0.50
1:C:68:LEU:HD22	1:C:404:PHE:CE2	2.47	0.50
1:C:81:ASN:HD22	1:C:83:HIS:CE1	2.30	0.50
1:C:272:PRO:HG2	1:C:298:TRP:CD2	2.46	0.50
1:A:39:MET:HE3	1:A:216:GLU:OE2	2.12	0.50
1:A:137:ASN:HD22	1:A:137:ASN:H	1.59	0.50
1:A:351:PRO:O	1:A:353:PRO:HD3	2.12	0.50
1:B:18:SER:HB3	1:B:328:ALA:HB1	1.92	0.50
1:C:224:ALA:N	1:C:278:SER:O	2.42	0.50
1:A:137:ASN:HD21	1:A:139:ALA:HB3	1.75	0.50
1:C:42:ARG:HD2	1:C:421:PHE:O	2.12	0.50
1:C:51:TYR:HD1	1:C:78:TRP:HD1	1.60	0.50
1:B:239:TYR:CG	1:B:240:SER:N	2.80	0.50
1:C:82:MET:HE3	1:C:98:ILE:HD12	1.93	0.50
1:C:273:GLU:N	1:C:300:GLN:HE22	2.09	0.50
1:C:248:ASN:HD21	1:C:257:ALA:H	1.58	0.50
1:C:123:LEU:CD1	1:C:153:ALA:HB2	2.42	0.49
1:C:108:PHE:HB2	1:C:118:GLY:O	2.11	0.49
1:A:355:GLN:O	1:A:356:ASN:ND2	2.41	0.49
1:C:304:LEU:CD1	2:C:501:LDA:H11	2.43	0.49
1:A:220:ASN:HB3	1:A:282:ARG:CB	2.42	0.49
1:A:301:PHE:CE2	1:A:319:GLU:HG3	2.47	0.49
1:B:39:MET:HE1	1:B:135:ARG:HH22	1.77	0.49
1:A:354:ALA:HA	1:A:357:ARG:HG2	1.93	0.49
1:C:62:SER:O	1:C:65:GLY:N	2.29	0.49
1:C:137:ASN:ND2	1:C:139:ALA:H	2.09	0.49
1:C:164:GLN:CG	1:C:165:LEU:H	2.26	0.49
1:C:291:TYR:N	1:C:291:TYR:CD2	2.79	0.49
1:B:137:ASN:ND2	1:B:140:TRP:H	2.07	0.49
1:B:239:TYR:OH	1:B:256:THR:O	2.18	0.49
1:B:354:ALA:O	1:B:355:GLN:HB3	2.13	0.49
1:C:1:ALA:CB	1:C:4:GLN:HB3	2.43	0.49
1:C:20:GLU:CB	1:C:32:ARG:HD3	2.42	0.49
1:C:312:ASP:O	1:C:314:LEU:HD13	2.12	0.49
1:C:28:GLY:HA2	1:C:83:HIS:CD2	2.48	0.49
1:C:51:TYR:CD1	1:C:78:TRP:HD1	2.30	0.49
1:C:70:ALA:HB1	1:C:73:ILE:CG2	2.42	0.49
1:B:359:ILE:O	1:B:362:PRO:HG3	2.13	0.49
1:A:103:GLY:HA2	1:A:123:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:HA	1:A:197:THR:HB	1.95	0.48
1:C:156:GLU:OE2	1:C:196:LYS:HE2	2.13	0.48
1:C:223:TYR:HE2	1:C:291:TYR:HH	1.61	0.48
1:C:333:TYR:N	1:C:341:PHE:O	2.39	0.48
1:A:121:THR:OG1	1:A:157:ARG:NH2	2.45	0.48
1:A:306:ALA:HB3	1:A:315:PHE:HB3	1.94	0.48
1:B:177:GLN:HE21	1:B:177:GLN:HA	1.79	0.48
1:B:332:THR:HG22	1:B:334:TYR:CE1	2.48	0.48
1:C:19:GLY:HA2	1:C:278:SER:HB2	1.95	0.48
1:C:326:ARG:HG3	1:C:348:ASP:HB3	1.94	0.48
1:A:321:PHE:CE2	1:A:352:VAL:HG22	2.49	0.48
1:C:6:ASN:O	1:C:7:GLU:CB	2.60	0.48
1:C:157:ARG:CB	1:C:197:THR:HG22	2.43	0.48
1:A:352:VAL:CG1	1:A:357:ARG:HA	2.42	0.48
1:B:170:ILE:CG2	1:B:185:ALA:HB2	2.43	0.48
1:B:307:THR:O	1:B:314:LEU:HD22	2.13	0.48
1:C:33:ASN:HB2	1:C:226:THR:HG21	1.94	0.48
1:A:366:ARG:HD3	1:A:390:MET:HE3	1.94	0.48
1:B:9:SER:O	1:B:11:SER:N	2.40	0.48
1:C:35:ALA:C	1:C:37:ILE:N	2.67	0.48
1:B:137:ASN:C	1:B:137:ASN:HD22	2.17	0.48
1:C:1:ALA:HB1	1:C:4:GLN:HB3	1.96	0.48
1:C:20:GLU:HB2	1:C:32:ARG:CD	2.44	0.48
1:C:252:LEU:C	1:C:254:ILE:H	2.17	0.48
1:B:281:ASN:HB2	1:B:289:ILE:CG2	2.43	0.48
1:B:322:LYS:HG3	1:B:351:PRO:O	2.13	0.48
1:C:20:GLU:CB	1:C:32:ARG:CD	2.92	0.48
1:C:23:ILE:HG23	1:C:29:ASN:ND2	2.28	0.48
1:C:250:TYR:O	1:C:252:LEU:N	2.47	0.48
