



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:01 PM UTC

PDB ID : 2R4P / pdb_00002r4p
Title : Crystal structure of the long-chain fatty acid transporter FadL mutant G212E
Authors : Hearn, E.M.; Patel, D.R.; Lepore, B.W.; Indic, M.; van den Berg, B.
Deposited on : 2007-08-31
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

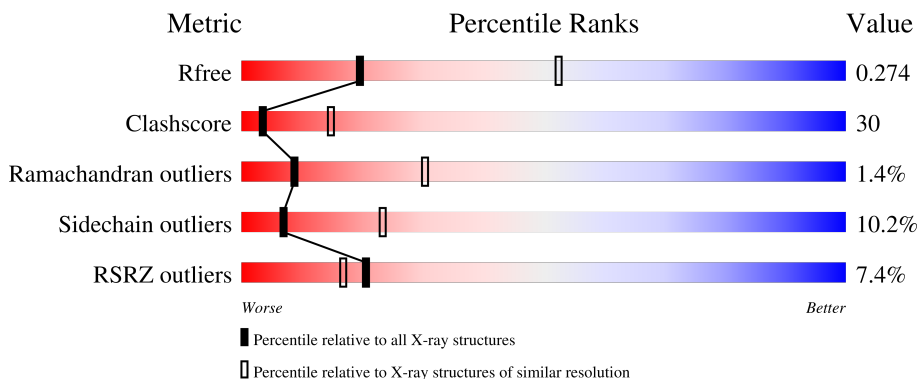
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	427	4% 51% 40% 7%
1	B	427	11% 50% 41% 7%

2 Entry composition

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

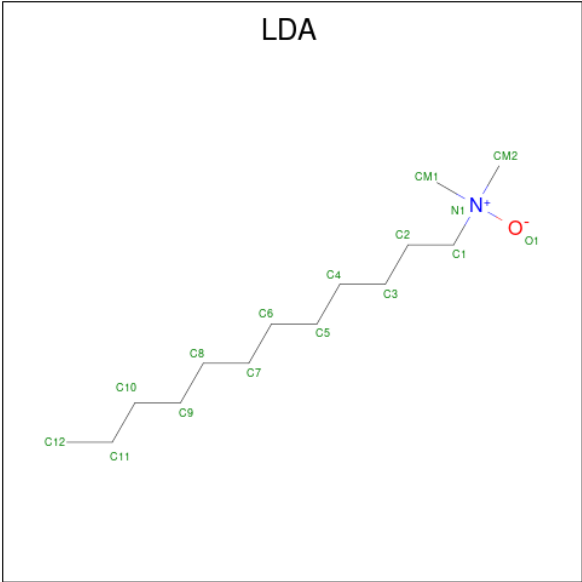
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	GLU	GLY	engineered 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	212	GLU	GLY	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

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).

