



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:34 PM UTC

PDB ID : 1T1L / pdb_00001t1l
Title : Crystal structure of the long-chain fatty acid transporter FadL
Authors : van den Berg, B.; Black, P.N.; Clemons Jr., W.M.; Rapoport, T.A.
Deposited on : 2004-04-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

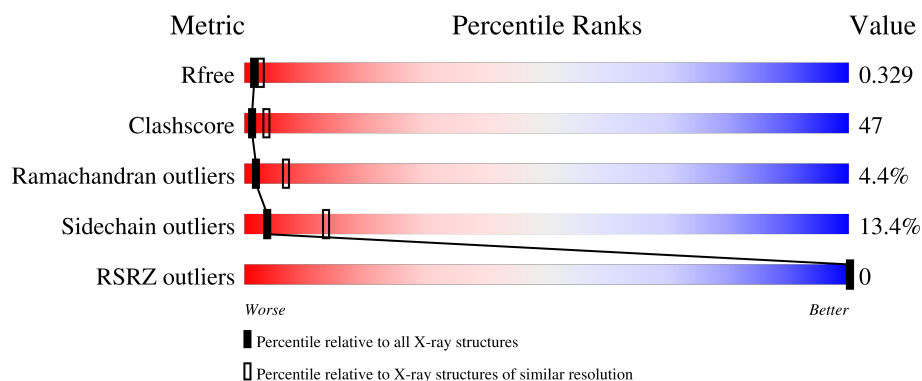
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	
1	B	427	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6642 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

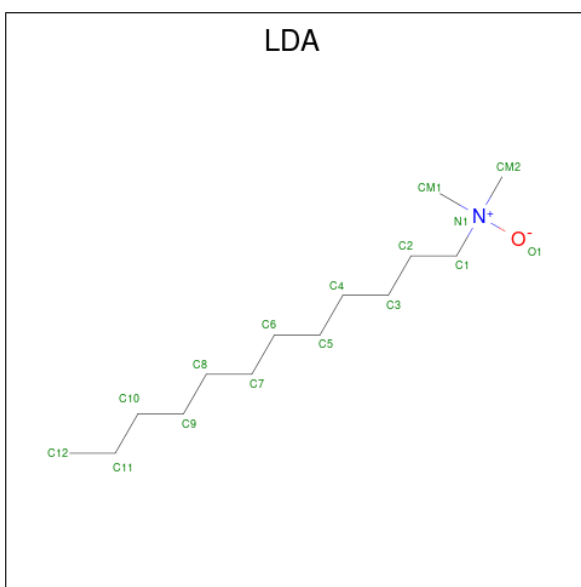
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3252	2057	552	637	6			
1	B	421	Total	C	N	O	S	0	0	0
			3252	2057	552	637	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	expression tag	UNP P10384
A	423	HIS	-	expression tag	UNP P10384
A	424	HIS	-	expression tag	UNP P10384
A	425	HIS	-	expression tag	UNP P10384
A	426	HIS	-	expression tag	UNP P10384
A	427	HIS	-	expression tag	UNP P10384
B	422	HIS	-	expression tag	UNP P10384
B	423	HIS	-	expression tag	UNP P10384
B	424	HIS	-	expression tag	UNP P10384
B	425	HIS	-	expression tag	UNP P10384
B	426	HIS	-	expression tag	UNP P10384
B	427	HIS	-	expression tag	UNP P10384

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (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		

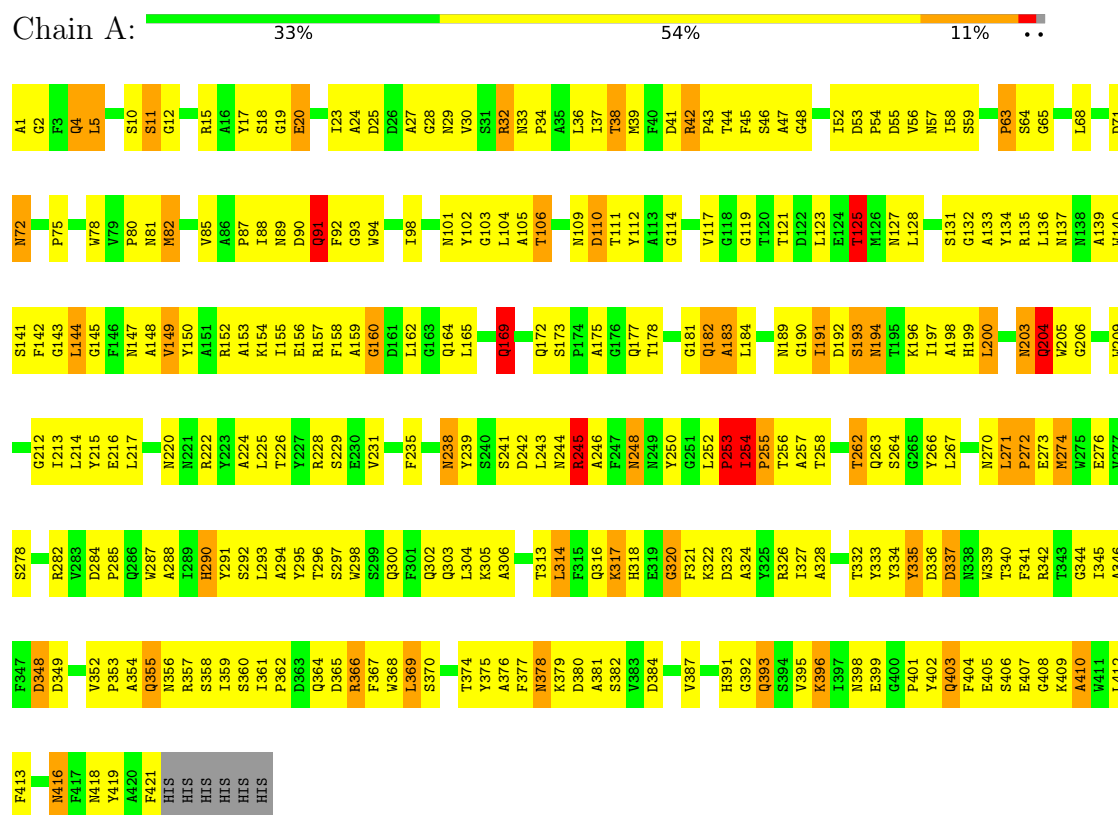
- Molecule 3 is water.

