



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:43 AM UTC

PDB ID : 3B9N / pdb_00003b9n
Title : Crystal structure of long-chain alkane monooxygenase (LadA)
Authors : Li, L.; Yang, W.; Xu, F.; Bartlam, M.; Rao, Z.
Deposited on : 2007-11-06
Resolution : 2.70 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
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

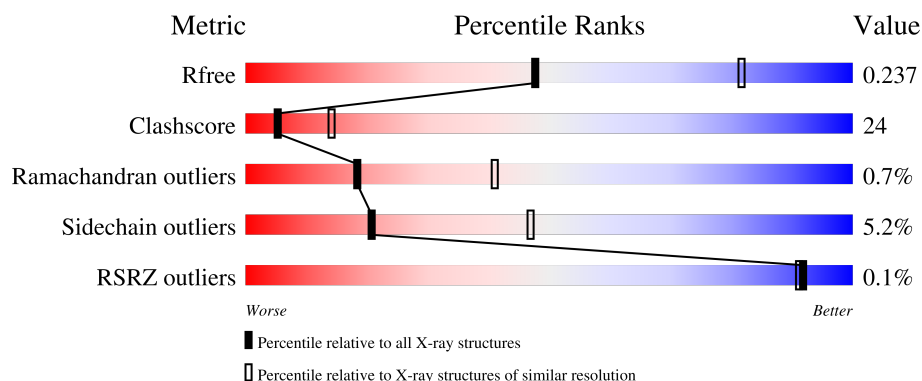
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	440	 56% 37% 5% •
1	B	440	 53% 40% 5% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7369 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 Alkane monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3513	2243	609	647	14			
1	B	434	Total	C	N	O	S	0	0	0
			3520	2248	609	648	15			

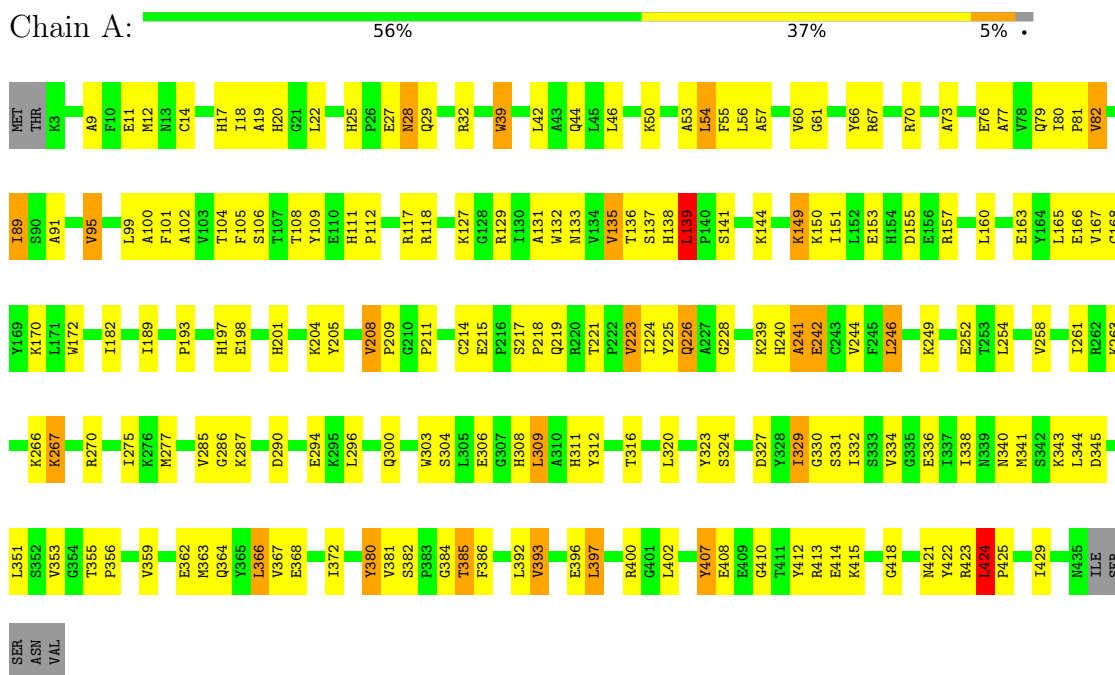
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	172	Total	O	0	0
			172	172		
2	B	164	Total	O	0	0
			164	164		

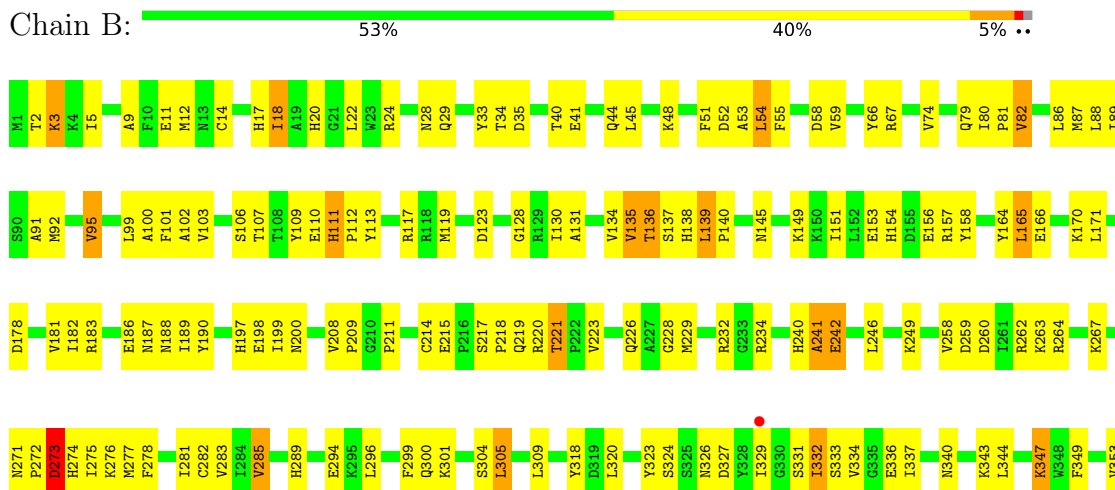
3 Residue-property plots [i](#)

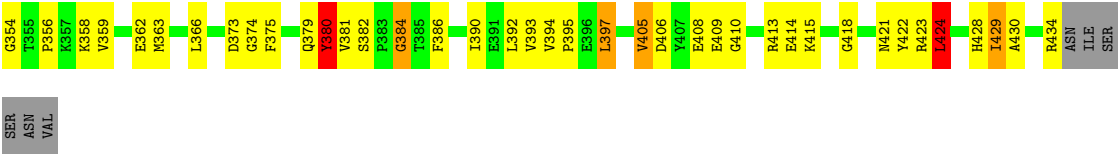
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Alkane monooxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.50Å 77.50Å 323.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 72.0 (50.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	19.30 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.249 0.184 , 0.237	Depositor DCC
R_{free} test set	2160 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtrriage
Anisotropy	0.846	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7369	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4297e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/3606	0.98	21/4877 (0.4%)
1	B	0.42	0/3613	1.00	22/4886 (0.5%)
All	All	0.42	0/7219	0.99	43/9763 (0.4%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ILE	N-CA-C	11.81	121.75	110.30