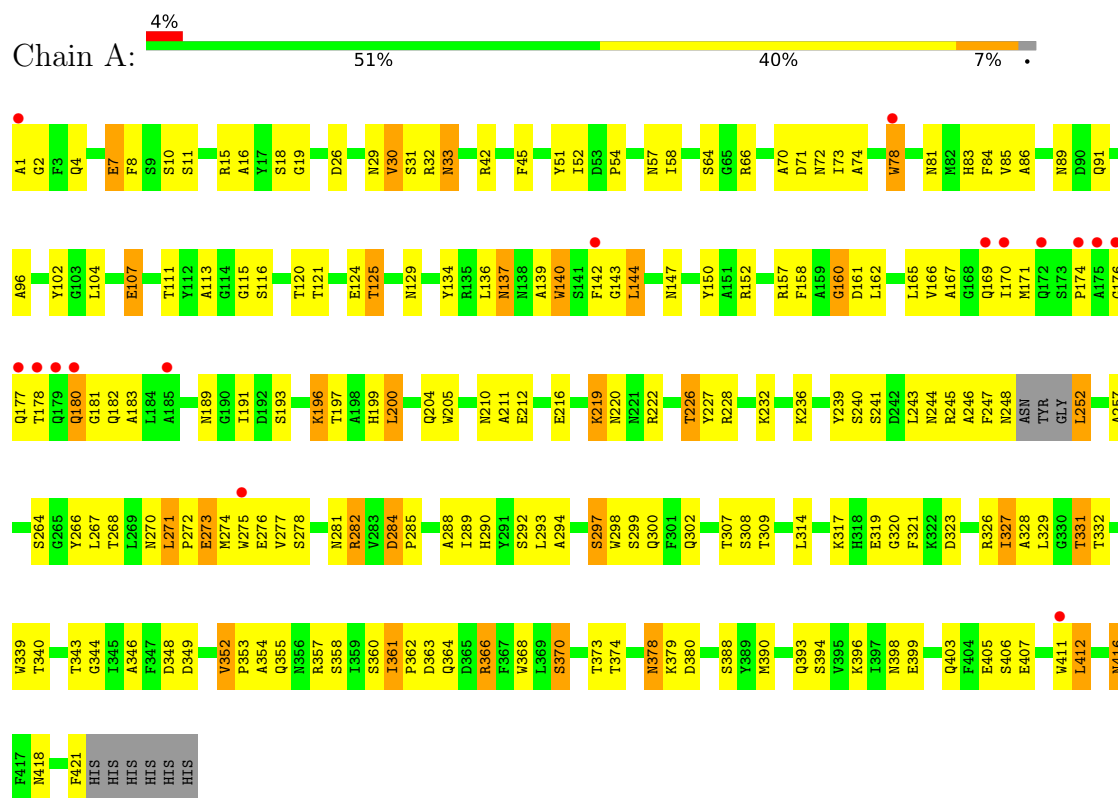


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		

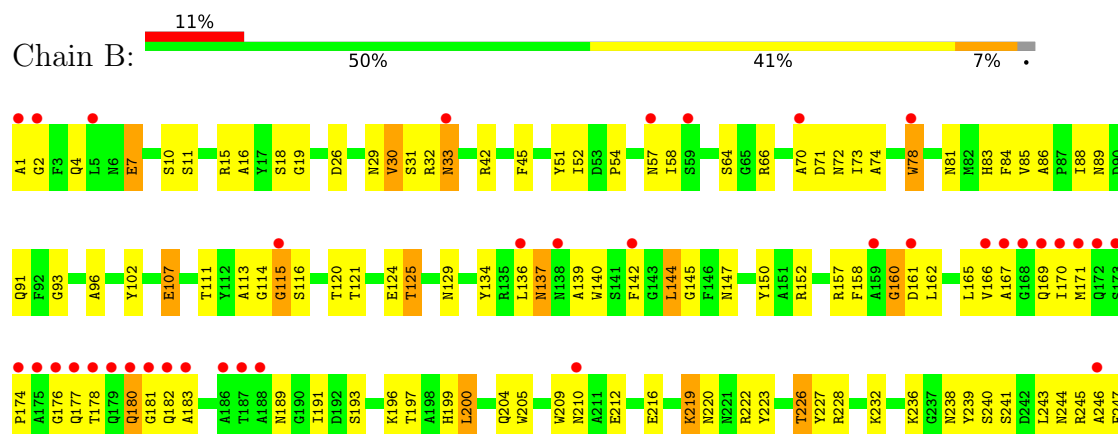
3 Residue-property plots

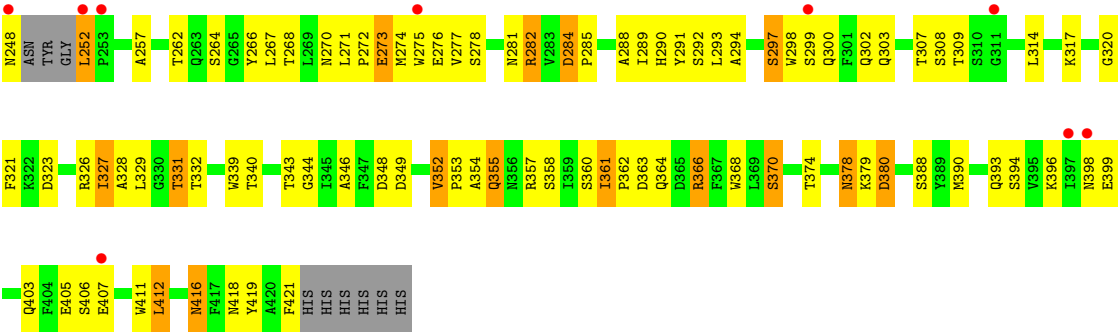
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Long-chain fatty acid transport protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.51Å 69.97Å 84.15Å 90.00° 100.84° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (10.00-2.90) 95.9 (10.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.267 , 0.288 0.255 , 0.274	Depositor DCC
R_{free} test set	2245 reflections (7.58%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6496	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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	0.51	0/3319	0.97	13/4518 (0.3%)
1	B	0.47	0/3319	0.95	14/4518 (0.3%)
All	All	0.49	0/6638	0.96	27/9036 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ASN	CA-C-N	8.58	130.56	119.84
1	A	33	ASN	C-N-CA	8.58	130.56	119.84
1	B	33	ASN	CA-C-N	8.27	130.18	119.84
1	B	33	ASN	C-N-CA	8.27	130.18	119.84
1	B	29	ASN	N-CA-C	7.49	119.53	111.36
1	A	29	ASN	N-CA-C	7.21	119.21	111.36
1	A	352	VAL	N-CA-C	6.28	114.10	107.76
1	A	271	LEU	CA-C-N	5.97	125.99	119.90
1	A	271	LEU	C-N-CA	5.97	125.99	119.90
1	A	273	GLU	N-CA-C	-5.77	103.08	110.53
1	B	183	ALA	N-CA-C	-5.68	106.33	113.20
1	B	352	VAL	N-CA-C	5.63	113.45	107.76
1	A	366	ARG	N-CA-C	5.61	118.60	109.24
1	A	140	TRP	N-CA-C	5.57	118.89	109.76
1	B	273	GLU	N-CA-C	-5.55	103.37	110.53
1	B	339	TRP	N-CA-C	5.52	118.47	109.59
1	B	271	LEU	CA-C-N	5.42	125.43	119.90
1	B	271	LEU	C-N-CA	5.42	125.43	119.90
1	A	183	ALA	N-CA-C	-5.42	106.64	113.20
1	A	339	TRP	N-CA-C	5.40	118.28	109.59
1	A	370	SER	N-CA-C	5.37	117.24	109.07
1	A	7	GLU	N-CA-C	5.29	118.20	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	SER	N-CA-C	5.28	117.09	109.07
1	B	380	ASP	N-CA-C	-5.26	107.88	114.56
1	B	7	GLU	N-CA-C	5.23	118.11	108.58
1	B	366	ARG	N-CA-C	5.09	117.74	109.24
1	B	303	GLN	N-CA-C	5.01	115.15	108.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3232	0	3013	183	0
1	B	3232	0	3013	189	0
2	A	16	0	31	5	0
2	B	16	0	31	5	0
All	All	6496	0	6088	372	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 30.