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

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



L412	T343	V277	N201
F413	G344	S278	G202
G414	I345	G279	N203
T415	A346	I280	Q204
M416	F347	N281	M205
F417	D348	R282	G206
M418	S349	V283	F207
A420	G350	D284	—
F421	P351	P285	A211
HIS	V352	Q286	G212
HIS	P353	N287	T213
HIS	A354	A288	L214
HIS	Q355	I289	Y215
HIS	N356	H290	E216
HIS	R357	I291	L217
HIS	S358	S292	D218
HIS	I359	I293	K219
	S360	A294	N220
	P361	Y295	N221
	P362	T296	R222
	D363	S297	Y223
	G364	M298	A224
	P365	S299	L225
	K366	Q300	T226
	F367	F301	Y227
	M368	Q302	—
	L369	Q303	E230
	S370	L304	V231
		K305	K232
		A306	T233
	T374	T307	—
	Y375	S308	G237
	A376	T309	N238
	K379	S310	Y239
	D380	—	S240
		L314	S241
	V383	F315	—
	D384	Q316	Y250
		K317	G251
	S388	H318	L252
		F319	P253
	H391	G320	T254
	G392	F321	P255
	Q393	K322	—
	S394	D323	A257
	V395	A324	—
	K396	Y325	T262
		R326	Q263
	E399	—	—
	G400	L329	Y266
	P401	T332	L267
	Y402	Y333	T268
		Y334	L269
	E405	Y335	N270
	S406	—	L271
	E407	W339	P272
	G408	N340	E273
	K409	F341	M274
	A410	T340	M275
	P411	P412	F276

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.02Å 122.02Å 164.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	11.99 – 2.80 11.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (11.99-2.80) 98.6 (11.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.298 , 0.331 0.298 , 0.329	Depositor DCC
R_{free} test set	1638 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.447 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6642	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.56	0/3341	1.13	33/4549 (0.7%)
1	B	0.57	0/3341	1.09	27/4549 (0.6%)
All	All	0.57	0/6682	1.11	60/9098 (0.7%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ILE	N-CA-C	12.75	136.42	108.88
1	A	254	ILE	CA-C-N	-12.20	104.60	119.84
1	A	254	ILE	C-N-CA	-12.20	104.60	119.84
1	A	271	LEU	CA-C-N	11.21	133.86	119.84
1	A	271	LEU	C-N-CA	11.21	133.86	119.84
1	B	283	VAL	N-CA-C	10.88	121.26	112.12
1	A	337	ASP	N-CA-C	-9.16	102.10	113.28
1	A	217	LEU	N-CA-C	-8.85	101.92	112.89
1	B	254	ILE	N-CA-C	8.60	127.47	108.88
1	B	219	LYS	N-CA-C	-8.10	101.57	112.26
1	B	284	ASP	CA-C-N	-7.67	112.31	119.82
1	B	284	ASP	C-N-CA	-7.67	112.31	119.82
1	A	4	GLN	N-CA-C	7.27	122.85	113.18
1	B	91	GLN	CA-CB-CG	-7.12	99.85	114.10
1	B	4	GLN	N-CA-C	7.09	122.61	113.18
1	B	299	SER	N-CA-C	-6.68	105.20	113.15
1	A	250	TYR	N-CA-C	-6.66	104.86	114.12
1	A	169	GLN	N-CA-C	-6.63	105.00	113.23
1	B	300	GLN	N-CA-C	-6.63	105.16	113.18
1	B	396	LYS	N-CA-C	-6.62	100.72	110.52
1	A	235	PHE	N-CA-C	6.33	118.90	109.59
1	A	193	SER	N-CA-C	6.25	117.89	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	GLN	N-CA-C	-6.20	105.55	113.23
1	B	250	TYR	N-CA-C	-6.11	103.91	113.02
1	A	20	GLU	N-CA-C	-6.05	102.12	110.35
1	B	369	LEU	N-CA-C	-6.01	99.35	108.67
1	A	63	PRO	N-CA-C	-5.97	105.59	113.65
1	B	91	GLN	N-CA-C	-5.91	107.88	114.62
1	B	254	ILE	CA-C-N	-5.81	112.57	119.84
1	B	254	ILE	C-N-CA	-5.81	112.57	119.84
1	B	11	SER	N-CA-C	-5.80	104.33	111.40
1	A	11	SER	N-CA-C	-5.78	104.34	111.40
1	A	255	PRO	N-CA-C	-5.66	100.80	112.47
1	B	252	LEU	CA-C-N	5.62	126.86	119.84
1	B	252	LEU	C-N-CA	5.62	126.86	119.84
1	A	393	GLN	N-CA-C	5.62	117.51	109.14
1	A	204	GLN	N-CA-C	5.61	117.94	109.41
1	A	370	SER	N-CA-C	5.60	117.69	109.24
1	B	284	ASP	N-CA-C	-5.52	99.48	108.82
1	A	177	GLN	N-CA-C	-5.52	106.55	113.28
1	A	91	GLN	N-CA-C	-5.47	108.38	114.62
1	B	63	PRO	N-CA-C	-5.47	105.93	113.53
1	B	317	LYS	N-CA-C	-5.47	101.21	109.85
1	B	125	THR	N-CA-C	5.44	117.77	108.90
1	A	91	GLN	N-CA-CB	-5.43	102.61	111.18
1	A	248	ASN	N-CA-C	5.41	118.08	110.23
1	A	222	ARG	N-CA-C	5.39	117.00	108.96
1	A	203	ASN	N-CA-C	5.38	116.20	107.32
1	B	20	GLU	N-CA-C	-5.35	103.28	110.24
1	A	406	SER	N-CA-C	5.33	117.75	109.60
1	A	149	VAL	N-CA-C	5.29	115.72	107.99
1	B	173	SER	CA-C-N	5.25	126.41	119.84
1	B	173	SER	C-N-CA	5.25	126.41	119.84
1	A	172	GLN	N-CA-C	-5.23	106.75	113.23
1	A	125	THR	N-CA-C	5.21	117.39	108.90
1	A	344	GLY	N-CA-C	5.17	118.61	110.91
1	B	149	VAL	N-CA-C	5.13	115.48	107.99
1	A	183	ALA	N-CA-C	-5.08	107.08	113.28
1	A	224	ALA	N-CA-C	5.07	117.51	109.50
1	A	91	GLN	CA-CB-CG	-5.03	104.04	114.10

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	298	0
1	B	3252	0	3033	299	0
2	A	16	0	31	8	0
2	B	16	0	31	6	0
3	A	52	0	0	16	0
3	B	54	0	0	26	0
All	All	6642	0	6128	594	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 47.

