



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:01 PM UTC

PDB ID : 1BSL / pdb_00001bsl
Title : STRUCTURE OF ALKANAL MONOOXYGENASE BETA CHAIN
Authors : Rayment, I.; Holden, H.M.; Thoden, J.B.; Baldwin, T.O.
Deposited on : 1996-10-22
Resolution : 1.95 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

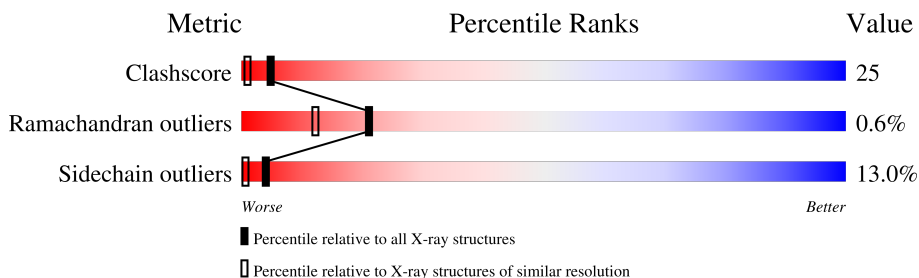
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	324	 55% 30% 13%
1	B	324	 45% 42% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6116 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 BACTERIAL LUCIFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	2	0
			2559	1612	441	491	15			
1	B	324	Total	C	N	O	S	0	3	0
			2568	1616	440	497	15			

- Molecule 2 is water.

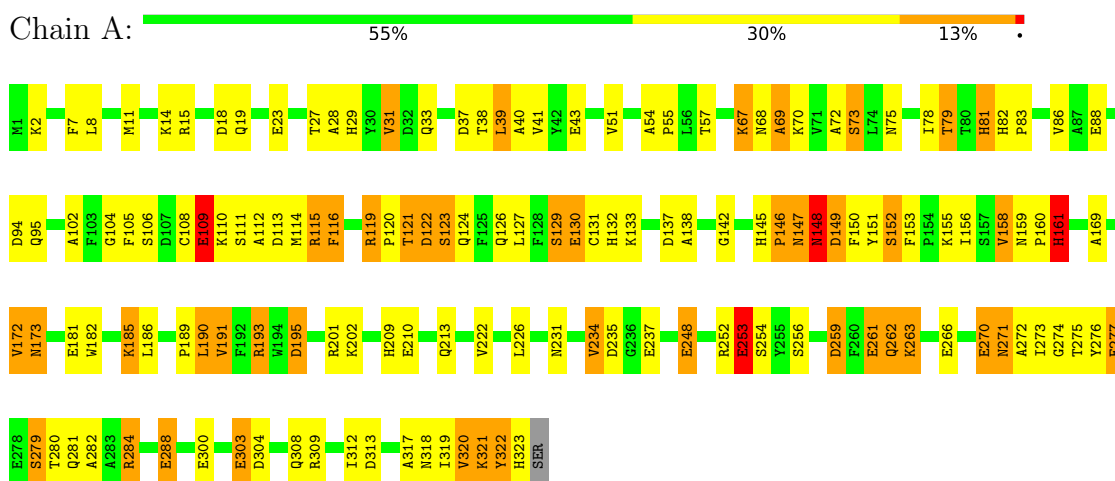
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	586	Total	O	0	0
			586	586		
2	B	403	Total	O	0	0
			403	403		

3 Residue-property plots

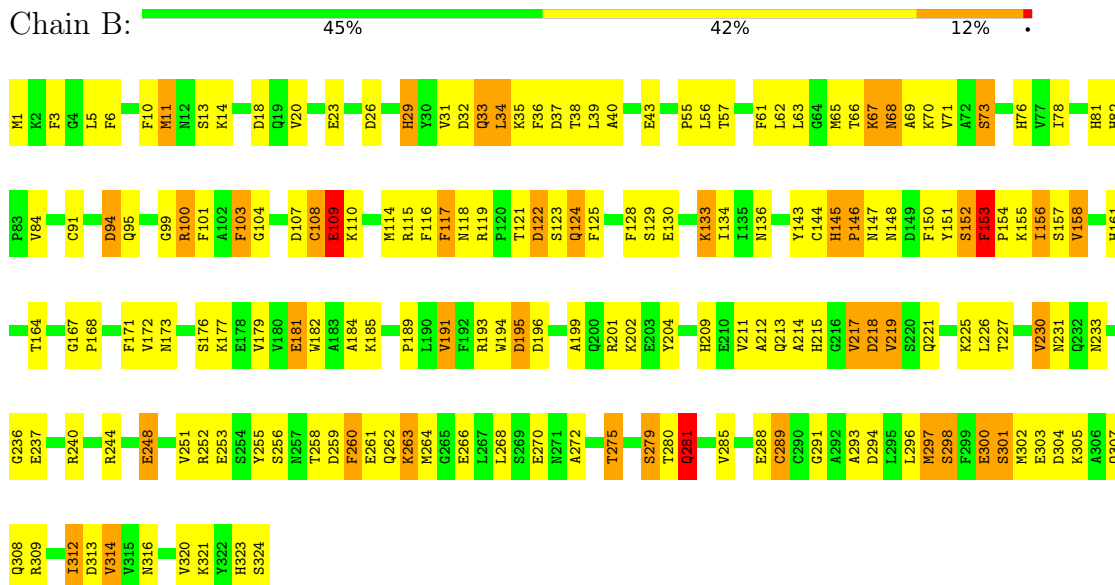
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: BACTERIAL LUCIFERASE



• Molecule 1: BACTERIAL LUCIFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.80Å 62.00Å 218.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.95)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6116	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.28	10/2629 (0.4%)	1.86	62/3556 (1.7%)
1	B	1.33	10/2640 (0.4%)	1.93	70/3570 (2.0%)
All	All	1.31	20/5269 (0.4%)	1.90	132/7126 (1.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	0
All	All	1	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	LYS	CE-NZ	9.20	1.76	1.49
1	A	29	HIS	ND1-CE1	7.64	1.40	1.32
1	A	190	LEU	CA-CB	7.20	1.64	1.53
1	A	231	ASN	CA-CB	7.18	1.62	1.52
1	B	312	ILE	CA-CB	-6.90	1.46	1.54
1	A	88	GLU	CD-OE1	6.58	1.37	1.25
1	B	32	ASP	CG-OD1	6.31	1.37	1.25
1	A	155	LYS	CE-NZ	-5.96	1.31	1.49
1	B	230	VAL	CA-CB	-5.89	1.47	1.54
1	B	297	MET	CA-C	-5.84	1.45	1.52
1	B	261	GLU	CD-OE1	5.50	1.35	1.25