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:SER:HB3	1:B:314:LEU:HD21	1.28	1.13
1:A:308:SER:HB3	1:A:314:LEU:HD21	1.29	1.08
1:B:58:ILE:HB	1:B:70:ALA:HB3	1.39	1.02
1:A:58:ILE:HB	1:A:70:ALA:HB3	1.41	0.98
1:A:390:MET:HE3	1:A:412:LEU:HD21	1.45	0.97
1:B:32:ARG:HD2	1:B:228:ARG:HH22	1.29	0.97
1:A:32:ARG:HD2	1:A:228:ARG:HH22	1.25	0.95
1:A:396:LYS:HE3	1:A:405:GLU:OE2	1.67	0.94
1:A:33:ASN:HD22	1:A:226:THR:HG21	1.31	0.94
1:A:248:ASN:HD21	1:A:257:ALA:H	1.15	0.93
1:B:33:ASN:HD22	1:B:226:THR:HG21	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ILE:HG12	2:B:502:LDA:HM23	1.51	0.92
1:B:396:LYS:HE3	1:B:405:GLU:OE2	1.70	0.91
1:B:326:ARG:HG3	1:B:348:ASP:HB3	1.53	0.90
1:A:326:ARG:HG3	1:A:348:ASP:HB3	1.52	0.90
1:B:390:MET:HE3	1:B:412:LEU:HD21	1.52	0.89
1:B:248:ASN:HD21	1:B:257:ALA:H	1.14	0.89
1:B:267:LEU:HD23	1:B:268:THR:N	1.94	0.83
1:A:32:ARG:HD2	1:A:228:ARG:NH2	1.93	0.83
1:A:267:LEU:HD23	1:A:268:THR:N	1.93	0.83
1:B:11:SER:HB3	1:B:15:ARG:NH2	1.94	0.82
1:A:11:SER:HB3	1:A:15:ARG:NH2	1.94	0.82
1:A:302:GLN:HE22	1:A:320:GLY:HA2	1.44	0.82
1:B:302:GLN:HE22	1:B:320:GLY:HA2	1.43	0.82
1:A:284:ASP:OD1	1:A:285:PRO:HD2	1.81	0.80
1:B:32:ARG:HD2	1:B:228:ARG:NH2	1.97	0.79
1:B:284:ASP:OD1	1:B:285:PRO:HD2	1.82	0.79
1:A:45:PHE:CE1	1:A:421:PHE:HE1	2.00	0.79
1:A:267:LEU:HD13	2:A:501:LDA:H81	1.64	0.78
1:B:45:PHE:CE1	1:B:421:PHE:HE1	2.01	0.78
1:B:281:ASN:HB2	1:B:289:ILE:HG22	1.64	0.78
1:B:212:GLU:HG3	1:B:226:THR:HG22	1.67	0.77
1:A:378:ASN:O	1:A:379:LYS:HB2	1.85	0.76
1:A:281:ASN:HB2	1:A:289:ILE:HG22	1.67	0.76
1:A:232:LYS:HG2	1:A:270:ASN:ND2	2.01	0.74
1:A:248:ASN:ND2	1:A:257:ALA:H	1.86	0.74
1:B:248:ASN:ND2	1:B:257:ALA:H	1.85	0.74
1:B:33:ASN:ND2	1:B:226:THR:HG21	2.03	0.74
1:A:33:ASN:ND2	1:A:226:THR:HG21	2.03	0.74
1:A:212:GLU:HG3	1:A:226:THR:HG22	1.69	0.74
1:B:252:LEU:HD12	1:B:252:LEU:N	2.03	0.74
1:B:232:LYS:HG2	1:B:270:ASN:ND2	2.02	0.73
1:A:252:LEU:N	1:A:252:LEU:HD12	2.05	0.72
1:A:58:ILE:HD13	1:A:406:SER:HB3	1.71	0.72
1:A:102:TYR:O	1:A:125:THR:HB	1.89	0.72
1:B:134:TYR:CE1	1:B:136:LEU:HD23	2.25	0.71
1:B:308:SER:CB	1:B:314:LEU:HD21	2.15	0.71
1:B:378:ASN:O	1:B:379:LYS:HB2	1.90	0.71
1:B:52:ILE:HG12	1:B:412:LEU:CD1	2.20	0.71
1:A:343:THR:HG22	1:A:344:GLY:N	2.06	0.70
1:B:52:ILE:HG12	1:B:412:LEU:HD13	1.73	0.70
1:A:113:ALA:O	1:A:160:GLY:HA3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HB3	2:A:501:LDA:H111	1.73	0.70
1:A:45:PHE:HE1	1:A:421:PHE:CE1	2.09	0.70
1:A:308:SER:CB	1:A:314:LEU:HD21	2.16	0.70
1:B:113:ALA:O	1:B:160:GLY:HA3	1.91	0.70
1:B:343:THR:HG22	1:B:344:GLY:N	2.06	0.69
1:B:58:ILE:HD13	1:B:406:SER:HB3	1.74	0.69
1:A:178:THR:HG22	1:A:180:GLN:H	1.57	0.69
1:B:302:GLN:NE2	1:B:320:GLY:HA2	2.07	0.69
1:A:45:PHE:HE1	1:A:421:PHE:HE1	1.40	0.68
1:A:52:ILE:HG12	1:A:412:LEU:CD1	2.22	0.68
1:B:102:TYR:O	1:B:125:THR:HB	1.93	0.68
1:A:134:TYR:CE1	1:A:136:LEU:HD23	2.29	0.68
1:B:45:PHE:HE1	1:B:421:PHE:CE1	2.12	0.67
1:B:4:GLN:NE2	1:B:274:MET:HE1	2.10	0.67
1:B:150:TYR:CE2	1:B:152:ARG:HG3	2.30	0.67
1:B:178:THR:HG22	1:B:180:GLN:H	1.61	0.66
1:A:52:ILE:HG12	1:A:412:LEU:HD13	1.75	0.66
1:A:302:GLN:NE2	1:A:320:GLY:HA2	2.09	0.65
1:A:361:ILE:HG12	2:A:501:LDA:O1	1.95	0.65
1:B:398:ASN:OD1	1:B:403:GLN:HG2	1.97	0.64
1:A:150:TYR:CE2	1:A:152:ARG:HG3	2.32	0.64
1:B:199:HIS:C	1:B:200:LEU:HD12	2.23	0.64
1:B:19:GLY:HA2	1:B:278:SER:HB2	1.79	0.64
1:B:45:PHE:HE1	1:B:421:PHE:HE1	1.42	0.64
1:B:45:PHE:CE1	1:B:421:PHE:CE1	2.85	0.64
1:B:248:ASN:HD21	1:B:257:ALA:N	1.93	0.63
1:A:390:MET:HE3	1:A:412:LEU:CD2	2.23	0.63
1:A:267:LEU:HD23	1:A:267:LEU:C	2.23	0.62
1:A:378:ASN:OD1	1:A:380:ASP:HB2	2.00	0.62
1:A:199:HIS:C	1:A:200:LEU:HD12	2.24	0.62
1:A:4:GLN:NE2	1:A:274:MET:HE1	2.14	0.62
1:A:398:ASN:OD1	1:A:403:GLN:HG2	2.00	0.62
1:B:81:ASN:HD22	1:B:83:HIS:CE1	2.18	0.62
1:A:232:LYS:HG2	1:A:270:ASN:HD22	1.64	0.61
1:B:390:MET:HE3	1:B:412:LEU:CD2	2.27	0.61
1:A:19:GLY:HA2	1:A:278:SER:HB2	1.82	0.61
1:B:232:LYS:HG2	1:B:270:ASN:HD22	1.66	0.61
1:A:107:GLU:O	1:A:107:GLU:HG2	2.00	0.61
1:B:267:LEU:HD23	1:B:267:LEU:C	2.25	0.61
1:A:45:PHE:CE1	1:A:421:PHE:CE1	2.84	0.60