1:A:354:ALA:HA	1:A:357:ARG:HG3	1.95	0.47
1:B:13:LEU:HD11	1:B:388:SER:CB	2.43	0.47
1:B:308:SER:CB	1:B:314:LEU:HD11	2.44	0.47
1:C:81:ASN:HD22	1:C:83:HIS:HE1	1.61	0.47
1:C:108:PHE:CG	1:C:118:GLY:O	2.67	0.47
1:A:151:ALA:HB3	1:A:233:ILE:HD13	1.95	0.47
1:A:304:LEU:HD12	2:A:506:LDA:H11	1.94	0.47
1:B:9:SER:C	1:B:11:SER:H	2.16	0.47
1:B:159:ALA:O	1:B:160:GLY:O	2.31	0.47
1:C:46:SER:HA	1:C:417:PHE:O	2.14	0.47
1:C:139:ALA:HB1	1:C:215:TYR:CE2	2.49	0.47
1:A:158:PHE:HA	1:A:197:THR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:SER:O	1:B:416:ASN:ND2	2.46	0.47
1:B:10:SER:HB3	1:B:416:ASN:HD22	1.75	0.47
1:B:124:GLU:HB2	1:B:152:ARG:HB2	1.95	0.47
1:C:381:ALA:HA	1:C:418:ASN:O	2.13	0.47
1:C:396:LYS:HD2	1:C:396:LYS:N	2.28	0.47
1:B:169:GLN:HA	1:B:169:GLN:OE1	2.13	0.47
1:C:51:TYR:HD1	1:C:78:TRP:CD1	2.31	0.47
1:C:20:GLU:OE2	1:C:20:GLU:CA	2.60	0.47
1:C:233:ILE:HD12	1:C:269:LEU:HD23	1.97	0.47
1:C:269:LEU:CD2	1:C:271:LEU:HD21	2.45	0.47
1:A:6:ASN:N	1:A:6:ASN:ND2	2.62	0.47
1:A:284:ASP:CG	1:A:285:PRO:HD2	2.35	0.47
1:C:18:SER:OG	1:C:290:HIS:CD2	2.65	0.47
1:C:21:GLY:HA2	1:C:36:LEU:CD1	2.35	0.47
1:A:116:SER:HA	1:A:158:PHE:O	2.14	0.47
1:A:380:ASP:OD2	1:A:380:ASP:N	2.47	0.47
1:B:90:ASP:OD2	1:B:90:ASP:N	2.35	0.47
1:B:165:LEU:C	1:B:167:ALA:H	2.18	0.47
1:B:334:TYR:N	1:B:334:TYR:CD1	2.83	0.47
1:A:52:ILE:HG22	1:A:54:PRO:HD3	1.96	0.47
1:A:80:PRO:O	1:A:81:ASN:HB3	2.15	0.47
1:A:304:LEU:CD1	2:A:506:LDA:H11	2.45	0.47
1:B:297:SER:O	1:B:300:GLN:HG3	2.14	0.47
1:C:317:LYS:HD3	1:C:318:HIS:N	2.30	0.47
1:B:334:TYR:O	1:B:335:TYR:C	2.52	0.47
1:C:58:ILE:O	1:C:70:ALA:N	2.45	0.47
1:C:64:SER:CB	1:C:165:LEU:HD21	2.34	0.47
1:B:216:GLU:HB3	1:B:222:ARG:HB3	1.96	0.47
1:B:235:PHE:HB2	1:B:267:LEU:O	2.15	0.47
1:A:256:THR:OG1	1:A:314:LEU:HA	2.15	0.46
1:A:304:LEU:O	1:A:316:GLN:HA	2.14	0.46
1:C:18:SER:HB3	1:C:328:ALA:HB1	1.97	0.46
1:C:171:MET:HE2	1:C:171:MET:HA	1.96	0.46
1:C:229:SER:C	1:C:230:GLU:O	2.51	0.46
1:A:24:ALA:HB2	1:A:36:LEU:HD22	1.96	0.46
1:C:343:THR:CG2	1:C:344:GLY:N	2.78	0.46
1:A:89:ASN:C	1:A:91:GLN:H	2.19	0.46
1:A:162:LEU:HD21	1:A:401:PRO:HG3	1.98	0.46
1:A:374:THR:HG23	1:A:384:ASP:OD2	2.16	0.46
1:B:393:GLN:HE21	1:B:393:GLN:CA	2.25	0.46
1:C:273:GLU:H	1:C:300:GLN:HE22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:HB1	1:A:298:TRP:HE1	1.81	0.46
1:B:191:ILE:HD11	1:B:247:PHE:CZ	2.50	0.46
1:B:354:ALA:HB2	1:B:357:ARG:NH2	2.30	0.46
1:A:46:SER:HB2	1:A:418:ASN:ND2	2.31	0.46
1:A:62:SER:HB3	1:A:68:LEU:HD21	1.96	0.46
1:C:26:ASP:O	1:C:28:GLY:N	2.49	0.46
1:A:7:GLU:OE2	1:A:52:ILE:HD11	2.16	0.46
1:B:137:ASN:HD22	1:B:137:ASN:N	2.13	0.46
1:B:286:GLN:O	1:B:333:TYR:HD1	1.99	0.46
1:B:354:ALA:HB2	1:B:357:ARG:CZ	2.45	0.46
1:C:155:ILE:HD11	2:C:501:LDA:C6	2.45	0.46
1:B:19:GLY:N	1:B:292:SER:HB3	2.26	0.46