1	A	270	GLU	CD-OE1	5.30	1.35	1.25
1	B	280	THR	CA-CB	5.23	1.61	1.53
1	B	95	GLN	CA-CB	5.22	1.61	1.53
1	A	259	ASP	CG-OD1	5.19	1.35	1.25
1	B	40	ALA	CA-CB	-5.19	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	ASP	CG-OD1	5.17	1.35	1.25
1	A	109	GLU	CD-OE2	5.13	1.35	1.25
1	A	161[A]	HIS	N-CA	-5.05	1.39	1.45
1	A	161[B]	HIS	N-CA	-5.05	1.39	1.45

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ASN	CB-CA-C	11.23	131.41	110.63
1	B	29	HIS	CA-CB-CG	-11.21	102.59	113.80
1	B	37	ASP	CA-CB-CG	-10.13	102.47	112.60
1	A	29	HIS	CA-CB-CG	-9.80	104.00	113.80
1	A	161[A]	HIS	CB-CA-C	8.81	125.75	109.54
1	A	161[B]	HIS	CB-CA-C	8.81	125.75	109.54
1	A	319	ILE	CB-CA-C	-8.72	100.55	112.24
1	B	145	HIS	CB-CA-C	-8.64	100.44	111.15
1	A	191	VAL	N-CA-CB	8.45	122.55	111.90
1	A	313	ASP	CA-CB-CG	-8.18	104.42	112.60
1	B	20	VAL	N-CA-CB	8.18	119.59	110.51
1	B	11	MET	N-CA-CB	-8.13	98.86	111.05
1	A	148	ASN	CA-CB-CG	7.94	120.54	112.60
1	A	161[A]	HIS	N-CA-C	-7.94	99.30	110.50
1	A	161[B]	HIS	N-CA-C	-7.94	99.30	110.50
1	A	234	VAL	CB-CA-C	-7.93	101.66	112.04
1	A	79	THR	CB-CA-C	7.92	124.14	110.68
1	B	57	THR	CA-CB-OG1	-7.68	98.08	109.60
1	B	70	LYS	N-CA-CB	-7.48	98.22	110.41
1	B	191	VAL	CB-CA-C	7.48	119.63	110.73
1	A	190	LEU	CB-CA-C	-7.47	97.07	110.36
1	A	318	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	B	158	VAL	N-CA-CB	-7.42	102.13	111.41
1	B	314	VAL	CB-CA-C	-7.42	102.48	111.97
1	A	94	ASP	CA-CB-CG	7.27	119.87	112.60
1	B	26	ASP	CB-CA-C	-7.21	98.83	110.79
1	A	271	ASN	N-CA-CB	7.13	120.64	110.44
1	B	168	PRO	CB-CA-C	-7.02	102.41	111.46
1	A	120	PRO	N-CA-CB	6.99	109.43	103.35
1	A	7	PHE	CA-CB-CG	-6.92	106.88	113.80
1	B	76	HIS	CA-CB-CG	-6.91	106.89	113.80
1	A	33	GLN	N-CA-CB	6.74	120.83	110.46
1	A	222	VAL	CB-CA-C	6.71	119.08	110.96
1	B	23	GLU	CB-CG-CD	6.64	123.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161[A]	HIS	N-CA-CB	-6.63	100.63	110.17
1	A	161[B]	HIS	N-CA-CB	-6.63	100.63	110.17