All (594) 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:HH11	1:A:245:ARG:HB2	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:199:HIS:C	1:A:200:LEU:HD23	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:B:396:LYS:N	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: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
1:A:127:ASN:HD21	1:A:147:ASN:HB2	1.44	0.80
1:B:200:LEU:O	1:B:201:ASN:HB3	1.81	0.79
1:B:34:PRO:HB2	1:B:143:GLY:HA3	1.63	0.79
1:B:273:GLU:HG2	3:B:457:HOH:O	1.83	0.79
1:A:34:PRO:HB2	1:A:143:GLY:HA3	1.63	0.78
1:A:57:ASN:HD22	1:A:72:ASN:H	1.31	0.78
1:A:298:TRP:O	1:A:321:PHE:HB2	1.83	0.78
1:B:88:ILE:HG22	1:B:89:ASN:OD1	1.84	0.77
1:A: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:HG2	1:B:282:ARG:NH1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:PHE:HA	3:B:471:HOH:O	1.91	0.68
1:B:280:TYR:HE1	1:B:288:ALA:HB1	1.58	0.68
1:A:149:VAL:O	1:A:206:GLY:N	2.26	0.68
1:B:367:PHE:CG	1:B:391:HIS:HB3	2.29	0.68
1:A:117:VAL:HG23	1:A:359:ILE:HD11	1.76	0.68
1:B:231:VAL:HB	1:B:271:LEU:HD12	1.75	0.68
1:A:244:ASN:HD22	1:A:245:ARG:H	1.40	0.68
1:B:339:TRP:CZ3	1:B:375:TYR:HB2	2.30	0.67
1:B:367:PHE:HB2	1:B:391:HIS:N	2.09	0.67
1:A:364:GLN:HE21	1:A:393:GLN:N	1.92	0.67
1:A:153:ALA:HB1	2:A:428:LDA:H102	1.77	0.67
1:A:409:LYS:O	1:A:410:ALA:HB2	1.95	0.66
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:395:VAL:C	1:B:396:LYS:HE3	2.21	0.65
1:B:357:ARG:HD2	1:B:395:VAL:HG21	1.77	0.65
1:A:282:ARG:NH2	1:A:285:PRO:O	2.29	0.65
1:A:209:TRP:O	1:A:229:SER:HB3	1.96	0.65
1:A:252:LEU:O	1:A:254:ILE:HG23	1.96	0.65
1:A:376:ALA:HA	1:A:382:SER:CB	2.26	0.65
1:A:403:GLN:HE21	1:A:403:GLN:HA	1.62	0.65
1:B:5:LEU:HD22	1:B:32:ARG:HH21	1.62	0.65
1:B:104:LEU:HD22	2:B:428:LDA:H31	1.79	0.64
1:A:5:LEU:HD22	1:A:32:ARG:HH21	1.63	0.64
1:B:279:GLY:HA3	1:B:291:TYR:CE1	2.33	0.64
1:B:117:VAL:HG23	1:B:359:ILE:HD11	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:HIS:O	1:B:239:TYR:HA	1.97	0.64
1:A:157:ARG:C	1:A:197:ILE:HG12	2.22	0.64
1:A:297:SER:HB2	1:A:300:GLN:OE1	1.97	0.64
1:B:360:SER:O	1:B:362:PRO:HD3	1.96	0.64
1:B:38:THR:HG21	1:B:135:ARG:HB2	1.81	0.63
1:B:173:SER:O	1:B:175:ALA:N	2.31	0.63
1:B:241:SER:HB2	3:B:449:HOH:O	1.97	0.63
1:A:231:VAL:HB	1:A:271:LEU:HB2	1.80	0.63
1:A:220:ASN:HD21	1:A:282:ARG:HD3	1.63	0.63
1:B:302:GLN:O	1:B:320:GLY:N	2.27	0.63
1:A:254:ILE:O	1:A:255:PRO:C	2.39	0.63
1:A:38:THR:HG21	1:A:135:ARG:HB2	1.81	0.63
1:A:117:VAL:HB	1:A:399:GLU:OE1	1.98	0.63
1:B:393:GLN:HE21	1:B:395:VAL:CG1	2.12	0.63
1:A:245:ARG:HB2	1:A:245:ARG:NH1	2.09	0.62
1:B:183:ALA:C	1:B:185:ALA:H	2.06	0.62
1:B:125:THR:HG22	1:B:150:TYR:O	1.98	0.62
1:A:156:GLU:HA	1:A:198:ALA:O	1.99	0.62
1:B:52:ILE:HG23	1:B:412:LEU:HD22	1.81	0.62
1:A:377:PHE:CD1	1:A:382:SER:HA	2.35	0.62
1:B:43:PRO:HA	1:B:85:VAL:O	2.00	0.62
1:B:303:GLN:NE2	1:B:316:GLN:HE22	1.97	0.62
1:B:364:GLN:CG	1:B:392:GLY:HA3	2.25	0.62
1:B:277:VAL:O	1:B:292:SER:HA	2.00	0.62
1:B:346:ALA:HB3	1:B:368:TRP:HB2	1.82	0.62
1:A:324:ALA:HB1	1:A:349:ASP:O	1.99	0.61
1:B:155:ILE:HG13	2:B:428:LDA:H111	1.81	0.61
1:B:55:ASP:HB3	1:B:409:LYS:HG3	1.83	0.61
1: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:203:ASN:C	1:A:204:GLN:NE2	2.60	0.59
1:B:90:ASP:OD1	1:B:90:ASP:O	2.19	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:A:189:ASN:HB3	3:A:472:HOH:O	2.02	0.59
1:A:136:LEU:HD22	1:A:142:PHE:CE1	2.37	0.59
1:B:232:LYS:HG2	1:B:270:ASN:HD21	1.63	0.59
1:A:282:ARG:NH1	1:A:334:TYR:CE1	2.70	0.59
1:A:364:GLN:CG	1:A:392:GLY:HA3	2.28	0.59
1:A:360:SER:O	1:A:362:PRO:HD3	2.02	0.59
1:B:308:SER:HB3	1:B:314:LEU:CD1	2.32	0.59
1:A:403:GLN:HA	1:A:403:GLN:NE2	2.18	0.59
1:B:411:TRP:HB3	1:B:413:PHE:CZ	2.37	0.58
1:A:149:VAL:N	1:A:206:GLY:O	2.31	0.58
1:A:144:LEU:HD12	1:A:145:GLY:N	2.19	0.58
1:B:37:ILE:C	1:B:39:MET:H	2.10	0.58
1:B:396:LYS:HG3	1:B:405:GLU:OE1	2.02	0.58
1:A:184:LEU:HB2	3:A:444:HOH:O	2.02	0.58
1:B:383:VAL:CG2	1:B:384:ASP:N	2.65	0.58
1:A: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:393:GLN:NE2	1:B:395:VAL:CG1	2.67	0.58
1:A:37:ILE:C	1:A:39:MET:H	2.11	0.57
1:A:297:SER:HA	1:A:323:ASP:OD1	2.04	0.57