1:B:191:ILE:HD11	1:B:247:PHE:CE2	2.51	0.46
1:C:158:PHE:HA	1:C:197:THR:H	1.80	0.46
1:C:317:LYS:HD3	1:C:318:HIS:H	1.80	0.46
1:A:62:SER:CB	1:A:68:LEU:HD21	2.46	0.46
1:B:304:LEU:CD1	2:B:503:LDA:C1	2.94	0.46
1:A:220:ASN:HB3	1:A:282:ARG:HB2	1.99	0.45
1:B:164:GLN:HG3	1:B:189:ASN:ND2	2.31	0.45
1:B:228:ARG:HB3	1:B:274:MET:CB	2.46	0.45
1:C:11:SER:HB2	1:C:384:ASP:OD1	2.16	0.45
1:B:135:ARG:NH2	1:B:216:GLU:OE2	2.50	0.45
1:B:155:ILE:HG13	2:B:503:LDA:H92	1.98	0.45
1:C:7:GLU:HB3	1:C:50:VAL:HG21	1.99	0.45
1:C:45:PHE:CG	1:C:46:SER:N	2.84	0.45
1:C:58:ILE:CD1	1:C:406:SER:HB2	2.47	0.45
1:C:109:ASN:O	1:C:111:THR:N	2.47	0.45
1:B:162:LEU:O	1:B:166:VAL:HG23	2.16	0.45
1:B:343:THR:HA	1:B:370:SER:O	2.16	0.45
1:C:137:ASN:ND2	1:C:140:TRP:N	2.60	0.45
1:A:10:SER:CB	1:A:416:ASN:HD22	2.29	0.45
1:C:51:TYR:CD1	1:C:78:TRP:CD1	3.05	0.45
1:B:114:GLY:HA2	1:B:402:TYR:CZ	2.52	0.45
1:C:123:LEU:HD12	1:C:153:ALA:HB2	1.98	0.45
1:A:158:PHE:CA	1:A:197:THR:HB	2.47	0.45
1:A:199:HIS:HE1	1:B:192:ASP:OD1	1.99	0.45
1:A:303:GLN:NE2	1:A:316:GLN:HG3	2.32	0.45
1:B:216:GLU:CB	1:B:222:ARG:HB3	2.47	0.45
1:B:324:ALA:CB	1:B:351:PRO:HG3	2.46	0.45
1:C:42:ARG:NH1	1:C:420:ALA:HB1	2.31	0.45
1:C:281:ASN:O	1:C:288:ALA:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ILE:CD1	2:C:501:LDA:H22	2.16	0.45
1:A:248:ASN:O	1:A:250:TYR:CD2	2.70	0.45
2:B:503:LDA:H51	2:B:503:LDA:H21	1.29	0.45
1:C:334:TYR:CD2	1:C:340:THR:HG23	2.52	0.45
1:C:393:GLN:HA	1:C:393:GLN:NE2	2.28	0.45
1:A:3:PHE:O	1:A:3:PHE:CD2	2.70	0.45
1:B:121:THR:OG1	1:B:157:ARG:NH2	2.49	0.45
1:B:378:ASN:O	1:B:379:LYS:CB	2.60	0.45
1:A:68:LEU:HD23	1:A:68:LEU:N	2.32	0.44
1:A:159:ALA:O	1:A:160:GLY:O	2.35	0.44
1:A:185:ALA:O	1:A:187:THR:N	2.50	0.44
1:B:103:GLY:HA2	1:B:123:LEU:O	2.17	0.44
1:C:154:LYS:HA	1:C:200:LEU:O	2.17	0.44
1:C:216:GLU:HA	1:C:222:ARG:HB3	1.99	0.44
1:A:5:LEU:HD13	1:A:102:TYR:HA	1.99	0.44
1:A:15:ARG:NH1	1:A:20:GLU:OE1	2.50	0.44
1:B:129:ASN:CG	1:B:130:LEU:N	2.70	0.44
1:B:272:PRO:HG2	1:B:298:TRP:CD2	2.51	0.44
1:C:348:ASP:O	1:C:348:ASP:OD2	2.36	0.44
1:C:343:THR:HG22	1:C:344:GLY:N	2.32	0.44
1:A:51:TYR:OH	1:A:76:THR:HG21	2.18	0.44
1:B:305:LYS:HD3	1:B:316:GLN:NE2	2.33	0.44
1:B:91:GLN:NE2	1:B:135:ARG:O	2.51	0.44
1:B:326:ARG:HB2	1:B:348:ASP:CB	2.48	0.44
1:C:238:ASN:HD22	1:C:262:THR:CG2	2.30	0.44
1:A:40:PHE:CD1	1:A:40:PHE:N	2.85	0.44
1:A:361:ILE:HG22	1:A:361:ILE:O	2.17	0.44
1:B:248:ASN:HD21	1:B:256:THR:HA	1.82	0.44
1:B:321:PHE:CE2	1:B:352:VAL:HG22	2.53	0.44
1:B:377:PHE:HB2	1:B:381:ALA:HB3	1.99	0.44
1:B:378:ASN:OD1	1:B:380:ASP:N	2.38	0.44
1:C:13:LEU:HD13	1:C:17:TYR:OH	2.18	0.44
1:A:11:SER:OG	1:A:15:ARG:NH2	2.51	0.44
1:A:366:ARG:NH1	2:A:505:LDA:H12	2.32	0.44
1:B:254:ILE:HD13	1:B:254:ILE:H	1.83	0.44
1:B:343:THR:CG2	1:B:344:GLY:N	2.80	0.44
1:C:27:ALA:O	1:C:28:GLY:C	2.56	0.44
1:A:15:ARG:NH1	1:A:20:GLU:OE2	2.49	0.44