1	B	147	ASN	N-CA-CB	-6.61	100.39	111.96
1	A	129	SER	N-CA-CB	6.58	119.79	110.12
1	B	36	PHE	CA-CB-CG	-6.56	107.24	113.80
1	B	189	PRO	CB-CA-C	-6.54	101.28	110.63
1	B	144	CYS	N-CA-CB	6.51	122.79	111.13
1	B	280	THR	N-CA-CB	-6.51	100.55	110.12
1	A	235	ASP	CA-CB-CG	6.50	119.10	112.60
1	B	191	VAL	N-CA-CB	6.41	120.31	112.10
1	B	116	PHE	CA-CB-CG	-6.41	107.39	113.80
1	B	219	VAL	N-CA-CB	-6.37	101.87	110.54
1	B	68	ASN	CA-CB-CG	6.33	118.93	112.60
1	A	303	GLU	CB-CA-C	6.32	121.43	110.68
1	B	100	ARG	CD-NE-CZ	6.32	133.25	124.40
1	B	100	ARG	NE-CZ-NH2	-6.29	113.54	119.20
1	B	136	ASN	N-CA-CB	-6.27	100.56	110.22
1	B	296	LEU	N-CA-CB	6.23	121.15	110.68
1	A	189	PRO	N-CA-CB	6.18	109.15	103.15
1	B	69	ALA	N-CA-CB	6.18	120.93	110.49
1	B	195	ASP	N-CA-CB	6.17	120.16	110.46
1	A	69	ALA	N-CA-C	6.17	119.41	110.28
1	A	73	SER	N-CA-CB	6.15	119.48	109.95
1	A	79	THR	CA-CB-OG1	6.12	118.78	109.60
1	B	146	PRO	N-CA-CB	6.05	109.02	103.15
1	A	304	ASP	CA-CB-CG	5.99	118.59	112.60
1	B	70	LYS	CA-CB-CG	-5.99	102.12	114.10
1	B	196	ASP	CA-CB-CG	5.99	118.59	112.60
1	B	313	ASP	CA-C-N	-5.96	113.05	120.56
1	B	313	ASP	C-N-CA	-5.96	113.05	120.56
1	B	218	ASP	N-CA-CB	5.95	119.15	110.58
1	A	72	ALA	N-CA-C	5.95	118.45	109.23
1	B	117	PHE	CA-CB-CG	-5.93	107.87	113.80
1	B	109	GLU	N-CA-CB	-5.91	101.46	110.26
1	B	94	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	215	HIS	CA-CB-CG	-5.87	107.93	113.80
1	B	217	VAL	N-CA-C	5.87	116.64	108.89
1	B	172	VAL	N-CA-C	5.86	116.37	108.17
1	B	300	GLU	N-CA-C	5.86	119.24	111.75
1	A	95	GLN	CB-CG-CD	5.83	122.52	112.60
1	A	318	ASN	CB-CG-ND2	5.79	125.09	116.40
1	B	108	CYS	N-CA-CB	5.79	118.63	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	PHE	CB-CA-C	5.77	117.77	109.92
1	B	73	SER	N-CA-C	-5.72	99.96	109.46
1	A	132	HIS	CA-CB-CG	-5.71	108.09	113.80
1	A	119	ARG	N-CA-CB	5.70	118.66	110.11
1	A	40	ALA	N-CA-CB	5.70	119.86	110.69
1	B	167	GLY	CA-C-N	5.69	125.62	119.76
1	B	167	GLY	C-N-CA	5.69	125.62	119.76