1:A:81:ASN:HD22	1:A:83:HIS:CE1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:HB2	1:A:245:ARG:NH1	2.16	0.60
1:B:191:ILE:HD12	1:B:191:ILE:H	1.67	0.60
1:B:361:ILE:HD11	2:B:502:LDA:HM12	1.84	0.60
1:B:378:ASN:OD1	1:B:380:ASP:HB2	2.02	0.60
1:A:343:THR:CG2	1:A:344:GLY:N	2.65	0.60
1:B:42:ARG:HD2	1:B:421:PHE:O	2.02	0.59
1:B:343:THR:CG2	1:B:344:GLY:N	2.65	0.59
1:A:236:LYS:HD3	1:A:266:TYR:CE2	2.37	0.59
1:A:191:ILE:H	1:A:191:ILE:HD12	1.68	0.58
1:A:297:SER:HA	1:A:323:ASP:CG	2.28	0.58
1:B:245:ARG:NH1	1:B:245:ARG:HB2	2.18	0.58
1:B:276:GLU:HG3	1:B:294:ALA:HB2	1.84	0.58
1:B:297:SER:HA	1:B:323:ASP:CG	2.29	0.58
1:B:177:GLN:HA	1:B:182:GLN:HE21	1.69	0.58
1:B:219:LYS:HE2	1:B:219:LYS:HA	1.85	0.58
1:B:236:LYS:HD3	1:B:266:TYR:CE2	2.38	0.58
1:B:370:SER:HB3	1:B:388:SER:OG	2.03	0.57
1:A:326:ARG:CG	1:A:348:ASP:HB3	2.31	0.57
1:B:11:SER:HB3	1:B:15:ARG:HH22	1.68	0.57
1:A:58:ILE:HD13	1:A:406:SER:CB	2.33	0.57
1:A:42:ARG:HD2	1:A:421:PHE:O	2.05	0.57
1:A:393:GLN:HE21	1:A:394:SER:H	1.52	0.57
1:B:107:GLU:O	1:B:107:GLU:HG2	2.04	0.57
1:B:176:GLY:O	1:B:182:GLN:HG3	2.05	0.57
1:B:121:THR:HG21	2:B:502:LDA:HM22	1.86	0.57
1:B:30:VAL:HG11	1:B:85:VAL:HG21	1.86	0.56
1:B:57:ASN:ND2	1:B:72:ASN:H	2.04	0.56
1:B:393:GLN:HE21	1:B:394:SER:H	1.52	0.56
1:A:248:ASN:HD21	1:A:257:ALA:N	1.94	0.56
1:A:177:GLN:HA	1:A:182:GLN:HE21	1.71	0.55
1:A:30:VAL:HG11	1:A:85:VAL:HG21	1.87	0.55
1:B:10:SER:HB2	1:B:416:ASN:HB2	1.87	0.55
1:A:290:HIS:HE1	1:A:332:THR:OG1	1.90	0.55
1:B:136:LEU:HD12	1:B:140:TRP:HB2	1.88	0.55
1:A:144:LEU:HD23	1:A:210:ASN:O	2.06	0.55
1:A:219:LYS:HE2	1:A:219:LYS:HA	1.88	0.55
1:B:169:GLN:HA	1:B:169:GLN:OE1	2.06	0.55
1:B:134:TYR:CD1	1:B:136:LEU:HD23	2.41	0.55
1:B:243:LEU:O	1:B:257:ALA:HB1	2.07	0.55
1:A:176:GLY:O	1:A:182:GLN:HG3	2.06	0.54
1:A:57:ASN:ND2	1:A:72:ASN:H	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:ND2	1:A:140:TRP:H	2.05	0.54
1:A:134:TYR:CD1	1:A:136:LEU:HD23	2.41	0.54
1:B:346:ALA:HB3	1:B:368:TRP:HB2	1.89	0.54
1:A:10:SER:HB2	1:A:416:ASN:HB2	1.89	0.54
1:A:81:ASN:HD22	1:A:83:HIS:HE1	1.55	0.54
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.07	0.54
1:A:276:GLU:HG3	1:A:294:ALA:HB2	1.89	0.54
1:A:239:TYR:CG	1:A:240:SER:N	2.76	0.54
1:A:11:SER:HB3	1:A:15:ARG:HH22	1.72	0.54
1:B:167:ALA:CB	1:B:189:ASN:HB2	2.37	0.54
1:B:239:TYR:CG	1:B:240:SER:N	2.76	0.54
1:B:58:ILE:HD13	1:B:406:SER:CB	2.36	0.54
1:A:246:ALA:O	1:A:248:ASN:N	2.41	0.53
1:B:113:ALA:C	1:B:160:GLY:HA3	2.33	0.53
1:B:144:LEU:HD23	1:B:210:ASN:O	2.07	0.53
1:A:167:ALA:CB	1:A:189:ASN:HB2	2.39	0.53
1:B:411:TRP:C	1:B:412:LEU:HD22	2.34	0.53
1:A:104:LEU:HD23	2:A:501:LDA:H12	1.90	0.53
1:B:137:ASN:ND2	1:B:140:TRP:H	2.05	0.53
1:A:346:ALA:HB3	1:A:368:TRP:HB2	1.91	0.53
1:A:136:LEU:HD12	1:A:140:TRP:HB2	1.90	0.53
1:B:81:ASN:HD22	1:B:83:HIS:HE1	1.56	0.52
1:B:1:ALA:HB1	1:B:4:GLN:HB3	1.91	0.52
1:B:246:ALA:O	1:B:248:ASN:N	2.42	0.52
1:A:89:ASN:ND2	1:A:91:GLN:H	2.07	0.52
1:A:113:ALA:C	1:A:160:GLY:HA3	2.34	0.52
1:A:227:TYR:HD1	1:A:275:TRP:NE1	2.08	0.52
1:B:326:ARG:CG	1:B:348:ASP:HB3	2.32	0.52
1:A:292:SER:O	1:A:327:ILE:HD13	2.09	0.52
1:B:292:SER:O	1:B:327:ILE:HD13	2.09	0.52
1:A:166:VAL:O	1:A:170:ILE:HG13	2.10	0.51
1:B:7:GLU:N	1:B:7:GLU:CD	2.68	0.51
1:B:354:ALA:HA	1:B:357:ARG:HG3	1.92	0.51
1:A:243:LEU:O	1:A:257:ALA:HB1	2.10	0.51
1:B:89:ASN:ND2	1:B:91:GLN:H	2.09	0.51
1:B:178:THR:HG22	1:B:180:GLN:HB2	1.92	0.51
1:A:26:ASP:HB2	1:A:418:ASN:ND2	2.25	0.51
1:B:26:ASP:HB2	1:B:418:ASN:ND2	2.26	0.51
1:B:220:ASN:HB3	1:B:282:ARG:HB3	1.93	0.51
1:A:137:ASN:C	1:A:137:ASN:HD22	2.19	0.51
1:B:137:ASN:C	1:B:137:ASN:HD22	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:HB	1:A:181:GLY:H	1.76	0.51
1:A:273:GLU:HG3	1:A:297:SER:OG	2.11	0.51
1:A:411:TRP:C	1:A:412:LEU:HD22	2.36	0.51
1:A:178:THR:HG22	1:A:180:GLN:HB2	1.92	0.50
1:B:18:SER:HB3	1:B:328:ALA:HB1	1.92	0.50
1:A:361:ILE:O	1:A:363:ASP:N	2.44	0.50
1:B:216:GLU:HB3	1:B:222:ARG:HB3	1.93	0.50
1:A:18:SER:HB3	1:A:328:ALA:HB1	1.92	0.50
1:A:1:ALA:HB1	1:A:4:GLN:HB3	1.94	0.50
1:B:58:ILE:HB	1:B:70:ALA:CB	2.27	0.50
1:B:273:GLU:HG3	1:B:297:SER:OG	2.10	0.50