1:A:216:GLU:HB2	1:A:222:ARG:HB3	2.00	0.44
1:A:280:TYR:C	1:A:280:TYR:CD2	2.91	0.44
1:B:280:TYR:CD2	1:B:281:ASN:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ASN:ND2	1:C:71:ASP:HA	2.33	0.44
1:A:6:ASN:O	1:A:17:TYR:CE1	2.70	0.44
1:A:214:LEU:O	1:A:214:LEU:HD23	2.18	0.44
1:B:165:LEU:C	1:B:167:ALA:N	2.72	0.44
1:B:304:LEU:HD13	2:B:503:LDA:C1	2.48	0.44
1:B:352:VAL:HA	1:B:353:PRO:HD3	1.82	0.44
1:C:1:ALA:HB1	1:C:4:GLN:CB	2.48	0.44
1:C:15:ARG:HG2	1:C:342:ARG:HD3	2.00	0.44
1:B:7:GLU:OE2	2:B:504:LDA:HM12	2.18	0.43
1:B:178:THR:CG2	1:B:181:GLY:H	2.31	0.43
1:B:361:ILE:N	1:B:362:PRO:HD3	2.32	0.43
1:B:137:ASN:HD21	1:B:139:ALA:HB3	1.82	0.43
1:B:155:ILE:HD11	2:B:503:LDA:H71	2.00	0.43
1:B:256:THR:OG1	1:B:314:LEU:HA	2.17	0.43
1:B:36:LEU:HD23	1:B:214:LEU:HD13	2.00	0.43
1:B:78:TRP:O	1:B:80:PRO:HD3	2.17	0.43
1:B:113:ALA:HB1	1:B:161:ASP:OD2	2.18	0.43
1:C:181:GLY:C	1:C:183:ALA:H	2.21	0.43
2:C:502:LDA:H12	2:C:502:LDA:H41	1.89	0.43
1:A:36:LEU:O	1:A:39:MET:HB2	2.19	0.43
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.83	0.43
1:A:350:SER:HA	1:A:351:PRO:HD3	1.83	0.43
1:B:13:LEU:HA	1:B:17:TYR:CZ	2.54	0.43
1:C:195:THR:O	1:C:197:THR:N	2.51	0.43
1:A:3:PHE:O	1:A:3:PHE:HD2	2.01	0.43
1:A:15:ARG:O	1:A:16:ALA:HB3	2.19	0.43
1:A:34:ALA:HB1	1:A:131:SER:OG	2.18	0.43
1:B:303:GLN:NE2	1:B:316:GLN:NE2	2.63	0.43
1:C:43:PRO:HA	1:C:85:VAL:O	2.18	0.43
1:C:273:GLU:N	1:C:300:GLN:NE2	2.65	0.43
1:C:334:TYR:CD2	1:C:340:THR:CG2	3.02	0.43
1:C:345:ILE:CG2	1:C:346:ALA:N	2.82	0.43
1:A:21:GLY:HA2	1:A:36:LEU:HD11	2.00	0.43
1:B:13:LEU:HD11	1:B:388:SER:HB2	2.01	0.43
1:B:378:ASN:OD1	1:B:379:LYS:N	2.52	0.43
1:C:19:GLY:H	1:C:292:SER:HB3	1.82	0.43
1:C:170:ILE:HA	1:C:173:SER:HB3	2.00	0.43
1:A:223:TYR:N	1:A:223:TYR:CD1	2.86	0.43
1:B:13:LEU:CD1	1:B:388:SER:HB2	2.48	0.43
1:C:57:ASN:ND2	1:C:71:ASP:OD2	2.52	0.43
1:C:112:TYR:HE2	1:C:404:PHE:HE2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LEU:H	1:C:165:LEU:HD23	1.83	0.43
1:A:5:LEU:CD1	1:A:103:GLY:H	2.32	0.43
1:A:86:ALA:HA	1:A:87:PRO:HD3	1.69	0.43
1:A:419:TYR:HE2	1:A:421:PHE:CD1	2.37	0.43
1:B:58:ILE:HD13	1:B:406:SER:HB2	1.99	0.43
1:B:252:LEU:HD23	1:B:254:ILE:HG13	2.01	0.43
1:C:321:PHE:CD2	1:C:352:VAL:HG22	2.52	0.43
1:C:345:ILE:HG22	1:C:346:ALA:N	2.34	0.43
1:C:391:HIS:ND1	1:C:392:GLY:N	2.67	0.43
1:C:404:PHE:CD1	1:C:404:PHE:N	2.86	0.43
1:B:250:TYR:O	1:B:251:GLY:C	2.57	0.43
1:C:20:GLU:HB3	1:C:32:ARG:HD2	2.01	0.43
1:C:62:SER:C	1:C:64:SER:N	2.71	0.43
1:C:326:ARG:HG3	1:C:326:ARG:NH1	2.34	0.43
1:B:10:SER:O	1:B:13:LEU:HB3	2.18	0.42
1:B:43:PRO:HA	1:B:85:VAL:O	2.19	0.42
1:B:55:ASP:O	1:B:408:GLY:HA2	2.19	0.42
1:B:117:VAL:HG23	1:B:359:ILE:HD11	2.01	0.42
1:B:266:TYR:HB2	1:B:307:THR:OG1	2.19	0.42
1:C:33:ASN:ND2	1:C:226:THR:HG22	2.34	0.42
1:C:243:LEU:HD23	1:C:243:LEU:HA	1.84	0.42