1	B	242	GLU	N-CA-C	-9.36	102.37	113.88
1	A	139	LEU	CA-C-N	8.90	129.47	119.32
1	A	139	LEU	C-N-CA	8.90	129.47	119.32
1	A	380	TYR	N-CA-C	-8.73	103.21	114.04
1	A	136	THR	N-CA-C	-8.33	96.17	109.59
1	A	242	GLU	N-CA-C	-8.30	103.67	113.88
1	A	89	ILE	N-CA-C	8.01	118.56	110.23
1	B	111	HIS	CA-C-N	7.81	128.53	119.47
1	B	111	HIS	C-N-CA	7.81	128.53	119.47
1	B	380	TYR	N-CA-C	-7.46	104.78	114.04
1	B	139	LEU	CA-C-N	7.35	127.21	119.05
1	B	139	LEU	C-N-CA	7.35	127.21	119.05
1	A	241	ALA	N-CA-C	7.16	120.61	110.23
1	A	208	VAL	CA-C-N	6.76	126.22	118.85
1	A	208	VAL	C-N-CA	6.76	126.22	118.85
1	B	264	ARG	N-CA-C	-6.61	104.47	112.54
1	B	208	VAL	CA-C-N	6.59	126.53	119.28
1	B	208	VAL	C-N-CA	6.59	126.53	119.28
1	A	424	LEU	CA-C-N	6.50	126.42	119.85
1	A	424	LEU	C-N-CA	6.50	126.42	119.85
1	A	224	ILE	N-CA-C	6.41	117.06	107.51
1	B	109	TYR	N-CA-C	6.01	120.42	112.72
1	A	160	LEU	N-CA-C	-5.76	105.08	111.36
1	B	136	THR	N-CA-C	-5.70	101.59	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	TYR	N-CA-C	5.63	120.41	112.93
1	A	60	VAL	N-CA-C	-5.58	107.29	112.43
1	A	393	VAL	N-CA-C	5.52	115.72	110.53
1	B	241	ALA	N-CA-C	5.44	117.91	110.24
1	B	331	SER	N-CA-C	-5.36	107.39	114.04
1	B	20	HIS	N-CA-C	5.30	117.91	109.96
1	A	223	VAL	N-CA-C	-5.29	102.75	109.58
1	B	111	HIS	N-CA-C	5.27	116.05	109.57
1	A	39	TRP	N-CA-C	5.27	117.02	111.28
1	B	240	HIS	N-CA-C	5.16	119.32	112.72
1	A	407	TYR	N-CA-C	5.15	117.35	110.35
1	B	273	ASP	N-CA-C	-5.11	107.05	113.28
1	B	304	SER	N-CA-C	5.11	116.63	108.41
1	B	405	VAL	N-CA-C	-5.07	107.89	112.96
1	B	221	THR	CA-C-N	-5.06	115.02	120.03
1	B	221	THR	C-N-CA	-5.06	115.02	120.03
1	A	108	THR	N-CA-C	5.05	119.15	112.89
1	A	304	SER	N-CA-C	5.03	116.50	108.41

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	3513	0	3410	167	0
1	B	3520	0	3423	177	0
2	A	172	0	0	10	0
2	B	164	0	0	11	0
All	All	7369	0	6833	337	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 24.