1:B:289:ILE:HD12	1:B:331:THR:HB	1.93	0.50
1:A:66:ARG:HH11	1:A:161:ASP:HB3	1.76	0.50
1:A:89:ASN:CG	1:A:91:GLN:H	2.20	0.50
1:A:111:THR:HA	1:A:193:SER:HB3	1.93	0.50
1:A:216:GLU:HB3	1:A:222:ARG:HB3	1.94	0.50
1:A:220:ASN:HB3	1:A:282:ARG:HB3	1.93	0.50
1:B:66:ARG:HH11	1:B:161:ASP:HB3	1.77	0.49
1:B:378:ASN:O	1:B:379:LYS:CB	2.60	0.49
1:A:354:ALA:HA	1:A:357:ARG:HG3	1.93	0.49
1:A:137:ASN:ND2	1:A:139:ALA:H	2.10	0.49
1:A:358:SER:HB2	1:A:399:GLU:OE1	2.11	0.49
1:B:111:THR:HA	1:B:193:SER:HB3	1.95	0.49
1:A:54:PRO:HG2	1:A:74:ALA:O	2.12	0.49
1:A:289:ILE:HD12	1:A:331:THR:HB	1.92	0.49
1:B:73:ILE:HD11	1:B:362:PRO:HG2	1.94	0.49
1:B:361:ILE:HG12	2:B:502:LDA:CM2	2.32	0.49
1:B:361:ILE:O	1:B:363:ASP:N	2.44	0.49
1:A:246:ALA:C	1:A:248:ASN:H	2.20	0.49
1:A:370:SER:HB3	1:A:388:SER:OG	2.11	0.49
1:B:54:PRO:HG2	1:B:74:ALA:O	2.13	0.49
1:A:212:GLU:CG	1:A:226:THR:HG22	2.42	0.49
1:B:31:SER:HB3	1:B:83:HIS:HD2	1.78	0.48
1:B:166:VAL:O	1:B:170:ILE:HG13	2.13	0.48
1:B:246:ALA:C	1:B:248:ASN:H	2.21	0.48
1:B:290:HIS:HE1	1:B:332:THR:OG1	1.95	0.48
1:A:7:GLU:CD	1:A:7:GLU:N	2.71	0.48
1:B:293:LEU:HD13	1:B:327:ILE:HG12	1.95	0.48
1:A:137:ASN:HD21	1:A:140:TRP:H	1.61	0.48
1:B:200:LEU:HD12	1:B:200:LEU:N	2.28	0.48
1:B:178:THR:HB	1:B:181:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLN:NE2	1:A:274:MET:CE	2.77	0.48
1:B:4:GLN:NE2	1:B:274:MET:CE	2.76	0.48
1:B:239:TYR:CE2	1:B:314:LEU:HB3	2.48	0.48
1:A:64:SER:HB3	1:A:165:LEU:HD21	1.96	0.48
1:A:174:PRO:C	1:A:176:GLY:H	2.22	0.48
1:B:51:TYR:HD1	1:B:78:TRP:HD1	1.60	0.48
1:A:51:TYR:HD1	1:A:78:TRP:CD1	2.32	0.47
1:B:89:ASN:CG	1:B:91:GLN:H	2.22	0.47
1:B:51:TYR:HD1	1:B:78:TRP:CD1	2.32	0.47
1:B:212:GLU:CG	1:B:226:THR:HG22	2.40	0.47
1:A:298:TRP:HB3	1:A:321:PHE:HB3	1.97	0.47
1:A:51:TYR:HD1	1:A:78:TRP:HD1	1.61	0.47
1:B:137:ASN:ND2	1:B:139:ALA:H	2.12	0.47
1:B:137:ASN:HD21	1:B:140:TRP:H	1.61	0.47
1:B:147:ASN:ND2	1:B:210:ASN:OD1	2.46	0.47
1:B:31:SER:HB3	1:B:83:HIS:CD2	2.49	0.47
1:B:177:GLN:HA	1:B:182:GLN:NE2	2.29	0.47
1:B:1:ALA:HB1	1:B:4:GLN:CB	2.45	0.47
1:B:358:SER:HB2	1:B:399:GLU:OE1	2.14	0.47
1:B:30:VAL:CG1	1:B:85:VAL:HG21	2.44	0.46
1:B:30:VAL:HG23	1:B:30:VAL:O	2.16	0.46
1:A:227:TYR:HD1	1:A:275:TRP:CD1	2.33	0.46
1:A:378:ASN:O	1:A:379:LYS:CB	2.56	0.46
1:B:7:GLU:CD	1:B:7:GLU:H	2.24	0.46
1:B:16:ALA:HB2	1:B:370:SER:OG	2.16	0.46
1:A:31:SER:HB3	1:A:83:HIS:HD2	1.79	0.46
1:A:58:ILE:CD1	1:A:406:SER:HB3	2.42	0.46
1:A:66:ARG:NH1	1:A:161:ASP:HB3	2.30	0.46
1:A:364:GLN:HG3	1:A:393:GLN:O	2.16	0.46
1:B:64:SER:HB3	1:B:165:LEU:HD21	1.98	0.46
1:B:137:ASN:ND2	1:B:137:ASN:C	2.73	0.46
1:B:298:TRP:HB3	1:B:321:PHE:HB3	1.96	0.46
1:A:227:TYR:CD1	1:A:275:TRP:NE1	2.84	0.46
1:B:66:ARG:NH1	1:B:161:ASP:HB3	2.30	0.46
1:B:199:HIS:O	1:B:239:TYR:HA	2.16	0.46
1:A:281:ASN:O	1:A:288:ALA:HA	2.16	0.46
1:B:174:PRO:C	1:B:176:GLY:H	2.22	0.46
1:A:73:ILE:HD11	1:A:362:PRO:HG2	1.98	0.45
1:A:232:LYS:NZ	1:A:270:ASN:HD21	2.14	0.45
1:A:246:ALA:C	1:A:248:ASN:N	2.73	0.45
1:B:58:ILE:CD1	1:B:406:SER:HB3	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:C	1:B:248:ASN:N	2.74	0.45
1:A:177:GLN:HA	1:A:182:GLN:NE2	2.31	0.45
1:A:191:ILE:HD12	1:A:191:ILE:N	2.32	0.45
1:A:319:GLU:OE1	2:A:501:LDA:HM23	2.16	0.45
1:B:227:TYR:HD1	1:B:275:TRP:NE1	2.15	0.45
1:B:284:ASP:CG	1:B:285:PRO:HD2	2.42	0.45
1:A:200:LEU:HD12	1:A:200:LEU:N	2.30	0.45
1:A:284:ASP:CG	1:A:285:PRO:HD2	2.41	0.45
1:B:228:ARG:HB3	1:B:274:MET:HB3	1.98	0.45
1:B:116:SER:HA	1:B:158:PHE:O	2.17	0.45
1:B:177:GLN:CD	1:B:177:GLN:H	2.25	0.45
1:A:30:VAL:CG1	1:A:85:VAL:HG21	2.46	0.45
1:A:360:SER:C	1:A:362:PRO:HD3	2.42	0.45
1:B:241:SER:HB3	1:B:257:ALA:HA	1.99	0.45
1:B:297:SER:C	1:B:299:SER:H	2.24	0.45
1:A:340:THR:HB	1:A:374:THR:HB	1.99	0.45
1:A:252:LEU:N	1:A:252:LEU:CD1	2.76	0.45
1:B:121:THR:OG1	1:B:157:ARG:NH2	2.50	0.45
1:A:1:ALA:HB1	1:A:4:GLN:CB	2.47	0.44
1:A:31:SER:HB3	1:A:83:HIS:CD2	2.52	0.44
1:A:239:TYR:CE2	1:A:314:LEU:HB3	2.51	0.44
1:B:348:ASP:OD2	1:B:366:ARG:HB2	2.16	0.44
1:A:302:GLN:NE2	1:A:302:GLN:HA	2.33	0.44
1:B:157:ARG:HA	1:B:157:ARG:HD3	1.74	0.44
1:A:121:THR:OG1	1:A:157:ARG:NH2	2.51	0.44