1	B	20	VAL	N-CA-C	5.68	116.33	110.36
1	B	68	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	201	ARG	NE-CZ-NH2	-5.68	114.09	119.20
1	B	152[A]	SER	N-CA-CB	5.68	119.77	110.90
1	B	152[B]	SER	N-CA-CB	5.68	119.77	110.90
1	A	317	ALA	CA-C-O	5.68	126.77	120.63
1	A	57	THR	CA-CB-OG1	-5.58	101.22	109.60
1	A	73	SER	N-CA-C	-5.58	100.89	109.76
1	B	181	GLU	CB-CG-CD	-5.58	103.12	112.60
1	B	69	ALA	N-CA-C	5.56	122.65	110.80
1	A	137	ASP	CB-CA-C	-5.54	102.14	110.90
1	A	193	ARG	N-CA-C	5.54	118.57	109.76
1	A	106	SER	N-CA-C	5.53	117.38	109.14
1	B	294	ASP	CA-CB-CG	-5.52	107.08	112.60
1	A	75	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	288	GLU	N-CA-CB	5.47	118.75	110.28
1	A	253	GLU	N-CA-C	5.46	118.28	111.24
1	A	130	GLU	CB-CG-CD	5.46	121.88	112.60
1	B	67	LYS	N-CA-C	-5.45	108.41	114.62
1	B	201	ARG	N-CA-CB	5.44	118.12	110.12
1	A	277	GLU	CB-CG-CD	5.43	121.83	112.60
1	A	195	ASP	CA-CB-CG	-5.42	107.18	112.60
1	B	103	PHE	N-CA-C	5.39	117.78	107.75
1	B	259	ASP	N-CA-CB	5.38	117.92	109.69
1	A	320	VAL	N-CA-CB	-5.37	103.24	110.54
1	B	10	PHE	N-CA-CB	5.36	117.92	109.83
1	A	122	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	160	PRO	N-CA-CB	5.31	108.44	102.60
1	A	81	HIS	N-CA-CB	-5.31	102.36	110.85
1	B	172	VAL	CB-CA-C	-5.29	102.94	110.83
1	A	102	ALA	N-CA-CB	5.28	119.55	110.68
1	B	199	ALA	N-CA-CB	-5.28	102.36	110.01
1	B	91	CYS	N-CA-CB	5.28	117.88	110.12
1	A	148	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	300	GLU	N-CA-C	5.22	118.43	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ALA	CB-CA-C	5.21	119.44	110.79
1	B	275	THR	CA-CB-OG1	-5.20	101.80	109.60
1	B	100	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	A	75	ASN	CB-CA-C	-5.14	103.60	112.44
1	B	171	PHE	N-CA-CB	5.14	120.09	110.99
1	A	41	VAL	N-CA-C	5.12	115.23	107.75
1	A	81	HIS	CA-CB-CG	-5.12	108.69	113.80
1	B	279	SER	CA-CB-OG	-5.12	100.87	111.10
1	A	131	CYS	N-CA-CB	5.10	117.40	110.01
1	B	184	ALA	N-CA-CB	-5.09	102.63	110.12