All (337) 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:332:ILE:HD11	1:B:336:GLU:HB2	1.48	0.95
1:B:45:LEU:HD12	1:B:48:LYS:HE3	1.45	0.95
1:B:275:ILE:HG22	1:B:277:MET:HE3	1.53	0.89
1:A:422:TYR:HD1	1:A:423:ARG:HG3	1.40	0.87
1:B:359:VAL:HG12	1:B:363:MET:HE2	1.57	0.86
1:A:53:ALA:HB2	1:A:100:ALA:HB3	1.59	0.84
1:A:380:TYR:H	1:A:385:THR:HG21	1.46	0.81
1:A:277:MET:HA	1:A:277:MET:HE2	1.64	0.80
1:A:285:VAL:HG12	1:A:359:VAL:HG21	1.65	0.79
1:A:219:GLN:NE2	1:A:413:ARG:H	1.81	0.78
1:B:332:ILE:HD13	1:B:333:SER:N	1.97	0.78
1:A:29:GLN:NE2	1:A:32:ARG:HH11	1.81	0.78
1:A:324:SER:HB3	1:A:327:ASP:OD1	1.84	0.77
1:A:144:LYS:HG2	1:B:209:PRO:HG2	1.67	0.76
1:B:234:ARG:HD2	1:B:260:ASP:OD1	1.85	0.76
1:A:226:GLN:HB2	1:A:241:ALA:HB2	1.68	0.76
1:A:150:LYS:HD2	1:A:150:LYS:O	1.85	0.76
1:A:28:ASN:ND2	1:A:382:SER:H	1.84	0.75
1:A:239:LYS:HG2	1:A:429:ILE:HD11	1.67	0.75
1:A:117:ARG:HG3	1:A:214:CYS:SG	2.27	0.74
1:B:267:LYS:HB3	2:B:571:HOH:O	1.86	0.73
1:A:149:LYS:H	1:A:149:LYS:HD3	1.53	0.72
1:A:422:TYR:CD1	1:A:423:ARG:HG3	2.24	0.72
1:A:275:ILE:HG22	1:A:277:MET:HE3	1.71	0.72
1:A:345:ASP:HB3	1:A:351:LEU:HD23	1.72	0.72
1:B:318:TYR:CG	1:B:329:ILE:HD11	2.25	0.71
1:A:296:LEU:HD12	1:A:353:VAL:HG21	1.73	0.70
1:B:258:VAL:HG13	1:B:277:MET:HG3	1.74	0.70
1:A:336:GLU:HG2	1:A:340:ASN:ND2	2.07	0.69
1:A:285:VAL:CG1	1:A:359:VAL:HG21	2.21	0.69
1:B:275:ILE:HG22	1:B:277:MET:CE	2.20	0.69
1:B:28:ASN:ND2	1:B:382:SER:H	1.90	0.69
1:B:277:MET:HE2	1:B:277:MET:HA	1.75	0.68
1:B:267:LYS:HE2	2:B:571:HOH:O	1.93	0.68
1:A:29:GLN:HE22	1:A:32:ARG:HH11	1.40	0.67
1:B:226:GLN:NE2	1:B:228:GLY:H	1.92	0.67
1:B:324:SER:HB3	1:B:327:ASP:OD1	1.94	0.66
1:B:53:ALA:HB2	1:B:100:ALA:HB3	1.78	0.66
1:B:226:GLN:HE22	1:B:228:GLY:N	1.93	0.66
1:B:363:MET:HE1	1:B:393:VAL:HG11	1.79	0.65
1:B:332:ILE:CD1	1:B:336:GLU:HB2	2.23	0.65
1:A:106:SER:HA	1:A:135:VAL:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASN:HD22	1:B:29:GLN:H	1.45	0.65
1:B:106:SER:HA	1:B:135:VAL:O	1.97	0.65
1:A:340:ASN:HA	1:A:343:LYS:CD	2.26	0.65
1:B:2:THR:HG23	1:B:3:LYS:NZ	2.12	0.64
1:B:226:GLN:HE22	1:B:228:GLY:H	1.43	0.64
1:B:276:LYS:HA	1:B:373:ASP:OD1	1.97	0.64
1:A:138:HIS:CD2	1:A:139:LEU:H	2.16	0.64
1:A:217:SER:HB2	1:A:218:PRO:HD2	1.80	0.64
1:B:40:THR:O	1:B:44:GLN:HG3	1.98	0.64
1:A:219:GLN:HE21	1:A:413:ARG:H	1.45	0.63
1:A:149:LYS:H	1:A:149:LYS:CD	2.07	0.63
1:A:166:GLU:HG2	1:A:170:LYS:HE3	1.81	0.62
1:A:267:LYS:HB2	2:A:514:HOH:O	1.99	0.62
1:B:17:HIS:CD2	1:B:18:ILE:HD12	2.34	0.62
1:B:33:TYR:CE2	1:B:34:THR:HG23	2.35	0.62
1:A:80:ILE:HD11	2:B:654:HOH:O	2.00	0.62
1:A:306:GLU:HB2	2:A:566:HOH:O	2.00	0.61
1:B:2:THR:HG23	1:B:3:LYS:HZ3	1.65	0.61
1:B:305:LEU:O	1:B:309:LEU:HD23	2.01	0.61
1:B:181:VAL:HG21	1:B:215:GLU:OE1	2.00	0.61
1:B:226:GLN:HB2	1:B:241:ALA:HB2	1.81	0.61