1:A:57:ASN:HD22	1:A:72:ASN:N	2.02	0.57
1:A:103:GLY:N	2:A:428:LDA:HM23	2.19	0.57
1:A:243:LEU:HD12	3:A:458:HOH:O	2.03	0.57
1:A:68:LEU:CD1	1:A:402:TYR:HB3	2.35	0.57
1:B:54:PRO:HD2	1:B:75:PRO:O	2.04	0.57
1:B:339:TRP:HZ3	1:B:375:TYR:HB2	1.68	0.57
1:A:37:ILE:HB	1:A:133:ALA:HB3	1.86	0.57
1:B:333:TYR:HB3	1:B:341:PHE:HB2	1.85	0.57
1:B:136:LEU:HD22	1:B:142:PHE:CE1	2.40	0.57
1:A:18:SER:O	1:A:23:ILE:HD11	2.05	0.57
1:A:376:ALA:HA	1:A:382:SER:HB3	1.87	0.57
1:A:157:ARG:HB3	1:A:197:ILE:HD11	1.86	0.56
1:A:54:PRO:HD2	1:A:75:PRO:O	2.04	0.56
1:A:106:THR:HG21	1:A:360:SER:HA	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ALA:O	1:A:193:SER:HA	2.04	0.56
1:A:387:VAL:HG22	1:A:413:PHE:HD2	1.70	0.56
1:B:288:ALA:O	1:B:289:ILE:HG13	2.04	0.56
1:A:381:ALA:HB2	1:A:419:TYR:HD1	1.70	0.56
1:B:18:SER:O	1:B:23:ILE:HD11	2.05	0.56
1:B:343:THR:HG22	1:B:344:GLY:N	2.21	0.56
1:A:284:ASP:HB3	1:A:287:TRP:H	1.69	0.56
1:B:11:SER:HB2	1:B:15:ARG:NH2	2.20	0.56
1:B:37:ILE:HB	1:B:133:ALA:HB3	1.87	0.56
1:A:34:PRO:HB2	1:A:143:GLY:CA	2.34	0.56
1:B:157:ARG:C	1:B:197:ILE:HG12	2.31	0.56
1:A:102:TYR:HB3	2:A:428:LDA:HM21	1.87	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: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
1:B:64:SER:HB3	1:B:165:LEU:HG	1.88	0.56
1:B:157:ARG:O	1:B:197:ILE:HG12	2.06	0.55
1:B:317:LYS:HD3	1:B:318:HIS:N	2.21	0.55
1:A:33:ASN:HB3	1:A:36:LEU:HD12	1.89	0.55
1:A:253:PRO:HB2	3:A:480:HOH:O	2.06	0.55
1:A:377:PHE:CE1	1:A:382:SER:HA	2.40	0.55
1:B:308:SER:HB3	1:B:314:LEU:HD13	1.89	0.55
1:A:245:ARG:HH12	1:A:258:THR:C	2.14	0.55
1:A:220:ASN:ND2	1:A:282:ARG:HD3	2.21	0.55
1:B:33:ASN:HB3	1:B:36:LEU:HD12	1.88	0.55
1:A:136:LEU:HD22	1:A:142:PHE:HE1	1.71	0.55
1:B:86:ALA:HB1	3:B:466:HOH:O	2.06	0.55
1:B:178:THR:O	1:B:182:GLN:HG3	2.07	0.55
1:A:127:ASN:HD22	1:A:127:ASN:C	2.12	0.55
1:A:354:ALA:O	1:A:357:ARG:HG3	2.07	0.55
1:A:41:ASP:OD1	1:A:42:ARG:HD3	2.07	0.55
1:B:12:GLY:CA	1:B:15:ARG:NH1	2.70	0.55
1:A:123:LEU:HD22	2:A:428:LDA:H51	1.89	0.54
1:A:131:SER:HB3	1:A:145:GLY:HA3	1.88	0.54
1:A:178:THR:C	1:A:182:GLN:NE2	2.65	0.54
1:A:378:ASN:N	1:A:378:ASN:HD22	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:A:90:ASP:O	2.24	0.54
1:A:282:ARG:HA	1:A:288:ALA:CB	2.38	0.54
1:B:57:ASN:HD22	1:B:72:ASN:N	1.99	0.54
1:B:366:ARG:HB3	1:B:367:PHE:HD1	1.73	0.54
1:B:192:ASP:OD2	1:B:195:THR:OG1	2.26	0.54
1:A:19:GLY:HA2	1:A:278:SER:HB2	1.90	0.53
1:B:68:LEU:HD11	1:B:402:TYR:HB3	1.90	0.53
1:B:384:ASP:O	1:B:415:THR:HA	2.09	0.53
1:A:364:GLN:NE2	1:A:393:GLN:H	2.01	0.53
1:B:324:ALA:HB1	1:B:349:ASP:O	2.09	0.53
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.73	0.53
1:B: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:B:360:SER:C	1:B:362:PRO:HD3	2.33	0.53
1:A:155:ILE:HG13	2:A:428:LDA:H101	1.90	0.53
1:A:317:LYS:HD3	1:A:318:HIS:N	2.24	0.53
1:B:218:ASP:CG	1:B:219:LYS:N	2.65	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:23:ILE:HB	1:A:29:ASN:HD21	1.74	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:B:112:TYR:CE2	1:B:114:GLY:HA3	2.45	0.52
1:B:143:GLY:O	1:B:211:ALA:HB1	2.08	0.52
1:A:293:LEU:HD13	1:A:327:ILE:HD13	1.90	0.52
1:A:398:ASN:OD1	1:A:403:GLN:NE2	2.42	0.52
1:B:220:ASN:O	1:B:282:ARG:HB3	2.08	0.52
1:B:364:GLN:HG3	1:B:392:GLY:CA	2.30	0.52
1:A:101:ASN:ND2	1:A:127:ASN:HB2	2.25	0.52
1:A:220:ASN:ND2	1:A:282:ARG:HB3	2.25	0.52
1:B:291:TYR:HB3	1:B:329:LEU:HD23	1.91	0.52
1:B:139:ALA:C	3:B:451:HOH:O	2.53	0.52
1:B:299:SER:HA	1:B:321:PHE:O	2.09	0.52
1:B:322:LYS:NZ	1:B:352:VAL:N	2.57	0.52
1:A:18:SER:OG	1:A:290:HIS:HD2	1.91	0.52
1:A:346:ALA:O	1:A:368:TRP:N	2.37	0.52
1:B:153:ALA:HB1	2:B:428:LDA:H112	1.91	0.52
1:B:222:ARG:HG2	1:B:222:ARG:NH1	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:201:ASN:O	1:B:237:GLY:HA3	2.10	0.52
1:A:52:ILE:HG12	1:A:412:LEU:HD13	1.92	0.52
1:B:375:TYR:HB3	1:B:383:VAL:CG1	2.39	0.52
1:B:75:PRO:HD2	1:B:105:ALA:O	2.10	0.52
1:A:12:GLY:CA	1:A:15:ARG:NH1	2.71	0.52
1:A:98:ILE:CG1	1:A:128:LEU:HD23	2.34	0.52
1:B:23:ILE:HB	1:B:29:ASN:HD21	1.74	0.51
1:B:198:ALA:HA	3:B:449:HOH:O	2.09	0.51