1:B:227:TYR:HD1	1:B:275:TRP:CD1	2.36	0.44
1:A:299:SER:OG	1:A:323:ASP:OD2	2.33	0.44
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.88	0.44
1:B:364:GLN:O	1:B:366:ARG:HG3	2.18	0.44
1:A:177:GLN:CD	1:A:177:GLN:H	2.26	0.44
1:A:16:ALA:HB2	1:A:370:SER:OG	2.18	0.44
1:A:137:ASN:ND2	1:A:137:ASN:C	2.74	0.44
1:A:378:ASN:OD1	1:A:380:ASP:N	2.50	0.44
1:A:178:THR:C	1:A:180:GLN:N	2.75	0.44
1:B:302:GLN:NE2	1:B:302:GLN:HA	2.33	0.44
1:A:199:HIS:O	1:A:239:TYR:HA	2.18	0.43
1:A:244:ASN:C	1:A:246:ALA:N	2.76	0.43
1:A:299:SER:HA	1:A:321:PHE:O	2.18	0.43
1:A:364:GLN:O	1:A:366:ARG:HG3	2.17	0.43
1:A:228:ARG:HB3	1:A:274:MET:HB3	2.00	0.43
1:B:136:LEU:HD12	1:B:140:TRP:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:C	1:A:180:GLN:H	2.25	0.43
1:A:293:LEU:HD13	1:A:327:ILE:HG12	1.99	0.43
1:A:96:ALA:HA	1:A:129:ASN:O	2.19	0.43
1:B:299:SER:HA	1:B:321:PHE:O	2.18	0.43
1:B:355:GLN:HE21	1:B:355:GLN:HB2	1.64	0.43
1:A:30:VAL:O	1:A:30:VAL:HG23	2.18	0.43
1:A:267:LEU:C	1:A:267:LEU:CD2	2.91	0.43
1:B:348:ASP:OD2	1:B:348:ASP:O	2.37	0.43
1:A:7:GLU:CD	1:A:7:GLU:H	2.27	0.43
1:A:162:LEU:O	1:A:166:VAL:HG23	2.19	0.43
1:A:241:SER:HB3	1:A:257:ALA:HA	2.01	0.43
1:B:96:ALA:HA	1:B:129:ASN:O	2.19	0.43
1:B:114:GLY:O	1:B:115:GLY:C	2.61	0.43
1:B:340:THR:HB	1:B:374:THR:HB	2.01	0.43
1:A:348:ASP:OD2	1:A:366:ARG:HB2	2.19	0.43
1:B:134:TYR:CE1	1:B:136:LEU:CD2	2.99	0.43
1:A:116:SER:HA	1:A:158:PHE:O	2.19	0.43
1:A:171:MET:HE1	1:A:182:GLN:HG2	2.01	0.43
1:B:321:PHE:CZ	1:B:352:VAL:HG22	2.54	0.43
1:A:84:PHE:CZ	1:A:86:ALA:HB2	2.54	0.42
1:A:297:SER:C	1:A:299:SER:H	2.27	0.42
1:B:19:GLY:HA2	1:B:292:SER:HB3	2.01	0.42
1:A:136:LEU:HD12	1:A:140:TRP:CB	2.49	0.42
1:A:321:PHE:CZ	1:A:352:VAL:HG22	2.55	0.42
1:B:88:ILE:HG13	1:B:93:GLY:HA2	2.02	0.42
1:B:178:THR:C	1:B:180:GLN:H	2.27	0.42
1:A:196:LYS:HE3	1:A:196:LYS:HB2	1.89	0.42
1:B:272:PRO:HG2	1:B:298:TRP:CD2	2.54	0.42
1:B:355:GLN:H	1:B:355:GLN:HG3	1.40	0.42
1:A:191:ILE:H	1:A:191:ILE:CD1	2.33	0.42
1:A:272:PRO:HG2	1:A:298:TRP:CD2	2.54	0.42
1:B:232:LYS:NZ	1:B:270:ASN:HD21	2.18	0.42
1:B:281:ASN:O	1:B:288:ALA:HA	2.20	0.42
1:A:204:GLN:HG3	1:A:205:TRP:N	2.34	0.42
1:A:353:PRO:O	1:A:354:ALA:C	2.62	0.42
1:B:145:GLY:O	1:B:209:TRP:HA	2.20	0.42
1:B:177:GLN:CD	1:B:177:GLN:N	2.78	0.42
1:B:353:PRO:O	1:B:354:ALA:C	2.62	0.42
1:A:282:ARG:HG3	1:A:282:ARG:HH11	1.85	0.42
1:B:238:ASN:HB3	1:B:262:THR:CG2	2.50	0.42
1:A:273:GLU:H	1:A:300:GLN:HE22	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:THR:C	1:B:180:GLN:N	2.77	0.41
1:B:291:TYR:CD2	1:B:291:TYR:N	2.88	0.41
1:B:364:GLN:HG3	1:B:393:GLN:O	2.20	0.41
1:B:84:PHE:CZ	1:B:86:ALA:HB2	2.56	0.41
1:A:157:ARG:HA	1:A:157:ARG:HD3	1.75	0.41
1:B:162:LEU:O	1:B:166:VAL:HG23	2.21	0.41
1:B:378:ASN:OD1	1:B:380:ASP:N	2.53	0.41
1:B:191:ILE:HD12	1:B:191:ILE:N	2.31	0.41
1:B:267:LEU:C	1:B:267:LEU:CD2	2.92	0.41
1:A:147:ASN:ND2	1:A:210:ASN:OD1	2.46	0.41
1:B:282:ARG:HG3	1:B:282:ARG:HH11	1.85	0.41
1:B:58:ILE:CB	1:B:70:ALA:HB3	2.28	0.41
1:B:244:ASN:C	1:B:246:ALA:N	2.76	0.41
1:B:171:MET:HE1	1:B:182:GLN:HG2	2.01	0.41
1:B:227:TYR:CD1	1:B:275:TRP:NE1	2.89	0.41
1:B:239:TYR:O	1:B:240:SER:HB3	2.20	0.41
1:A:244:ASN:C	1:A:246:ALA:H	2.29	0.41
1:B:204:GLN:HG3	1:B:205:TRP:N	2.35	0.41
1:B:273:GLU:HG2	1:B:300:GLN:OE1	2.21	0.41
1:B:361:ILE:CD1	2:B:502:LDA:HM12	2.49	0.41
1:A:271:LEU:HA	1:A:272:PRO:HD3	1.83	0.41
1:B:380:ASP:O	1:B:419:TYR:HA	2.21	0.41
1:A:8:PHE:CD1	1:A:8:PHE:C	2.99	0.40
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.88	0.40
1:A:220:ASN:HB3	1:A:282:ARG:CB	2.51	0.40
1:A:177:GLN:CD	1:A:177:GLN:N	2.79	0.40
1:B:272:PRO:HA	1:B:300:GLN:NE2	2.36	0.40
1:B:360:SER:C	1:B:362:PRO:HD3	2.46	0.40
1:A:19:GLY:HA2	1:A:292:SER:HB3	2.03	0.40
1:A:143:GLY:O	1:A:211:ALA:HA	2.22	0.40
1:A:348:ASP:OD2	1:A:348:ASP:O	2.39	0.40
1:B:223:TYR:CD1	1:B:223:TYR:N	2.88	0.40
1:B:244:ASN:C	1:B:246:ALA:H	2.30	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	414/427 (97%)	382 (92%)	26 (6%)	6 (1%)	9	30
1	B	414/427 (97%)	376 (91%)	32 (8%)	6 (1%)	9	30
All	All	828/854 (97%)	758 (92%)	58 (7%)	12 (1%)	9	30