1:B:422:TYR:HD1	1:B:423:ARG:HG3	1.65	0.61
1:B:79:GLN:O	1:B:82:VAL:HG22	2.02	0.60
1:B:183:ARG:HG2	1:B:190:TYR:CE1	2.36	0.60
1:A:168:CYS:HB3	1:A:172:TRP:CZ3	2.36	0.60
1:B:186:GLU:H	1:B:186:GLU:CD	2.09	0.60
1:A:410:GLY:O	1:A:415:LYS:NZ	2.35	0.59
1:A:149:LYS:HD3	1:A:149:LYS:N	2.16	0.59
1:A:239:LYS:CG	1:A:429:ILE:HD11	2.32	0.59
1:B:271:ASN:OD1	1:B:273:ASP:HB2	2.03	0.59
1:B:329:ILE:CG2	1:B:337:ILE:HD12	2.32	0.59
1:A:356:PRO:HG3	1:A:392:LEU:HB3	1.83	0.59
1:A:244:VAL:HG11	1:A:261:ILE:HD13	1.83	0.59
1:B:359:VAL:CG1	1:B:363:MET:HE2	2.32	0.59
1:B:282:CYS:HB2	1:B:349:PHE:CE2	2.38	0.59
1:B:117:ARG:HG3	1:B:214:CYS:SG	2.43	0.58
1:B:282:CYS:HB2	1:B:349:PHE:HE2	1.68	0.58
1:A:363:MET:HE1	1:A:393:VAL:HG11	1.85	0.58
1:B:405:VAL:HG23	1:B:406:ASP:OD1	2.03	0.58
1:B:278:PHE:HA	1:B:374:GLY:O	2.04	0.58
1:A:105:PHE:HB3	1:A:132:TRP:NE1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:HG3	1:A:67:ARG:HH11	1.67	0.58
1:B:134:VAL:HG11	1:B:165:LEU:HD21	1.84	0.58
1:A:9:ALA:HB1	1:A:386:PHE:CZ	2.38	0.58
1:B:12:MET:HE2	1:B:58:ASP:HA	1.86	0.58
1:B:166:GLU:HG2	1:B:170:LYS:HE3	1.85	0.58
1:A:118:ARG:HD3	1:B:87:MET:HE3	1.85	0.57
1:A:340:ASN:HA	1:A:343:LYS:HD2	1.86	0.57
1:A:153:GLU:O	1:A:157:ARG:HG3	2.05	0.57
1:A:28:ASN:ND2	1:A:29:GLN:H	2.02	0.57
1:A:209:PRO:HD2	1:B:145:ASN:OD1	2.05	0.56
1:A:137:SER:O	1:A:157:ARG:NH1	2.36	0.56
1:B:137:SER:O	1:B:157:ARG:NH1	2.38	0.56
2:A:594:HOH:O	1:B:110:GLU:HG2	2.06	0.56
1:B:28:ASN:ND2	1:B:29:GLN:H	2.03	0.56
1:B:296:LEU:O	1:B:296:LEU:HD23	2.05	0.56
1:A:17:HIS:CD2	1:A:18:ILE:HD12	2.41	0.56
1:B:332:ILE:HD13	1:B:333:SER:H	1.68	0.56
1:A:359:VAL:HG12	1:A:363:MET:HE2	1.87	0.56
1:A:133:ASN:HA	1:A:225:TYR:HB2	1.86	0.56
1:B:198:GLU:HB3	1:B:209:PRO:O	2.06	0.56
1:A:381:VAL:HG13	1:A:384:GLY:HA3	1.88	0.56
1:A:223:VAL:HA	1:A:242:GLU:OE2	2.06	0.55
1:B:434:ARG:HG2	2:B:656:HOH:O	2.05	0.55
1:A:70:ARG:HD3	2:A:458:HOH:O	2.06	0.55
1:B:329:ILE:HG21	1:B:337:ILE:HD12	1.88	0.55
1:A:287:LYS:NZ	1:A:287:LYS:HB3	2.21	0.55
1:A:270:ARG:HD2	2:A:474:HOH:O	2.07	0.54
1:A:252:GLU:CD	1:A:252:GLU:H	2.15	0.54
1:A:19:ALA:HB2	1:A:380:TYR:CD1	2.43	0.54
1:A:138:HIS:O	1:A:139:LEU:C	2.51	0.54
1:B:379:GLN:NE2	1:B:382:SER:OG	2.41	0.54
1:B:45:LEU:O	1:B:48:LYS:HG3	2.07	0.54
1:B:182:ILE:HD11	1:B:189:ILE:CG2	2.38	0.54
1:B:111:HIS:CD2	1:B:113:TYR:H	2.25	0.53
1:B:285:VAL:HG21	1:B:393:VAL:CG2	2.39	0.53
1:A:138:HIS:CD2	1:A:139:LEU:HG	2.43	0.53
1:B:80:ILE:HA	1:B:81:PRO:C	2.33	0.53
1:A:138:HIS:CG	1:A:139:LEU:H	2.27	0.53
1:A:263:LYS:HA	1:A:266:LYS:HD3	1.91	0.53
1:B:12:MET:HE2	1:B:58:ASP:CA	2.39	0.53
1:A:329:ILE:HG22	1:A:330:GLY:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLY:O	1:B:229:MET:HE2	2.09	0.53
1:B:249:LYS:HB3	1:B:349:PHE:C	2.34	0.52