1	A	261	GLU	N-CA-CB	5.09	117.70	110.06
1	B	256	SER	N-CA-C	5.03	116.61	111.03
1	B	281	GLN	N-CA-CB	5.03	117.69	110.20
1	B	298	SER	N-CA-CB	5.02	118.81	110.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	69	ALA	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	322	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2559	0	2435	109	0
1	B	2568	0	2446	159	0
2	A	586	0	0	20	1
2	B	403	0	0	23	1
All	All	6116	0	4881	255	1

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 25.

All (255) 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:67:LYS:CE	1:B:67:LYS:NZ	1.76	1.46
1:B:114:MET:HE2	1:B:124:GLN:HG3	1.18	1.09
1:A:146:PRO:HG3	1:A:153:PHE:CE2	1.88	1.08
1:A:146:PRO:HD3	1:A:153:PHE:CE1	1.97	0.99
1:B:148:ASN:HD22	1:B:150:PHE:N	1.64	0.94
1:A:148:ASN:ND2	1:A:150:PHE:H	1.65	0.93
1:B:148:ASN:ND2	1:B:150:PHE:H	1.66	0.92
1:A:112:ALA:HA	1:A:115:ARG:NE	1.86	0.90
1:B:255:TYR:HB3	1:B:258:THR:CG2	2.02	0.90
1:B:301:SER:OG	2:B:710:HOH:O	1.90	0.89
1:B:148:ASN:ND2	1:B:151:TYR:H	1.70	0.89
1:B:35:LYS:HG3	1:B:321:LYS:HG3	1.56	0.88
1:A:148:ASN:HD22	1:A:150:PHE:N	1.73	0.87
1:B:263:LYS:NZ	2:B:717:HOH:O	2.02	0.86
1:A:148:ASN:ND2	1:A:150:PHE:N	2.23	0.86
1:A:116:PHE:CZ	1:B:156:ILE:HG12	2.10	0.86
1:A:55:PRO:HD2	2:A:380:HOH:O	1.76	0.86
1:B:248:GLU:HG3	2:B:444:HOH:O	1.75	0.86
1:A:146:PRO:HG3	1:A:153:PHE:CZ	2.13	0.82
1:B:148:ASN:HD22	1:B:150:PHE:H	0.85	0.81
1:B:255:TYR:HB3	1:B:258:THR:HG21	1.64	0.79
1:B:35:LYS:H	1:B:316:ASN:HD21	1.28	0.79
1:B:33:GLN:HG2	1:B:34:LEU:HD23	1.65	0.79
1:A:37:ASP:O	1:A:70:LYS:HB2	1.84	0.78
1:A:27:THR:O	1:A:31:VAL:HG13	1.84	0.77
1:A:146:PRO:HG3	1:A:153:PHE:CD2	2.19	0.77
1:B:109:GLU:HB2	2:B:668:HOH:O	1.85	0.77
1:A:148:ASN:HD22	1:A:150:PHE:H	1.27	0.76
1:A:116:PHE:HZ	1:B:156:ILE:HG12	1.51	0.75
1:A:69:ALA:HA	2:A:387:HOH:O	1.87	0.74
1:B:181:GLU:HG2	1:B:211:VAL:HG21	1.68	0.74
1:A:321:LYS:HD2	1:A:322:TYR:CZ	2.21	0.74
1:B:114:MET:HE2	1:B:124:GLN:CG	2.10	0.73
1:A:146:PRO:HD2	1:A:153:PHE:O	1.89	0.73