All (12) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [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	330/338 (98%)	296 (90%)	34 (10%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	330/338 (98%)	297 (90%)	33 (10%)	7	24
All	All	660/676 (98%)	593 (90%)	67 (10%)	7	23

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	71	ASP
1	A	78	TRP
1	A	107	GLU
1	A	120	THR
1	A	124	GLU
1	A	125	THR
1	A	137	ASN
1	A	142	PHE
1	A	144	LEU
1	A	180	GLN
1	A	197	THR
1	A	200	LEU
1	A	219	LYS
1	A	226	THR
1	A	252	LEU
1	A	264	SER
1	A	277	VAL
1	A	282	ARG
1	A	284	ASP
1	A	297	SER
1	A	307	THR
1	A	309	THR
1	A	317	LYS
1	A	327	ILE
1	A	329	LEU
1	A	331	THR
1	A	349	ASP
1	A	355	GLN
1	A	361	ILE
1	A	373	THR
1	A	407	GLU
1	A	412	LEU
1	A	416	ASN
1	B	30	VAL
1	B	71	ASP

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Mol	Chain	Res	Type
1	B	78	TRP
1	B	107	GLU
1	B	120	THR
1	B	124	GLU
1	B	125	THR
1	B	137	ASN
1	B	142	PHE
1	B	144	LEU
1	B	180	GLN
1	B	197	THR
1	B	200	LEU
1	B	219	LYS
1	B	226	THR
1	B	252	LEU
1	B	264	SER
1	B	277	VAL
1	B	282	ARG
1	B	284	ASP
1	B	297	SER
1	B	307	THR
1	B	309	THR
1	B	317	LYS
1	B	327	ILE
1	B	329	LEU
1	B	331	THR
1	B	349	ASP
1	B	355	GLN
1	B	361	ILE
1	B	407	GLU
1	B	412	LEU
1	B	416	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	33	ASN
1	A	57	ASN
1	A	72	ASN
1	A	81	ASN
1	A	83	HIS
1	A	127	ASN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	138	ASN
1	A	182	GLN
1	A	220	ASN
1	A	248	ASN
1	A	270	ASN
1	A	281	ASN
1	A	290	HIS
1	A	300	GLN
1	A	302	GLN
1	A	303	GLN
1	A	316	GLN
1	A	338	ASN
1	A	355	GLN
1	A	356	ASN
1	A	364	GLN
1	A	393	GLN
1	A	416	ASN
1	A	418	ASN
1	B	4	GLN
1	B	33	ASN
1	B	57	ASN
1	B	72	ASN
1	B	81	ASN
1	B	83	HIS
1	B	127	ASN
1	B	137	ASN
1	B	138	ASN
1	B	182	GLN
1	B	220	ASN
1	B	248	ASN
1	B	270	ASN
1	B	281	ASN
1	B	286	GLN
1	B	290	HIS
1	B	300	GLN
1	B	302	GLN
1	B	303	GLN
1	B	318	HIS
1	B	338	ASN
1	B	355	GLN
1	B	356	ASN