1:B:381:VAL:HG13	1:B:384:GLY:HA3	1.91	0.52
1:A:367:VAL:HA	1:A:372:ILE:HG12	1.91	0.52
1:A:413:ARG:NH1	1:A:424:LEU:HD13	2.24	0.52
1:B:3:LYS:HD2	1:B:3:LYS:O	2.09	0.52
1:A:151:ILE:N	1:A:151:ILE:HD12	2.24	0.52
1:B:363:MET:CE	1:B:393:VAL:HG11	2.39	0.52
1:B:51:PHE:HE1	1:B:390:ILE:HG12	1.75	0.52
1:B:111:HIS:HD2	1:B:113:TYR:H	1.57	0.52
1:A:239:LYS:HG2	1:A:429:ILE:CD1	2.36	0.52
1:A:340:ASN:HA	1:A:343:LYS:HD3	1.91	0.52
1:B:242:GLU:OE1	1:B:413:ARG:HD3	2.10	0.52
1:A:55:PHE:C	1:A:55:PHE:CD2	2.88	0.52
1:A:413:ARG:HG2	1:A:421:ASN:O	2.09	0.52
1:B:329:ILE:HG12	1:B:329:ILE:O	2.09	0.52
1:B:107:THR:HB	1:B:164:TYR:CD1	2.44	0.51
1:A:244:VAL:HB	1:A:277:MET:HE1	1.92	0.51
1:A:258:VAL:HG13	1:A:277:MET:HG3	1.92	0.51
1:B:112:PRO:HG3	1:B:164:TYR:CE1	2.45	0.51
1:A:79:GLN:O	1:A:82:VAL:HG22	2.11	0.51
1:A:312:TYR:CE1	1:A:316:THR:HG21	2.46	0.51
1:B:197:HIS:O	1:B:211:PRO:HB3	2.11	0.51
1:A:28:ASN:HD21	1:A:382:SER:H	1.59	0.51
1:A:254:LEU:O	1:A:258:VAL:HG23	2.11	0.51
1:A:300:GLN:OE1	1:A:344:LEU:HD12	2.10	0.51
1:A:22:LEU:HD23	1:A:380:TYR:O	2.11	0.50
1:B:300:GLN:NE2	1:B:344:LEU:HD13	2.26	0.50
1:B:413:ARG:HG2	1:B:421:ASN:O	2.10	0.50
1:A:198:GLU:HB3	1:A:209:PRO:O	2.11	0.50
1:A:393:VAL:HG12	1:A:397:LEU:HD22	1.93	0.50
1:A:296:LEU:HD23	1:A:296:LEU:O	2.11	0.50
1:A:144:LYS:CG	1:B:209:PRO:HG2	2.39	0.50
1:A:336:GLU:HG2	1:A:340:ASN:HD21	1.76	0.50
1:B:123:ASP:OD1	1:B:128:GLY:HA2	2.12	0.50
1:B:271:ASN:HB3	1:B:274:HIS:CD2	2.47	0.50
1:B:428:HIS:CE1	1:B:429:ILE:HD12	2.47	0.50
1:B:45:LEU:HD12	1:B:48:LYS:CE	2.30	0.50
1:B:178:ASP:HA	1:B:220:ARG:HH21	1.77	0.50
1:A:42:LEU:O	1:A:46:LEU:HG	2.11	0.50
1:B:340:ASN:HA	1:B:343:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLU:HB2	1:B:54:LEU:HD21	1.93	0.50
1:A:25:HIS:CD2	1:A:27:GLU:H	2.29	0.49
1:B:305:LEU:HD13	1:B:309:LEU:HD23	1.93	0.49
1:B:219:GLN:NE2	1:B:413:ARG:H	2.10	0.49
1:B:9:ALA:HB1	1:B:386:PHE:CZ	2.47	0.49
1:B:296:LEU:HD12	1:B:353:VAL:HG11	1.94	0.49
1:B:182:ILE:O	1:B:183:ARG:C	2.56	0.49
1:B:219:GLN:HE21	1:B:413:ARG:H	1.59	0.49
1:A:167:VAL:HG22	1:A:201:HIS:CD2	2.47	0.49
1:A:217:SER:HB2	1:A:218:PRO:CD	2.42	0.49
1:A:226:GLN:HE22	1:A:228:GLY:H	1.60	0.49
1:A:29:GLN:NE2	1:A:32:ARG:HD3	2.28	0.49
1:A:66:TYR:CZ	1:A:309:LEU:HD23	2.48	0.49
1:A:197:HIS:O	1:A:211:PRO:HB3	2.13	0.49
1:A:244:VAL:HG11	1:A:261:ILE:CD1	2.43	0.49
1:B:86:LEU:HD21	1:B:119:MET:HE3	1.95	0.48
1:B:332:ILE:HD11	1:B:336:GLU:CB	2.31	0.48
1:A:29:GLN:HE21	1:A:32:ARG:HD3	1.78	0.48
1:A:285:VAL:HG11	1:A:393:VAL:CG2	2.43	0.48
1:A:163:GLU:O	1:A:167:VAL:HG23	2.14	0.48
1:A:50:LYS:HA	1:A:407:TYR:CZ	2.49	0.48
1:B:289:HIS:HE1	2:B:587:HOH:O	1.96	0.48
1:A:204:LYS:NZ	2:A:545:HOH:O	2.46	0.48
1:B:262:ARG:NH1	1:B:272:PRO:O	2.46	0.47
1:A:53:ALA:HA	1:A:99:LEU:HD22	1.97	0.47
1:B:217:SER:HB2	1:B:218:PRO:HD2	1.95	0.47