1:A:54:ALA:HB2	2:B:328:HOH:O	1.88	0.72
1:A:82:HIS:O	1:A:86:VAL:HG23	1.89	0.72
1:A:121:THR:HG22	1:A:122:ASP:H	1.53	0.72
1:A:284:ARG:O	1:A:288:GLU:HG3	1.89	0.72
1:B:230:VAL:HG22	1:B:272:ALA:HB3	1.69	0.72
1:A:148:ASN:ND2	1:A:151:TYR:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASP:OD1	2:B:711:HOH:O	2.07	0.72
1:B:218:ASP:OD2	1:B:221:GLN:NE2	2.22	0.72
1:A:145:HIS:ND1	2:A:627:HOH:O	2.23	0.71
1:B:155:LYS:HE2	2:B:649:HOH:O	1.89	0.71
1:B:35:LYS:H	1:B:316:ASN:ND2	1.88	0.71
1:B:34:LEU:HD23	1:B:34:LEU:N	2.05	0.71
1:A:173:ASN:ND2	1:A:191:VAL:HG13	2.06	0.70
1:A:116:PHE:CE2	1:B:156:ILE:CD1	2.74	0.70
1:B:114:MET:CE	1:B:124:GLN:HG3	2.11	0.70
1:A:146:PRO:O	1:A:152:SER:HA	1.91	0.69
1:B:305:LYS:HD2	1:B:309:ARG:NH2	2.08	0.69
1:A:263:LYS:NZ	2:A:898:HOH:O	2.16	0.69
1:B:122:ASP:OD1	1:B:122:ASP:N	2.21	0.69
1:B:202:LYS:HZ3	1:B:289:CYS:HB3	1.55	0.69
1:B:133:LYS:NZ	2:B:391:HOH:O	2.25	0.69
1:A:185:LYS:NZ	2:A:462:HOH:O	2.25	0.68
1:A:209:HIS:O	1:A:213:GLN:HG3	1.94	0.68
1:A:321:LYS:HD2	1:A:322:TYR:CE2	2.29	0.68
1:B:109:GLU:HG2	2:B:654:HOH:O	1.94	0.68
1:B:251:VAL:HG12	1:B:260:PHE:CD1	2.29	0.67
1:A:18:ASP:OD1	1:B:161[B]:HIS:HE1	1.76	0.67
1:A:112:ALA:HA	1:A:115:ARG:CD	2.24	0.67
1:A:159:ASN:OD1	2:A:884:HOH:O	2.12	0.67
1:A:112:ALA:O	1:A:115:ARG:HG2	1.94	0.66
1:B:35:LYS:N	1:B:316:ASN:HD21	1.94	0.66
1:B:209:HIS:O	1:B:213:GLN:HG3	1.95	0.66
1:B:148:ASN:ND2	1:B:150:PHE:N	2.36	0.66
1:B:291:GLY:HA2	2:B:457:HOH:O	1.94	0.66
1:B:255:TYR:HB3	1:B:258:THR:HG22	1.78	0.65
1:B:219:VAL:HG13	2:B:482:HOH:O	1.97	0.65
1:A:271:ASN:HB2	1:A:273:ILE:HD12	1.79	0.65
1:A:109:GLU:OE1	2:A:403:HOH:O	2.15	0.65
1:B:82:HIS:CE1	1:B:84:VAL:HB	2.32	0.64
1:B:148:ASN:HD21	1:B:150:PHE:HB2	1.61	0.64
1:A:116:PHE:CE2	1:B:153:PHE:CE1	2.85	0.64
1:B:1:MET:HG2	1:B:293:ALA:O	1.97	0.64
1:A:127:LEU:HD13	1:A:150:PHE:CD1	2.34	0.63
1:A:116:PHE:CE2	1:B:156:ILE:HD13	2.34	0.63
1:B:218:ASP:CG	1:B:221:GLN:HE21	2.07	0.63