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Mol	Chain	Res	Type
1	B	364	GLN
1	B	393	GLN
1	B	416	ASN
1	B	418	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LDA	B	502	-	13,15,15	1.96	1 (7%)	14,17,17	1.52	2 (14%)
2	LDA	A	501	-	13,15,15	2.06	1 (7%)	14,17,17	1.72	4 (28%)

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	502	-	-	3/13/13/13	-
2	LDA	A	501	-	-	9/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LDA	O1-N1	-6.79	1.25	1.42
2	B	502	LDA	O1-N1	-6.67	1.25	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LDA	CM1-N1-C1	-3.99	101.85	110.23
2	B	502	LDA	CM1-N1-C1	-3.19	103.54	110.23
2	A	501	LDA	CM2-N1-C1	2.83	116.17	110.23
2	B	502	LDA	C9-C8-C7	-2.42	102.11	114.37
2	A	501	LDA	C9-C8-C7	-2.15	103.49	114.37
2	A	501	LDA	O1-N1-C1	2.12	114.46	109.27

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LDA	C2-C1-N1-O1
2	A	501	LDA	C2-C1-N1-CM1
2	A	501	LDA	C2-C1-N1-CM2
2	A	501	LDA	C11-C10-C9-C8
2	B	502	LDA	C11-C10-C9-C8
2	A	501	LDA	C1-C2-C3-C4
2	B	502	LDA	C2-C3-C4-C5
2	A	501	LDA	C3-C4-C5-C6
2	A	501	LDA	N1-C1-C2-C3
2	A	501	LDA	C6-C7-C8-C9
2	B	502	LDA	N1-C1-C2-C3
2	A	501	LDA	C7-C8-C9-C10

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	LDA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LDA	5	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, 95th 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	418/427 (97%)	0.14	16 (3%) 44 36	7, 31, 63, 92	0
1	B	418/427 (97%)	0.60	46 (11%) 10 9	16, 47, 90, 108	0
All	All	836/854 (97%)	0.37	62 (7%) 20 17	7, 38, 84, 108	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	GLY	5.0
1	B	183	ALA	5.0
1	B	181	GLY	4.6
1	B	188	ALA	4.5
1	B	175	ALA	4.2
1	A	178	THR	4.2
1	B	174	PRO	4.2
1	B	253	PRO	4.0
1	B	180	GLN	4.0
1	B	171	MET	3.8
1	B	178	THR	3.8
1	B	182	GLN	3.7
1	A	177	GLN	3.6
1	B	252	LEU	3.4
1	B	166	VAL	3.3
1	B	170	ILE	3.3
1	B	173	SER	3.3
1	B	187	THR	3.2
1	A	411	TRP	3.1
1	A	176	GLY	3.1
1	A	1	ALA	3.1
1	B	177	GLN	3.1
1	B	275	TRP	3.0
1	B	210	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	179	GLN	3.0
1	A	78	TRP	2.9
1	A	142	PHE	2.9
1	B	167	ALA	2.8
1	A	275	TRP	2.8
1	A	170	ILE	2.7
1	A	185	ALA	2.7
1	B	142	PHE	2.7
1	B	169	GLN	2.7
1	B	186	ALA	2.6
1	B	246	ALA	2.6
1	A	169	GLN	2.6
1	B	2	GLY	2.6
1	B	168	GLY	2.6
1	B	136	LEU	2.5
1	A	180	GLN	2.5
1	B	172	GLN	2.5
1	A	175	ALA	2.4
1	B	1	ALA	2.4
1	B	57	ASN	2.4
1	B	33	ASN	2.4
1	B	397	ILE	2.4
1	B	161	ASP	2.3
1	B	59	SER	2.3
1	B	407	GLU	2.3
1	B	115	GLY	2.2
1	B	78	TRP	2.2
1	B	299	SER	2.2
1	B	179	GLN	2.2
1	B	5	LEU	2.2
1	B	248	ASN	2.1
1	B	159	ALA	2.1
1	A	172	GLN	2.1
1	B	70	ALA	2.1
1	A	174	PRO	2.1
1	B	311	GLY	2.1
1	B	138	ASN	2.0
1	B	398	ASN	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	LDA	B	502	16/16	0.73	0.14	70,71,77,78	0
2	LDA	A	501	16/16	0.87	0.15	67,70,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.