1:A:18:ILE:HG22	1:A:19:ALA:N	2.29	0.47
1:A:226:GLN:HE22	1:A:228:GLY:N	2.13	0.47
1:A:166:GLU:CG	1:A:170:LYS:HE3	2.45	0.47
1:A:80:ILE:HA	1:A:81:PRO:C	2.40	0.47
1:A:363:MET:CE	1:A:393:VAL:HG11	2.44	0.47
1:B:112:PRO:HG3	1:B:164:TYR:CD1	2.50	0.47
1:A:286:GLY:O	1:A:356:PRO:HD3	2.15	0.46
1:A:364:GLN:O	1:A:368:GLU:HG3	2.15	0.46
1:B:17:HIS:CG	1:B:18:ILE:HD12	2.51	0.46
1:B:332:ILE:HG23	1:B:337:ILE:HG13	1.96	0.46
1:A:11:GLU:HB3	1:A:54:LEU:HD21	1.97	0.46
1:A:208:VAL:HA	1:A:209:PRO:HD3	1.73	0.46
1:A:287:LYS:HB3	1:A:287:LYS:HZ3	1.79	0.46
1:A:424:LEU:HA	1:A:425:PRO:HD3	1.76	0.46
1:A:89:ILE:HD12	1:A:101:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:HE2	1:A:320:LEU:HD21	1.79	0.46
1:B:410:GLY:O	1:B:415:LYS:NZ	2.49	0.46
1:B:53:ALA:HA	1:B:99:LEU:HD22	1.98	0.46
1:B:363:MET:HE1	1:B:393:VAL:CG1	2.45	0.46
1:B:59:VAL:O	1:B:59:VAL:HG23	2.16	0.46
1:B:386:PHE:O	1:B:390:ILE:HG13	2.16	0.46
1:B:413:ARG:CZ	1:B:424:LEU:HD13	2.45	0.46
1:B:424:LEU:HD23	1:B:430:ALA:HB3	1.97	0.46
1:B:66:TYR:O	1:B:67:ARG:HB2	2.16	0.46
1:B:390:ILE:HA	1:B:394:VAL:CG2	2.46	0.46
1:B:41:GLU:HG3	2:B:552:HOH:O	2.16	0.45
1:A:57:ALA:HA	1:A:104:THR:OG1	2.16	0.45
1:B:86:LEU:CD1	1:B:103:VAL:HG21	2.46	0.45
1:A:345:ASP:HB3	1:A:351:LEU:CD2	2.44	0.45
1:B:283:VAL:CG1	1:B:285:VAL:HG22	2.47	0.45
1:A:396:GLU:O	1:A:400:ARG:HG3	2.16	0.45
1:B:44:GLN:HG2	1:B:95:VAL:HG13	1.97	0.45
1:B:414:GLU:O	1:B:418:GLY:N	2.46	0.45
1:A:226:GLN:NE2	1:A:228:GLY:H	2.14	0.45
1:B:24:ARG:NH1	2:B:578:HOH:O	2.48	0.44
1:B:88:LEU:HB3	1:B:92:MET:HE2	1.97	0.44
1:A:296:LEU:CD1	1:A:353:VAL:HG21	2.45	0.44
2:A:441:HOH:O	1:B:215:GLU:HG2	2.17	0.44
1:B:219:GLN:O	1:B:221:THR:N	2.48	0.44
1:A:20:HIS:HE1	1:A:311:HIS:ND1	2.15	0.44
1:B:101:PHE:O	1:B:130:ILE:HD12	2.16	0.44
1:A:182:ILE:HD11	1:A:189:ILE:CG2	2.48	0.44
1:B:139:LEU:HA	1:B:140:PRO:HD3	1.77	0.44
1:A:242:GLU:OE1	1:A:413:ARG:HD3	2.18	0.44
1:A:362:GLU:O	1:A:366:LEU:HD22	2.16	0.44
1:A:414:GLU:O	1:A:418:GLY:N	2.45	0.44
1:B:226:GLN:HE22	1:B:228:GLY:CA	2.29	0.44
1:B:336:GLU:O	1:B:337:ILE:C	2.60	0.44
1:B:55:PHE:C	1:B:55:PHE:CD2	2.95	0.44
1:B:86:LEU:HD21	1:B:119:MET:CE	2.48	0.44
1:B:323:TYR:HB3	1:B:334:VAL:HG21	2.00	0.44
1:A:73:ALA:O	1:A:77:ALA:N	2.50	0.44
1:A:76:GLU:OE2	1:B:188:ASN:ND2	2.51	0.44
1:A:102:ALA:HA	1:A:131:ALA:HB3	2.00	0.44
1:A:381:VAL:O	1:A:385:THR:HG23	2.18	0.44
1:B:79:GLN:O	1:B:82:VAL:CG2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LEU:HD12	1:B:320:LEU:HB2	1.97	0.44
1:A:22:LEU:CD2	1:A:380:TYR:O	2.65	0.44
1:A:55:PHE:C	1:A:55:PHE:HD2	2.25	0.44
1:B:220:ARG:HD2	1:B:423:ARG:HD3	2.00	0.44
1:A:219:GLN:O	1:A:221:THR:N	2.50	0.44
1:B:408:GLU:O	1:B:409:GLU:C	2.59	0.44
1:A:215:GLU:HG2	2:B:548:HOH:O	2.18	0.43
1:B:296:LEU:HD23	1:B:296:LEU:C	2.42	0.43