1:B:143:TYR:CE1	1:B:157:SER:HB2	2.34	0.62
1:B:82:HIS:HE1	1:B:84:VAL:CG2	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASN:HD21	1:B:151:TYR:H	1.45	0.62
1:B:281:GLN:O	1:B:285:VAL:HG23	2.00	0.62
1:B:107:ASP:OD1	1:B:108:CYS:N	2.32	0.61
1:B:251:VAL:HG12	1:B:260:PHE:CE1	2.36	0.61
1:A:146:PRO:CD	1:A:153:PHE:CE1	2.78	0.61
1:B:324:SER:HB3	2:B:465:HOH:O	2.00	0.61
1:A:27:THR:HG23	1:A:309:ARG:NH1	2.15	0.60
1:A:161[B]:HIS:HB3	2:A:525:HOH:O	2.01	0.60
1:B:61:PHE:O	1:B:65:MET:HG2	2.01	0.60
1:B:248:GLU:OE2	1:B:252:ARG:NH1	2.35	0.60
1:A:275:THR:O	1:A:279:SER:HB2	2.01	0.60
1:A:116:PHE:CZ	1:B:153:PHE:CD1	2.89	0.60
1:B:108:CYS:SG	1:B:114:MET:HG2	2.41	0.60
1:A:145:HIS:O	1:A:147:ASN:ND2	2.35	0.60
1:B:305:LYS:HD2	1:B:309:ARG:HH22	1.66	0.60
1:A:148:ASN:HD21	1:A:151:TYR:H	1.50	0.59
1:B:67:LYS:NZ	1:B:67:LYS:CD	2.64	0.59
1:B:304:ASP:HB3	1:B:307:GLN:HB3	1.85	0.59
1:B:35:LYS:HB2	1:B:316:ASN:ND2	2.18	0.59
1:B:173:ASN:HD21	1:B:193:ARG:CG	2.16	0.59
1:A:169:ALA:HB2	2:A:703:HOH:O	2.02	0.58
1:B:125:PHE:HZ	1:B:182:TRP:CD1	2.22	0.58
1:A:271:ASN:CB	1:A:273:ILE:HD12	2.34	0.58
1:B:321:LYS:HE3	2:B:650:HOH:O	2.04	0.58
1:B:148:ASN:ND2	1:B:151:TYR:N	2.48	0.58
1:A:11:MET:HE1	2:A:338:HOH:O	2.03	0.58
1:B:94:ASP:OD1	1:B:164:THR:OG1	2.22	0.58
1:B:101:PHE:CE2	1:B:103:PHE:HB2	2.39	0.57
1:B:125:PHE:HZ	1:B:182:TRP:CG	2.22	0.57
1:A:110:LYS:HB2	1:A:113:ASP:HB2	1.85	0.57
1:A:116:PHE:CE2	1:B:156:ILE:HG12	2.39	0.57
1:B:31:VAL:HA	1:B:34:LEU:HG	1.86	0.57
1:B:63:LEU:HD23	1:B:71:VAL:HG23	1.87	0.57
1:B:143:TYR:HE1	1:B:157:SER:HB2	1.69	0.57
1:A:148:ASN:HD22	1:A:149:ASP:N	2.02	0.57
1:B:66:THR:OG1	1:B:100:ARG:NH2	2.39	0.56
1:A:68:ASN:HA	2:A:388:HOH:O	2.04	0.56
1:B:125:PHE:CZ	1:B:182:TRP:CD1	2.94	0.56
1:B:148:ASN:ND2	1:B:150:PHE:HB2	2.21	0.56
1:B:176:SER:OG	1:B:179:VAL:HG23	2.06	0.56
1:B:145:HIS:CD2	1:B:155:LYS:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:CD2	1:B:71:VAL:HG23	2.36	0.55
1:A:253:GLU:HG2	1:A:254:SER:N	2.20	0.55