1:B:290:HIS:HE1	1:B:332:THR:OG1	2.01	0.42
1:B:326:ARG:HA	1:B:348:ASP:CB	2.49	0.42
1:B:52:ILE:C	1:B:54:PRO:HD3	2.39	0.42
1:B:280:TYR:C	1:B:280:TYR:HD2	2.22	0.42
1:C:33:ASN:ND2	1:C:226:THR:CG2	2.82	0.42
1:B:165:LEU:O	1:B:167:ALA:N	2.52	0.42
1:C:20:GLU:HA	1:C:29:ASN:ND2	2.34	0.42
1:C:68:LEU:HD23	1:C:113:ALA:HB3	2.01	0.42
1:C:383:VAL:HG22	1:C:384:ASP:N	2.34	0.42
1:A:195:THR:O	1:A:196:LYS:C	2.57	0.42
1:A:220:ASN:HB3	1:A:282:ARG:HB3	2.01	0.42
1:B:58:ILE:HG12	1:B:73:ILE:HD13	2.00	0.42
1:B:249:ASN:O	1:B:250:TYR:CG	2.73	0.42
1:C:8:PHE:C	1:C:8:PHE:CD2	2.92	0.42
1:C:20:GLU:HB3	1:C:32:ARG:CD	2.50	0.42
1:C:129:ASN:HB2	1:C:147:ASN:OD1	2.19	0.42
1:C:135:ARG:HG3	1:C:137:ASN:O	2.19	0.42
1:A:33:ASN:C	1:A:35:ALA:N	2.72	0.42
1:A:158:PHE:C	1:A:197:THR:HB	2.39	0.42
1:C:236:LYS:HD3	1:C:266:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:THR:HA	1:C:371:ALA:HA	2.01	0.42
1:A:127:ASN:ND2	1:A:149:VAL:HG22	2.34	0.42
1:A:168:GLY:O	1:A:169:GLN:C	2.58	0.42
1:B:172:GLN:O	1:B:173:SER:CB	2.68	0.42
1:B:232:LYS:HE2	1:B:270:ASN:ND2	2.34	0.42
1:C:164:GLN:HG2	1:C:165:LEU:H	1.83	0.42
1:A:10:SER:HB3	1:A:416:ASN:HD22	1.85	0.42
1:B:137:ASN:ND2	1:B:137:ASN:N	2.67	0.42
1:A:120:THR:HB	1:A:156:GLU:HB2	2.02	0.42
1:B:243:LEU:HD22	1:B:247:PHE:CE1	2.55	0.42
1:B:347:PHE:CE1	1:B:365:ASP:HB3	2.53	0.42
1:C:101:ASN:C	1:C:102:TYR:CD1	2.94	0.42
1:A:153:ALA:HB1	2:A:506:LDA:H82	2.01	0.42
1:B:325:TYR:O	1:B:348:ASP:HB2	2.19	0.42
1:A:89:ASN:HD22	1:A:90:ASP:N	2.11	0.41
1:A:121:THR:HG21	2:A:506:LDA:H21	2.02	0.41
1:C:59:SER:OG	1:C:405:GLU:HB3	2.19	0.41
1:B:32:ARG:HH11	1:B:32:ARG:CG	2.29	0.41
1:B:167:ALA:HB1	1:B:185:ALA:O	2.20	0.41
1:B:402:TYR:CB	1:B:404:PHE:CE1	3.03	0.41
1:B:263:GLN:OE1	1:B:314:LEU:HD21	2.20	0.41
1:C:42:ARG:NH1	1:C:420:ALA:O	2.53	0.41
1:A:404:PHE:CD1	1:A:404:PHE:N	2.89	0.41
1:A:4:GLN:O	1:A:5:LEU:HD12	2.21	0.41
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.84	0.41
1:C:361:ILE:HG22	1:C:361:ILE:O	2.19	0.41
1:A:30:VAL:HG21	1:A:85:VAL:HG22	2.03	0.41
1:C:117:VAL:HG23	1:C:359:ILE:HD11	2.02	0.41
1:C:218:ASP:OD1	1:C:218:ASP:C	2.59	0.41
1:C:231:VAL:O	1:C:231:VAL:HG12	2.20	0.41
1:A:6:ASN:HD22	1:A:6:ASN:H	1.69	0.41
1:A:326:ARG:CG	1:A:348:ASP:HB3	2.47	0.41
1:A:334:TYR:HA	1:A:340:THR:HG23	2.02	0.41
1:B:342:ARG:NH2	1:B:374:THR:OG1	2.48	0.41
1:C:170:ILE:O	1:C:170:ILE:HG22	2.20	0.41
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.90	0.41
1:A:317:LYS:HD3	1:A:318:HIS:N	2.35	0.41
1:A:346:ALA:HB3	1:A:368:TRP:HB2	2.03	0.41
1:B:112:TYR:OH	1:B:404:PHE:HE2	2.03	0.41
1:B:288:ALA:O	1:B:331:THR:HB	2.21	0.41
1:C:19:GLY:O	1:C:22:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ALA:HA	1:C:143:GLY:HA2	2.02	0.41
1:A:19:GLY:O	1:A:20:GLU:C	2.60	0.41
1:B:131:SER:HB3	1:B:145:GLY:HA3	2.00	0.41
1:B:291:TYR:O	1:B:291:TYR:CD1	2.74	0.41