1:B:356:PRO:HB3	1:B:392:LEU:O	2.18	0.43
1:A:204:LYS:HD3	1:A:205:TYR:CE2	2.53	0.43
1:B:305:LEU:HD13	1:B:309:LEU:CD2	2.48	0.43
1:A:14:CYS:HB3	1:A:82:VAL:HG13	1.99	0.43
1:A:67:ARG:HG3	1:A:67:ARG:NH1	2.32	0.43
1:A:296:LEU:HD23	1:A:296:LEU:C	2.44	0.43
1:B:409:GLU:OE1	1:B:409:GLU:N	2.51	0.43
1:B:135:VAL:HG13	1:B:136:THR:O	2.18	0.43
1:A:111:HIS:CG	1:A:112:PRO:HD2	2.53	0.43
1:A:106:SER:HA	1:A:135:VAL:HG12	2.01	0.43
1:B:22:LEU:HD23	1:B:380:TYR:O	2.19	0.43
1:B:151:ILE:HG23	1:B:157:ARG:HH21	1.84	0.43
1:A:323:TYR:HB3	1:A:334:VAL:HG21	2.00	0.43
1:B:281:ILE:HG22	1:B:375:PHE:HB3	2.01	0.43
1:B:347:LYS:HE3	1:B:347:LYS:HA	2.01	0.43
1:B:394:VAL:HB	1:B:395:PRO:HD3	2.00	0.43
1:A:300:GLN:CA	1:A:344:LEU:HD11	2.49	0.43
1:A:165:LEU:HD12	1:A:240:HIS:CG	2.54	0.43
1:A:332:ILE:CG2	1:A:336:GLU:HB3	2.48	0.43
1:B:182:ILE:HD11	1:B:189:ILE:HG22	1.99	0.43
1:B:242:GLU:OE2	1:B:413:ARG:NH1	2.51	0.43
1:B:86:LEU:HD12	1:B:103:VAL:HG21	2.01	0.42
1:B:259:ASP:O	1:B:263:LYS:HG2	2.18	0.42
1:A:100:ALA:HA	1:A:129:ARG:HB3	2.00	0.42
1:A:400:ARG:HB2	1:A:402:LEU:HD12	2.00	0.42
1:B:55:PHE:C	1:B:55:PHE:HD2	2.27	0.42
1:A:102:ALA:HA	1:A:131:ALA:O	2.20	0.42
1:B:119:MET:HA	1:B:119:MET:HE2	2.01	0.42
1:A:44:GLN:HG3	1:A:95:VAL:HG11	2.00	0.42
1:B:28:ASN:HD22	1:B:29:GLN:N	2.13	0.42
1:A:80:ILE:O	1:A:80:ILE:HG23	2.20	0.42
1:B:5:ILE:HG23	1:B:374:GLY:HA2	2.01	0.42
1:B:186:GLU:CD	1:B:186:GLU:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG12	1:A:246:LEU:HD12	2.01	0.42
1:B:429:ILE:HD12	1:B:430:ALA:H	1.84	0.42
1:A:303:TRP:CE2	1:A:308:HIS:NE2	2.88	0.42
1:B:187:ASN:O	1:B:189:ILE:HG13	2.20	0.42
1:B:199:ILE:O	1:B:200:ASN:C	2.62	0.42
1:B:294:GLU:OE2	1:B:294:GLU:HA	2.20	0.42
1:B:285:VAL:HA	1:B:354:GLY:O	2.20	0.42
1:A:244:VAL:HB	1:A:277:MET:CE	2.50	0.42
1:B:359:VAL:HG12	1:B:363:MET:CE	2.38	0.42
1:A:11:GLU:HG2	1:A:39:TRP:CZ3	2.55	0.41
1:A:309:LEU:HD12	1:A:341:MET:SD	2.60	0.41
1:B:111:HIS:HA	1:B:112:PRO:HD3	1.76	0.41
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.90	0.41
1:B:226:GLN:NE2	1:B:228:GLY:N	2.59	0.41
1:B:232:ARG:NH1	2:B:538:HOH:O	2.48	0.41
1:B:381:VAL:CG1	1:B:384:GLY:HA3	2.49	0.41
1:B:166:GLU:CG	1:B:170:LYS:HE3	2.48	0.41
1:A:334:VAL:O	1:A:338:ILE:HG13	2.20	0.41
1:A:408:GLU:HG2	2:A:471:HOH:O	2.19	0.41
1:B:14:CYS:HB2	2:B:531:HOH:O	2.20	0.41
1:B:171:LEU:HG	1:B:199:ILE:HD13	2.01	0.41
1:B:299:PHE:C	1:B:301:LYS:N	2.77	0.41
1:A:11:GLU:HG2	1:A:39:TRP:HZ3	1.85	0.41
1:A:11:GLU:HG3	1:A:12:MET:N	2.36	0.41
1:A:286:GLY:O	1:A:355:THR:HA	2.20	0.41
1:B:102:ALA:HA	1:B:131:ALA:HB3	2.02	0.41
1:B:223:VAL:HA	1:B:413:ARG:NH1	2.36	0.41
1:B:340:ASN:O	1:B:343:LYS:HG2	2.20	0.41
1:A:61:GLY:HA2	1:A:141:SER:OG	2.20	0.41
1:A:219:GLN:HE22	1:A:412:TYR:HB3	1.86	0.41
1:A:285:VAL:HG11	1:A:393:VAL:HG22	2.03	0.41