1:A:340:THR:HG21	1:A:342:ARG:HH21	1.75	0.51
1:A:393:GLN:O	1:A:407:GLU:HA	2.10	0.51
1:B: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:220:ASN:OD1	1:A:282:ARG:HD3	2.10	0.51
1:A:364:GLN:CG	1:A:408:GLY:HA3	2.24	0.51
1:A:200:LEU:HD23	1:A:200:LEU:N	2.25	0.51
1:A:267:LEU:HD13	2:A:428:LDA:H112	1.93	0.51
1:B:139:ALA:O	1:B:215:TYR:HA	2.10	0.51
1:B:162:LEU:HB2	3:B:444:HOH:O	2.10	0.51
1:B:232:LYS:HG2	1:B:270:ASN:HD22	1.71	0.51
1:A:403:GLN:HE21	1:A:403:GLN:CA	2.24	0.51
1:B:127:ASN:HD22	1:B:127:ASN:C	2.14	0.51
1:B:293:LEU:HA	1:B:326:ARG:O	2.11	0.51
1:B:45:PHE:CD1	1:B:45:PHE:C	2.89	0.51
1:A:45:PHE:C	1:A:45:PHE:CD1	2.88	0.50
1:B:63:PRO:C	1:B:65:GLY:H	2.19	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:297:SER:C	1:B:299:SER:H	2.20	0.50
1:A:94:TRP:HA	1:A:132:GLY:HA2	1.93	0.50
1:B:89:ASN:HB2	1:B:91:GLN:HG2	1.94	0.50
1:B:48:GLY:O	1:B:80:PRO:HA	2.12	0.50
1:B:366:ARG:NH2	1:B:393:GLN:OE1	2.44	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:266:TYR:HE1	1:B:309:THR:HG22	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASN:ND2	1:B:291:TYR:OH	2.45	0.49
1:B:345:ILE:CG2	1:B:346:ALA:N	2.75	0.49
1:B:355:GLN:C	1:B:356:ASN:OD1	2.55	0.49
1:A:23:ILE:HB	1:A:29:ASN:ND2	2.27	0.49
1:A:203:ASN:H	1:A:204:GLN:HE22	1.58	0.49
1:B:158:PHE:O	1:B:197:ILE:HD13	2.12	0.49
1:B:364:GLN:HG2	1:B:408:GLY:N	2.27	0.49
1:A:276:GLU:OE1	1:A:294:ALA:HB2	2.12	0.49
1:B:23:ILE:HB	1:B:29:ASN:ND2	2.28	0.49
1:B:315:PHE:HE2	1:B:317:LYS:HB2	1.77	0.49
1:B:34:PRO:HB2	1:B:143:GLY:CA	2.38	0.49
1:B:41:ASP:OD1	1:B:42:ARG:HD3	2.12	0.49
1:A:267:LEU:C	1:A:267:LEU:HD23	2.38	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:104:LEU:HD11	1:B:361:ILE:HG12	1.93	0.49
1:A:63:PRO:C	1:A:65:GLY:H	2.20	0.49
1:A:381:ALA:HB2	1:A:419:TYR:CD1	2.47	0.49
1:B:136:LEU:HD22	1:B:142:PHE:HE1	1.77	0.49
1:B:288:ALA:HB2	1:B:334:TYR:HE1	1.77	0.49
1:A:10:SER:HB2	1:A:416:ASN:HB2	1.95	0.49
1:B:70:ALA:HA	3:B:432:HOH:O	2.13	0.49
1:B:127:ASN:C	1:B:127:ASN:ND2	2.70	0.49
1:A:41:ASP:C	1:A:87:PRO:HG3	2.37	0.49
1:A:104:LEU:HB3	2:A:428:LDA:O1	2.13	0.49
1:B:109:ASN:O	1:B:111:THR:N	2.46	0.49
1:B:305:LYS:HE3	1:B:316:GLN:HE22	1.78	0.48
1:A:34:PRO:HD2	1:A:212:GLY:HA3	1.94	0.48
1:A:353:PRO:HB2	1:A:355:GLN:NE2	2.27	0.48
1:B:20:GLU:HB3	1:B:32:ARG:HG2	1.95	0.48
1:B:219:LYS:HB2	1:B:219:LYS:HE2	1.56	0.48
1:A:2:GLY:HA3	1:A:365:ASP:OD2	2.14	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:B:180:GLN:CG	1:B:184:LEU:HD22	2.44	0.48
1:B:281:ASN:O	1:B:282:ARG:C	2.55	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:127:ASN:C	1:A:127:ASN:ND2	2.70	0.48
1:A:178:THR:C	1:A:182:GLN:HE21	2.22	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:GLU:HA	1:B:294:ALA:HA	1.96	0.48
1:A:291:TYR:N	1:A:291:TYR:CD2	2.82	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: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:A:375:TYR:HE2	1:A:377:PHE:CD2	2.32	0.48
1:A:384:ASP:N	1:A:416:ASN:O	2.38	0.48
1:A:387:VAL:HG22	1:A:413:PHE:CD2	2.47	0.48
1:B:33:ASN:HB3	1:B:36:LEU:CD1	2.44	0.48
1:B:101:ASN:ND2	1:B:127:ASN:HB2	2.28	0.48
1:B:104:LEU:HD23	1:B:104:LEU:H	1.79	0.48
1:B:218:ASP:CG	1:B:219:LYS:H	2.21	0.48
1:A:305:LYS:CG	1:A:316:GLN:HE22	2.20	0.48
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.77	0.47
1:B:122:ASP:HB3	3:B:470:HOH:O	2.12	0.47
1:B:266:TYR:CE1	1:B:309:THR:HG22	2.48	0.47
1:A:75:PRO:HD2	1:A:105:ALA:O	2.13	0.47
1:B:272:PRO:C	3:B:457:HOH:O	2.57	0.47
1:A:238:ASN:N	1:A:238:ASN:ND2	2.60	0.47
1:B:32:ARG:HH22	1:B:274:MET:HE1	1.79	0.47
1:A:5:LEU:HD23	3:A:463:HOH:O	2.14	0.47
1:B:251:GLY:C	1:B:252:LEU:HD23	2.39	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:159:ALA:O	1:A:160:GLY:O	2.32	0.47
1:A:353:PRO:HB2	1:A:355:GLN:HE22	1.79	0.47
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
1:B:142:PHE:CD2	1:B:213:ILE:HG12	2.50	0.47
1:B:146:PHE:CE2	1:B:207:PHE:HD1	2.33	0.47
1:B:298:TRP:C	1:B:300:GLN:H	2.21	0.47
1:B:304:LEU:HB2	1:B:317:LYS:HB3	1.96	0.47
1:A:184:LEU:HD23	1:A:184:LEU:C	2.39	0.47
1:A:367:PHE:CE1	1:A:391:HIS:HB3	2.50	0.47
1:A:407:GLU:HG3	1:A:408:GLY:N	2.28	0.47
1:B:37:ILE:HB	1:B:133:ALA:CB	2.45	0.47