1:C:381:ALA:O	1:C:382:SER:HB3	2.21	0.41
1:B:321:PHE:N	1:B:321:PHE:CD2	2.89	0.40
1:C:402:TYR:HB2	1:C:404:PHE:CE1	2.55	0.40
1:A:142:PHE:CD1	1:A:142:PHE:N	2.89	0.40
1:B:128:LEU:HD12	1:B:205:TRP:CZ3	2.56	0.40
1:B:274:MET:HG2	1:B:296:THR:OG1	2.21	0.40
1:B:347:PHE:HA	1:B:366:ARG:O	2.21	0.40
1:C:33:ASN:OD1	1:C:33:ASN:C	2.60	0.40
1:C:157:ARG:HB2	1:C:197:THR:CG2	2.49	0.40
1:C:366:ARG:NH1	2:C:502:LDA:H21	2.36	0.40
1:A:356:ASN:O	1:A:357:ARG:C	2.60	0.40
1:A:131:SER:HB2	1:A:144:LEU:O	2.21	0.40
1:A:143:GLY:O	1:A:211:ALA:HA	2.21	0.40
1:A:162:LEU:O	1:A:165:LEU:HB2	2.22	0.40
1:B:177:GLN:HA	1:B:177:GLN:NE2	2.35	0.40
1:C:157:ARG:HH12	2:C:501:LDA:CM2	2.26	0.40
1:A:158:PHE:CD1	1:A:158:PHE:N	2.89	0.40
1:B:9:SER:C	1:B:11:SER:N	2.75	0.40
1:B:253:PRO:O	1:B:254:ILE:O	2.40	0.40
1:B:387:VAL:HA	1:B:412:LEU:O	2.21	0.40
1:C:52:ILE:HB	1:C:77:ALA:HB3	2.04	0.40
1:C:140:TRP:O	1:C:141:SER:HB2	2.21	0.40
1:C:359:ILE:O	1:C:362:PRO:HG3	2.22	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	408/427 (96%)	352 (86%)	43 (10%)	13 (3%)	4 22
1	B	419/427 (98%)	355 (85%)	42 (10%)	22 (5%)	2 12
1	C	412/427 (96%)	340 (82%)	55 (13%)	17 (4%)	3 17
All	All	1239/1281 (97%)	1047 (84%)	140 (11%)	52 (4%)	3 17

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	A	337	ASP
1	A	355	GLN
1	B	90	ASP
1	B	174	PRO
1	B	254	ILE
1	B	355	GLN
1	B	379	LYS
1	C	2	GLY
1	C	27	ALA
1	C	164	GLN
1	C	165	LEU
1	C	355	GLN
1	A	2	GLY
1	A	34	ALA
1	A	160	GLY
1	A	186	ALA
1	B	72	ASN
1	B	160	GLY
1	B	217	LEU
1	B	250	TYR
1	B	272	PRO
1	B	354	ALA
1	B	359	ILE
1	C	29	ASN
1	C	90	ASP
1	C	110	ASP
1	C	160	GLY
1	C	272	PRO
1	A	105	ALA
1	A	249	ASN
1	A	272	PRO
1	B	154	LYS
1	B	362	PRO

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Mol	Chain	Res	Type
1	C	7	GLU
1	C	28	GLY
1	C	196	LYS
1	C	219	LYS
1	C	349	ASP
1	B	365	ASP
1	C	382	SER
1	A	72	ASN
1	B	22	ALA
1	C	335	TYR
1	B	2	GLY
1	B	115	GLY
1	B	335	TYR
1	B	166	VAL
1	B	173	SER
1	B	118	GLY
1	A	63	PRO
1	A	163	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	323/336 (96%)	299 (93%)	24 (7%)	13 40
1	B	330/336 (98%)	291 (88%)	39 (12%)	5 21
1	C	326/336 (97%)	293 (90%)	33 (10%)	7 27
All	All	979/1008 (97%)	883 (90%)	96 (10%)	8 29

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	11	SER
1	A	39	MET
1	A	63	PRO

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Mol	Chain	Res	Type
1	A	72	ASN
1	A	78	TRP
1	A	89	ASN
1	A	121	THR
1	A	130	LEU
1	A	137	ASN
1	A	140	TRP
1	A	189	ASN
1	A	197	THR
1	A	203	ASN
1	A	214	LEU
1	A	275	TRP
1	A	278	SER
1	A	282	ARG
1	A	314	LEU
1	A	322	LYS
1	A	380	ASP
1	A	393	GLN
1	A	404	PHE
1	A	416	ASN
1	B	3	PHE
1	B	10	SER
1	B	15	ARG
1	B	32	ARG
1	B	39	MET
1	B	72	ASN
1	B	81	ASN
1	B	89	ASN
1	B	90	ASP
1	B	122	ASP
1	B	125	THR
1	B	137	ASN
1	B	141	SER
1	B	169	GLN
1	B	172	GLN
1	B	174	PRO