1:A:380:TYR:H	1:A:385:THR:CG2	2.24	0.41
1:B:3:LYS:HD2	1:B:3:LYS:C	2.46	0.41
1:B:35:ASP:HA	2:B:580:HOH:O	2.21	0.41
1:B:228:GLY:C	1:B:229:MET:HE2	2.45	0.40
1:A:55:PHE:HD2	1:A:56:LEU:N	2.20	0.40
1:B:397:LEU:HD12	1:B:397:LEU:HA	1.92	0.40
1:B:429:ILE:H	1:B:429:ILE:HG13	1.68	0.40
1:A:66:TYR:O	1:A:67:ARG:HB2	2.22	0.40
1:A:91:ALA:HA	1:B:91:ALA:HA	2.03	0.40
1:A:127:LYS:HG2	2:A:525:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:HIS:CE1	1:B:158:TYR:HE1	2.39	0.40
1:A:27:GLU:HG2	2:A:507:HOH:O	2.20	0.40
1:A:150:LYS:O	1:A:150:LYS:CD	2.63	0.40
1:B:80:ILE:HG13	1:B:81:PRO:HA	2.03	0.40
1:B:299:PHE:O	1:B:300:GLN:C	2.65	0.40
1:A:193:PRO:HA	1:B:74:VAL:HG11	2.02	0.40
1:A:290:ASP:O	1:A:294:GLU:HG3	2.21	0.40
1:B:358:LYS:O	1:B:362:GLU: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	431/440 (98%)	403 (94%)	25 (6%)	3 (1%)	18	41
1	B	432/440 (98%)	400 (93%)	29 (7%)	3 (1%)	18	41
All	All	863/880 (98%)	803 (93%)	54 (6%)	6 (1%)	18	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	SER
1	B	149	LYS
1	A	139	LEU
1	A	329	ILE
1	B	424	LEU
1	B	384	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	372/379 (98%)	356 (96%)	16 (4%)	26	54
1	B	373/379 (98%)	350 (94%)	23 (6%)	16	39
All	All	745/758 (98%)	706 (95%)	39 (5%)	21	47

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	54	LEU
1	A	82	VAL
1	A	95	VAL
1	A	135	VAL
1	A	149	LYS
1	A	155	ASP
1	A	226	GLN
1	A	246	LEU
1	A	249	LYS
1	A	267	LYS
1	A	309	LEU
1	A	366	LEU
1	A	385	THR
1	A	397	LEU
1	A	424	LEU
1	B	3	LYS
1	B	18	ILE
1	B	52	ASP
1	B	54	LEU
1	B	82	VAL
1	B	95	VAL
1	B	135	VAL
1	B	138	HIS
1	B	153	GLU
1	B	156	GLU
1	B	165	LEU

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Mol	Chain	Res	Type
1	B	246	LEU
1	B	273	ASP
1	B	285	VAL
1	B	305	LEU
1	B	326	ASN
1	B	332	ILE
1	B	347	LYS
1	B	366	LEU
1	B	380	TYR
1	B	397	LEU
1	B	424	LEU
1	B	429	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	20	HIS
1	A	25	HIS
1	A	28	ASN
1	A	29	GLN
1	A	31	HIS
1	A	68	GLN
1	A	133	ASN
1	A	138	HIS
1	A	154	HIS
1	A	219	GLN
1	A	226	GLN
1	A	274	HIS
1	A	297	ASN
1	A	339	ASN
1	A	340	ASN
1	A	376	ASN
1	A	379	GLN
1	A	421	ASN
1	B	20	HIS
1	B	28	ASN
1	B	29	GLN
1	B	111	HIS
1	B	179	ASN
1	B	219	GLN
1	B	226	GLN

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Mol	Chain	Res	Type
1	B	274	HIS
1	B	289	HIS
1	B	300	GLN
1	B	311	HIS
1	B	379	GLN
1	B	398	GLN

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](#)

There are no ligands in this entry.

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	433/440 (98%)	-0.38	0	100 100	20, 32, 54, 71	0
1	B	434/440 (98%)	-0.32	1 (0%)	91 90	19, 34, 58, 78	0
All	All	867/880 (98%)	-0.35	1 (0%)	92 91	19, 34, 56, 78	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ILE	3.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.