1:A:244:ASN:N	3:A:457:HOH:O	2.39	0.47
1:B:196:LYS:HD2	1:B:199:HIS:HB2	1.97	0.47
1:A:156:GLU:CD	1:A:196:LYS:HE3	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ILE:HG12	1:A:369:LEU:HD12	1.96	0.47
1:A:345:ILE:HA	1:A:368:TRP:O	2.16	0.46
1:A:348:ASP:OD2	1:A:348:ASP:N	2.47	0.46
1:B:41:ASP:C	1:B:87:PRO:HG3	2.40	0.46
1:B:180:GLN:NE2	1:B:184:LEU:CD2	2.78	0.46
1:A:190:GLY:O	1:A:191:ILE:C	2.58	0.46
1:A:215:TYR:CD1	1:A:215:TYR:C	2.93	0.46
1:B:345:ILE:HG22	1:B:346:ALA:N	2.30	0.46
1:A:140:TRP:CZ2	1:A:215:TYR:HD2	2.32	0.46
1:B:13:LEU:O	1:B:370:SER:OG	2.33	0.46
1:B:15:ARG:NH1	1:B:20:GLU:OE2	2.48	0.46
1:B:157:ARG:HG3	1:B:157:ARG:HH11	1.79	0.46
1:B:322:LYS:NZ	1:B:351:PRO:C	2.73	0.46
1:B:146:PHE:CZ	1:B:207:PHE:HD1	2.33	0.46
1:A:33:ASN:HB3	1:A:36:LEU:CD1	2.46	0.46
1:A:241:SER:HB3	1:A:258:THR:H	1.81	0.46
1:B:37:ILE:HG21	1:B:93:GLY:C	2.40	0.46
1:B:180:GLN:HE21	1:B:184:LEU:CD1	2.28	0.46
1:B:104:LEU:HD21	2:B:428:LDA:H52	1.97	0.46
1:B:152:ARG:NH1	1:B:203:ASN:HD21	2.14	0.46
1:B:307:THR:HA	1:B:314:LEU:H	1.80	0.46
1:A:395:VAL:HG23	1:A:395:VAL:O	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:183:ALA:C	1:B:185:ALA:N	2.74	0.46
1:A:169:GLN:O	1:A:173:SER:HB3	2.16	0.46
1:A:263:GLN:HB3	1:A:264:SER:H	1.48	0.46
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.79	0.45
1:A:352:VAL:HG12	1:A:353:PRO:O	2.16	0.45
1:A:90:ASP:H	1:A:91:GLN:HG2	1.82	0.45
1:A:340:THR:CG2	1:A:341:PHE:N	2.79	0.45
1:A:396:LYS:N	1:A:396:LYS:HE3	2.31	0.45
1:B:152:ARG:NH1	1:B:203:ASN:ND2	2.63	0.45
1:B:393:GLN:NE2	1:B:395:VAL:HG13	2.18	0.45
1:A:15:ARG:NH1	1:A:20:GLU:OE2	2.49	0.45
1:A:142:PHE:CD2	1:A:213:ILE:HG12	2.52	0.45
1:A:378:ASN:O	1:A:380:ASP:N	2.49	0.45
1:B:10:SER:CB	1:B:416:ASN:HD22	2.28	0.45
1:B:38:THR:CG2	1:B:135:ARG:HB2	2.46	0.45
1:B:187:THR:HA	3:B:468:HOH:O	2.16	0.45
1:A:321:PHE:CE2	1:A:352:VAL:HG22	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HG21	1:A:93:GLY:C	2.41	0.45
1:B:158:PHE:C	1:B:197:ILE:HG23	2.41	0.45
1:A:82:MET:HE2	1:B:82:MET:HE2	1.97	0.45
1:B:109:ASN:C	1:B:111:THR:N	2.75	0.45
1:A:302:GLN:OE1	1:A:320:GLY:HA2	2.17	0.45
1:B:32:ARG:HD2	1:B:32:ARG:HA	1.60	0.45
1:A:38:THR:CG2	1:A:135:ARG:HB2	2.46	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:197:ILE:O	3:A:458:HOH:O	2.21	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:B:342:ARG:HD3	3:B:465:HOH:O	2.17	0.45
1:B:37:ILE:HG21	1:B:93:GLY:O	2.16	0.45
1:A:17:TYR:HB2	1:A:326:ARG:HH22	1.82	0.44
1:B:4:GLN:OE1	1:B:348:ASP:HB3	2.17	0.44
1:B:102:TYR:CD1	1:B:271:LEU:HD22	2.52	0.44
1:B:241:SER:OG	1:B:257:ALA:HA	2.16	0.44
1:B:339:TRP:HA	1:B:339:TRP:CE3	2.52	0.44
1:A:59:SER:O	1:A:405:GLU:N	2.50	0.44
1:A:117:VAL:HB	1:A:399:GLU:CD	2.43	0.44
1:A:244:ASN:O	1:A:246:ALA:N	2.51	0.44
1:A:32:ARG:HD2	1:A:32:ARG:HA	1.59	0.44
1:A:36:LEU:O	1:A:39:MET:HB2	2.18	0.44
1:A:200:LEU:HD22	1:A:239:TYR:CD1	2.53	0.44
1:A:276:GLU:HA	1:A:294:ALA:HA	1.99	0.44
1:A:335:TYR:CD2	1:A:336:ASP:HB2	2.53	0.44
1:A:364:GLN:CB	1:A:392:GLY:HA3	2.47	0.44
1:A:378:ASN:N	1:A:378:ASN:ND2	2.66	0.44
1:A:154:LYS:HB3	3:A:448:HOH:O	2.18	0.44
1:A:355:GLN:O	1:A:356:ASN:ND2	2.50	0.44
1:A:376:ALA:HA	1:A:382:SER:HB2	1.97	0.44
1:A:25:ASP:OD2	1:A:334:TYR:OH	2.26	0.44
1:A:220:ASN:CG	1:A:282:ARG:HD3	2.43	0.44
1:B:160:GLY:N	3:B:444:HOH:O	2.51	0.44
1:B:322:LYS:HE2	3:B:481:HOH:O	2.18	0.44
1:A:239:TYR:HE2	1:A:256:THR:O	2.01	0.44
1:A:402:TYR:HB2	1:A:404:PHE:CE1	2.52	0.44
1:B:36:LEU:O	1:B:39:MET:HB2	2.17	0.44
1:B:357:ARG:CD	1:B:395:VAL:HG21	2.47	0.44
1:A:37:ILE:HB	1:A:133:ALA:CB	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:364:GLN:HG2	1:A:407:GLU:C	2.42	0.43
1:B:128:LEU:O	1:B:147:ASN:HA	2.18	0.43
1:B:325:TYR:H	1:B:349:ASP:HB3	1.81	0.43
1:A:44:THR:N	1:A:85:VAL:O	2.47	0.43
1:A:204:GLN:NE2	1:A:204:GLN:N	2.66	0.43
1:A:366:ARG:O	1:A:367:PHE:HB3	2.18	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:41:ASP:O	1:A:87:PRO:HG3	2.18	0.43
1:A:37:ILE:HG21	1:A:93:GLY:O	2.19	0.43
1:A:403:GLN:NE2	1:A:403:GLN:CA	2.82	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:27:ALA:HB2	1:B:44:THR:HG22	2.01	0.43