1	B	187	THR
1	B	189	ASN
1	B	197	THR
1	B	210	ASN
1	B	249	ASN
1	B	252	LEU

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Mol	Chain	Res	Type
1	B	263	GLN
1	B	264	SER
1	B	275	TRP
1	B	280	TYR
1	B	282	ARG
1	B	290	HIS
1	B	322	LYS
1	B	326	ARG
1	B	334	TYR
1	B	340	THR
1	B	349	ASP
1	B	358	SER
1	B	373	THR
1	B	393	GLN
1	B	403	GLN
1	B	406	SER
1	B	415	THR
1	C	5	LEU
1	C	6	ASN
1	C	39	MET
1	C	63	PRO
1	C	72	ASN
1	C	78	TRP
1	C	120	THR
1	C	121	THR
1	C	122	ASP
1	C	137	ASN
1	C	142	PHE
1	C	144	LEU
1	C	162	LEU
1	C	197	THR
1	C	203	ASN
1	C	214	LEU
1	C	217	LEU
1	C	219	LYS
1	C	263	GLN
1	C	275	TRP
1	C	282	ARG
1	C	284	ASP
1	C	285	PRO
1	C	303	GLN
1	C	322	LYS

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Mol	Chain	Res	Type
1	C	326	ARG
1	C	331	THR
1	C	349	ASP
1	C	355	GLN
1	C	364	GLN
1	C	393	GLN
1	C	396	LYS
1	C	404	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	29	ASN
1	A	57	ASN
1	A	72	ASN
1	A	89	ASN
1	A	127	ASN
1	A	137	ASN
1	A	147	ASN
1	A	189	ASN
1	A	199	HIS
1	A	210	ASN
1	A	248	ASN
1	A	300	GLN
1	A	303	GLN
1	A	316	GLN
1	A	355	GLN
1	A	356	ASN
1	A	393	GLN
1	A	416	ASN
1	A	418	ASN
1	B	6	ASN
1	B	57	ASN
1	B	72	ASN
1	B	83	HIS
1	B	127	ASN
1	B	129	ASN
1	B	137	ASN
1	B	177	GLN
1	B	189	ASN
1	B	270	ASN

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Mol	Chain	Res	Type
1	B	281	ASN
1	B	290	HIS
1	B	300	GLN
1	B	316	GLN
1	B	356	ASN
1	B	393	GLN
1	B	416	ASN
1	B	418	ASN
1	C	29	ASN
1	C	57	ASN
1	C	72	ASN
1	C	81	ASN
1	C	91	GLN
1	C	129	ASN
1	C	137	ASN
1	C	182	GLN
1	C	189	ASN
1	C	201	ASN
1	C	210	ASN
1	C	238	ASN
1	C	248	ASN
1	C	270	ASN
1	C	281	ASN
1	C	290	HIS
1	C	300	GLN
1	C	316	GLN
1	C	355	GLN
1	C	356	ASN
1	C	393	GLN
1	C	416	ASN
1	C	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LDA	B	503	-	12,15,15	2.19	1 (8%)	14,17,17	1.40	1 (7%)
2	LDA	A	505	-	12,15,15	1.96	1 (8%)	14,17,17	1.70	3 (21%)
2	LDA	A	506	-	12,15,15	2.03	1 (8%)	14,17,17	1.81	5 (35%)
2	LDA	B	504	-	12,15,15	1.94	1 (8%)	14,17,17	1.88	3 (21%)
2	LDA	C	501	-	12,15,15	2.16	1 (8%)	14,17,17	1.32	2 (14%)
2	LDA	C	502	-	12,15,15	2.06	1 (8%)	14,17,17	1.57	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	503	-	-	8/13/13/13	-
2	LDA	A	505	-	-	8/13/13/13	-
2	LDA	A	506	-	-	6/13/13/13	-
2	LDA	B	504	-	-	7/13/13/13	-
2	LDA	C	501	-	-	8/13/13/13	-
2	LDA	C	502	-	-	6/13/13/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	LDA	O1-N1	-7.25	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LDA	O1-N1	-7.16	1.25	1.42
2	A	506	LDA	O1-N1	-6.69	1.26	1.42
2	C	502	LDA	O1-N1	-6.63	1.26	1.42
2	A	505	LDA	O1-N1	-6.25	1.27	1.42
2	B	504	LDA	O1-N1	-6.20	1.27	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	504	LDA	CM1-N1-C1	-4.81	100.13	110.23
2	A	505	LDA	CM1-N1-C1	-4.01	101.82	110.23
2	A	506	LDA	CM1-N1-C1	-3.93	101.98	110.23
2	C	502	LDA	O1-N1-C1	3.00	116.62	109.27