1:B:180:GLN:HE21	1:B:184:LEU:HD11	1.83	0.43
1:B:297:SER:C	1:B:299:SER:N	2.77	0.43
1:B:326:ARG:HG3	1:B:348:ASP:OD2	2.17	0.43
1:A:152:ARG:HA	1:A:203:ASN:OD1	2.19	0.43
1:B:282:ARG:NH1	1:B:282:ARG:CG	2.72	0.43
1:A:37:ILE:C	1:A:39:MET:N	2.75	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:N	1:B:223:TYR:CD1	2.86	0.43
1:B:204:GLN:HG3	1:B:205:TRP:N	2.32	0.43
1:B:303:GLN:NE2	1:B:305:LYS:HE3	2.34	0.43
1:A:1:ALA:HB3	1:A:368:TRP:CZ2	2.54	0.43
1:A:333:TYR:N	1:A:341:PHE:O	2.49	0.43
1:B:18:SER:C	1:B:290:HIS:HB2	2.44	0.43
1:B:174:PRO:C	1:B:176:GLY:N	2.77	0.43
1:B:227:TYR:CE1	1:B:275:TRP:NE1	2.86	0.43
1:A:106:THR:O	1:A:106:THR:HG22	2.17	0.42
1:A:112:TYR:C	1:A:114:GLY:H	2.27	0.42
1:A:336:ASP:HA	3:A:461:HOH:O	2.18	0.42
1:B:112:TYR:C	1:B:114:GLY:H	2.27	0.42
1:B:225:LEU:HD12	1:B:277:VAL:CG1	2.49	0.42
1:A:56:VAL:HG13	1:A:407:GLU:O	2.18	0.42
1:A:360:SER:HB2	1:A:361:ILE:HD12	2.02	0.42
1:A:47:ALA:HA	1:A:81:ASN:O	2.19	0.42
1:A:135:ARG:NH1	1:A:137:ASN:O	2.42	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:CE2	1:B:32:ARG:HD3	2.54	0.42
1:B:342:ARG:NH1	3:B:465:HOH:O	2.52	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:4:GLN:NE2	1:A:326:ARG:HB2	2.34	0.42
1:A:155:ILE:O	1:A:199:HIS:HA	2.19	0.42
1:A:213:ILE:HG22	1:A:214:LEU:N	2.34	0.42
1:B:5:LEU:CD2	1:B:32:ARG:HH21	2.31	0.42
1:A:109:ASN:C	1:A:111:THR:N	2.76	0.42
1:A:244:ASN:C	1:A:246:ALA:N	2.78	0.42
1:B:141:SER:HB2	1:B:214:LEU:HB3	2.02	0.42
1:B:18:SER:O	1:B:290:HIS:HB2	2.20	0.42
1:B:91:GLN:HG2	1:B:91:GLN:H	1.41	0.42
1:B:54:PRO:CD	1:B:75:PRO:O	2.68	0.42
1:B:115:GLY:CA	3:B:464:HOH:O	2.68	0.42
1:A:353:PRO:CB	1:A:355:GLN:HE22	2.33	0.42
1:B:53:ASP:OD2	1:B:53:ASP:C	2.62	0.42
1:B:281:ASN:O	1:B:283:VAL:HG13	2.19	0.42
1:A:4:GLN:HA	3:A:467:HOH:O	2.20	0.41
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:B:364:GLN:HE21	1:B:393:GLN:C	2.28	0.41
1:A:33:ASN:OD1	1:A:212:GLY:HA3	2.20	0.41
1:A:244:ASN:ND2	1:A:244:ASN:C	2.78	0.41
1:A:306:ALA:O	1:A:314:LEU:HB2	2.21	0.41
1:B:305:LYS:CE	1:B:316:GLN:NE2	2.83	0.41
1:B:179:GLN:H	1:B:179:GLN:HG2	1.64	0.41
1:B: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:A:46:SER:OG	1:A:418:ASN:ND2	2.53	0.41
1:A:153:ALA:HB1	2:A:428:LDA:C10	2.49	0.41
1:A:238:ASN:HB2	1:A:262:THR:HG23	2.02	0.41
1:A:345:ILE:HG12	1:A:369:LEU:CD1	2.51	0.41
1:B:44:THR:N	1:B:85:VAL:O	2.44	0.41
1:B:161:ASP:OD1	1:B:161:ASP:C	2.63	0.41
1:B:334:TYR:O	1:B:335:TYR:C	2.63	0.41
1:A:155:ILE:HD11	1:A:304:LEU:HD21	2.01	0.41
1:B:37:ILE:C	1:B:39:MET:N	2.75	0.41
1:B:282:ARG:HD2	1:B:287:TRP:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:200:LEU:O	1:B:201:ASN:CB	2.58	0.41
1:A:5:LEU:CD2	1:A:32:ARG:HH21	2.33	0.41
1:A:33:ASN:HA	1:A:34:PRO:HD3	1.89	0.41
1:A:45:PHE:HD1	1:A:46:SER:N	2.19	0.41
1:A:209:TRP:H	1:A:229:SER:HB3	1.86	0.41
1:A:254:ILE:H	1:A:254:ILE:HG13	1.65	0.41
1:A:273:GLU:HG2	1:A:297:SER:OG	2.21	0.41
1:A:298:TRP:O	1:A:321:PHE:CB	2.62	0.41
1:B:10:SER:H	1:B:416:ASN:ND2	2.19	0.41
1:B:45:PHE:HD1	1:B:46:SER:N	2.19	0.41
1:B:267:LEU:C	1:B:267:LEU:HD23	2.46	0.41
1:B:306:ALA:HB3	1:B:315:PHE:HB3	2.03	0.41
1:B:322:LYS:HE2	3:B:441:HOH:O	2.20	0.41
1:B:361:ILE:O	1:B:362:PRO:C	2.63	0.41
1:B:106:THR:O	1:B:106:THR:HG22	2.20	0.41
1:B:364:GLN:HE21	1:B:393:GLN:N	2.19	0.41
1:B:411:TRP:HB3	1:B:413:PHE:CE1	2.55	0.41
1:B:284:ASP:C	1:B:286:GLN:N	2.76	0.40
1:B:388:SER:HB2	3:B:453:HOH:O	2.21	0.40
1:A:378:ASN:C	1:A:380:ASP:H	2.30	0.40
1:B:12:GLY:HA3	1:B:17:TYR:CE2	2.56	0.40
1:A:53:ASP:OD2	1:A:53:ASP:C	2.63	0.40
1:A:63:PRO:C	1:A:65:GLY:N	2.77	0.40
1:A:375:TYR:HE2	1:A:377:PHE:CE2	2.39	0.40
1:B:63:PRO:C	1:B:65:GLY:N	2.78	0.40
1:B:21:GLY:C	1:B:36:LEU:HD11	2.47	0.40
1:B:98:ILE:CG1	1:B:128:LEU:HD23	2.34	0.40
1:B:288:ALA:HB2	1:B:334:TYR:CE1	2.57	0.40
1:A:358:SER:HB2	3:A:462:HOH:O	2.21	0.40
1:A:384:ASP:OD2	1:A:418:ASN:OD1	2.39	0.40
1:B:282:ARG:NH2	1:B:285:PRO:O	2.52	0.40
1:B:308:SER:HB3	1:B:314:LEU:HD11	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/427 (98%)	346 (83%)	57 (14%)	16 (4%)	2	9
1	B	419/427 (98%)	340 (81%)	58 (14%)	21 (5%)	1	5
All	All	838/854 (98%)	686 (82%)	115 (14%)	37 (4%)	2	7

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	24	ALA
1	A	253	PRO
1	A	320	GLY
1	B	35	ALA
1	B	184	LEU
1	B	255	PRO
1	B	366	ARG
1	A	119	GLY
1	B	119	GLY
1	A	28	GLY
1	A	401	PRO
1	B	28	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/337 (98%)	290 (88%)	41 (12%)	4	16
1	B	331/337 (98%)	283 (86%)	48 (14%)	3	11
All	All	662/674 (98%)	573 (87%)	89 (13%)	4	13

All (89) 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	125	THR
1	A	141	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	144	LEU
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	204	GLN
1	A	216	GLU
1	A	225	LEU
1	A	226	THR
1	A	238	ASN
1	A	245	ARG
1	A	253	PRO
1	A	262	THR
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	348	ASP
1	A	355	GLN
1	A	366	ARG
1	A	369	LEU
1	A	374	THR
1	A	378	ASN
1	A	396	LYS
1	A	403	GLN
1	A	416	ASN
1	B	5	LEU
1	B	32	ARG
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	141	SER
1	B	162	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	164	GLN
1	B	169	GLN
1	B	174	PRO
1	B	179	GLN
1	B	217	LEU
1	B	219	LYS
1	B	225	LEU
1	B	230	GLU
1	B	240	SER
1	B	252	LEU
1	B	253	PRO
1	B	254	ILE
1	B	255	PRO
1	B	262	THR
1	B	263	GLN
1	B	273	GLU
1	B	277	VAL
1	B	283	VAL
1	B	285	PRO
1	B	289	ILE
1	B	290	HIS
1	B	300	GLN
1	B	307	THR
1	B	310	SER
1	B	314	LEU
1	B	325	TYR
1	B	339	TRP
1	B	349	ASP
1	B	356	ASN
1	B	364	GLN
1	B	366	ARG
1	B	370	SER
1	B	396	LYS
1	B	407	GLU
1	B	412	LEU
1	B	421	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	72	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	81	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	238	ASN
1	A	244	ASN
1	A	248	ASN
1	A	263	GLN
1	A	290	HIS
1	A	303	GLN
1	A	316	GLN
1	A	318	HIS
1	A	355	GLN
1	A	356	ASN
1	A	364	GLN
1	A	378	ASN
1	A	416	ASN
1	A	418	ASN
1	B	57	ASN
1	B	72	ASN
1	B	81	ASN
1	B	127	ASN
1	B	164	GLN
1	B	179	GLN
1	B	180	GLN
1	B	194	ASN
1	B	270	ASN
1	B	281	ASN
1	B	303	GLN
1	B	316	GLN
1	B	364	GLN
1	B	403	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 [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	428	-	13,15,15	2.00	1 (7%)	14,17,17	1.67	4 (28%)
2	LDA	A	428	-	13,15,15	1.90	1 (7%)	14,17,17	1.63	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	B	428	-	-	4/13/13/13	-
2	LDA	A	428	-	-	5/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	428	LDA	O1-N1	-6.89	1.25	1.42
2	A	428	LDA	O1-N1	-6.45	1.26	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	428	LDA	CM1-N1-C1	-3.97	101.89	110.23
2	A	428	LDA	CM1-N1-C1	-3.68	102.51	110.23
2	A	428	LDA	O1-N1-C1	2.49	115.38	109.27
2	B	428	LDA	O1-N1-C1	2.24	114.76	109.27
2	B	428	LDA	C9-C8-C7	-2.16	103.47	114.37
2	B	428	LDA	CM2-N1-C1	2.13	114.71	110.23
2	A	428	LDA	C9-C8-C7	-2.12	103.68	114.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 14 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	421/427 (98%)	-1.20	0 100 100	24, 41, 52, 63	0
1	B	421/427 (98%)	-1.16	0 100 100	26, 43, 59, 91	0
All	All	842/854 (98%)	-1.18	0 100 100	24, 41, 56, 91	0

There are no RSRZ outliers to report.

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

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(Å ²)	Q<0.9
2	LDA	A	428	16/16	0.99	0.06	56,60,72,73	0
2	LDA	B	428	16/16	0.99	0.07	53,57,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.