2	B	504	LDA	CM2-N1-C1	2.89	116.30	110.23
2	C	502	LDA	CM1-N1-C1	-2.86	104.23	110.23
2	B	503	LDA	CM1-N1-C1	-2.83	104.30	110.23
2	B	504	LDA	O1-N1-C1	2.74	116.00	109.27
2	A	505	LDA	O1-N1-C1	2.70	115.89	109.27
2	A	506	LDA	C6-C5-C4	-2.32	102.64	114.42
2	C	502	LDA	C9-C8-C7	-2.30	102.72	114.42
2	A	506	LDA	O1-N1-C1	2.26	114.82	109.27
2	A	505	LDA	C9-C8-C7	-2.25	103.02	114.42
2	A	506	LDA	C9-C8-C7	-2.24	103.05	114.42
2	A	506	LDA	CM2-N1-C1	2.16	114.78	110.23
2	C	501	LDA	CM2-N1-C1	2.13	114.71	110.23
2	C	501	LDA	CM1-N1-C1	-2.11	105.81	110.23

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	505	LDA	C2-C1-N1-O1
2	A	505	LDA	C2-C1-N1-CM1
2	A	505	LDA	C2-C1-N1-CM2
2	A	506	LDA	N1-C1-C2-C3
2	B	504	LDA	C2-C1-N1-O1
2	B	504	LDA	C2-C1-N1-CM2
2	C	501	LDA	C2-C1-N1-O1
2	C	501	LDA	C2-C1-N1-CM1
2	C	501	LDA	C2-C1-N1-CM2
2	C	502	LDA	C2-C1-N1-O1
2	C	502	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
2	C	502	LDA	C2-C1-N1-CM2
2	B	503	LDA	C2-C3-C4-C5
2	C	502	LDA	C1-C2-C3-C4
2	A	506	LDA	C11-C10-C9-C8
2	B	503	LDA	C11-C10-C9-C8
2	B	503	LDA	C3-C4-C5-C6
2	C	502	LDA	C11-C10-C9-C8
2	C	501	LDA	C6-C7-C8-C9
2	A	506	LDA	C1-C2-C3-C4
2	B	503	LDA	C1-C2-C3-C4
2	A	505	LDA	C3-C4-C5-C6
2	A	506	LDA	C3-C4-C5-C6
2	B	503	LDA	C7-C8-C9-C10
2	A	505	LDA	C6-C7-C8-C9
2	A	506	LDA	C7-C8-C9-C10
2	B	504	LDA	C11-C10-C9-C8
2	B	504	LDA	C2-C3-C4-C5
2	A	505	LDA	C1-C2-C3-C4
2	C	501	LDA	N1-C1-C2-C3
2	C	502	LDA	C2-C3-C4-C5
2	A	506	LDA	C2-C3-C4-C5
2	B	504	LDA	C7-C8-C9-C10
2	B	503	LDA	C2-C1-N1-CM2
2	B	504	LDA	C2-C1-N1-CM1
2	B	503	LDA	C6-C7-C8-C9
2	B	504	LDA	C3-C4-C5-C6
2	C	501	LDA	C1-C2-C3-C4
2	C	501	LDA	C2-C3-C4-C5
2	A	505	LDA	C11-C10-C9-C8
2	A	505	LDA	C2-C3-C4-C5
2	C	501	LDA	C11-C10-C9-C8
2	B	503	LDA	N1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	LDA	9	0
2	A	505	LDA	3	0
2	A	506	LDA	15	0
2	B	504	LDA	2	0
2	C	501	LDA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	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

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	412/427 (96%)	-0.25	3 (0%)	87	88	4, 20, 35, 50	0
1	B	421/427 (98%)	-0.21	5 (1%)	79	78	10, 24, 35, 46	0
1	C	416/427 (97%)	-0.21	1 (0%)	95	96	7, 25, 38, 45	0
All	All	1249/1281 (97%)	-0.22	9 (0%)	87	88	4, 23, 36, 50	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	PRO	3.1
1	A	184	LEU	2.9
1	B	185	ALA	2.7
1	A	181	GLY	2.4
1	B	181	GLY	2.3
1	C	78	TRP	2.2
1	A	183	ALA	2.1
1	B	178	THR	2.1
1	B	374	THR	2.1

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	LDA	C	502	16/16	0.72	0.51	30,37,47,47	0
2	LDA	A	505	16/16	0.80	0.36	25,29,30,30	0
2	LDA	B	504	16/16	0.82	0.37	22,32,37,37	0
2	LDA	C	501	16/16	0.91	0.38	18,21,31,31	0
2	LDA	B	503	16/16	0.91	0.31	23,26,39,40	0
2	LDA	A	506	16/16	0.92	0.32	21,30,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.