1:A:309:ARG:HA	1:A:312:ILE:HD12	1.88	0.55
1:A:308:GLN:O	1:A:312:ILE:HG13	2.07	0.55
1:A:116:PHE:CZ	1:B:156:ILE:CG1	2.89	0.54
1:A:138:ALA:O	1:A:142:GLY:N	2.33	0.54
1:A:133:LYS:HD3	2:A:418:HOH:O	2.08	0.54
1:B:308:GLN:O	1:B:312:ILE:HG13	2.07	0.54
1:B:35:LYS:HB2	1:B:316:ASN:HD21	1.72	0.53
1:A:146:PRO:CD	1:A:153:PHE:CD1	2.92	0.53
1:B:125:PHE:HZ	1:B:182:TRP:HB2	1.73	0.53
1:A:67:LYS:NZ	2:A:608:HOH:O	2.41	0.53
1:B:258:THR:HA	2:B:589:HOH:O	2.09	0.53
1:B:323:HIS:HA	2:B:638:HOH:O	2.09	0.53
1:B:3:PHE:HB3	1:B:297:MET:CE	2.38	0.53
1:B:153:PHE:HB2	1:B:154:PRO:HD2	1.92	0.52
1:B:302:MET:HE3	1:B:308:GLN:HG3	1.92	0.52
1:A:266:GLU:O	1:A:270:GLU:HG3	2.09	0.52
1:A:259:ASP:OD2	1:A:262:GLN:HB2	2.10	0.51
1:B:78:ILE:HD11	1:B:128:PHE:CE1	2.45	0.51
1:A:28:ALA:HA	1:A:39:LEU:HD21	1.91	0.51
1:A:146:PRO:HD3	1:A:153:PHE:CD1	2.42	0.51
1:B:117:PHE:O	1:B:119:ARG:HG2	2.11	0.51
1:A:82:HIS:ND1	1:A:83:PRO:HD2	2.25	0.51
1:B:251:VAL:CG1	1:B:260:PHE:CE1	2.94	0.51
1:B:82:HIS:HE1	1:B:84:VAL:HG23	1.76	0.51
1:A:272:ALA:O	1:A:279:SER:OG	2.29	0.51
1:A:111:SER:O	1:A:114:MET:HB2	2.11	0.51
1:B:115:ARG:NH2	2:B:544:HOH:O	2.35	0.50
1:B:262:GLN:HG3	2:B:716:HOH:O	2.11	0.50
1:B:35:LYS:CB	1:B:316:ASN:HD21	2.24	0.50
1:B:173:ASN:HA	1:B:191:VAL:CG1	2.41	0.50
1:A:27:THR:CG2	1:A:309:ARG:HH12	2.24	0.50
1:A:146:PRO:CG	1:A:153:PHE:CZ	2.92	0.49
1:A:277:GLU:O	1:A:281:GLN:HG3	2.11	0.49
1:B:298:SER:OG	1:B:300:GLU:OE1	2.30	0.49
1:A:276:TYR:O	1:A:280:THR:HG23	2.11	0.49
1:A:148:ASN:HD21	1:A:150:PHE:HB2	1.76	0.49
1:B:38:THR:HG22	1:B:39:LEU:N	2.27	0.49
1:B:275:THR:O	1:B:279:SER:HB3	2.11	0.49
1:B:264:MET:O	1:B:268:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ALA:O	1:B:217:VAL:HB	2.13	0.49
1:B:202:LYS:HG3	1:B:289:CYS:O	2.13	0.48
1:A:116:PHE:CZ	1:B:156:ILE:CG2	2.96	0.48
1:B:101:PHE:HE2	1:B:103:PHE:HB2	1.78	0.48
1:B:231:ASN:HD22	1:B:301:SER:HB2	1.78	0.48
1:A:79:THR:CG2	1:A:108:CYS:H	2.27	0.48
1:A:11:MET:HG2	1:A:51:VAL:CG1	2.44	0.47
1:A:126:GLN:HG2	2:A:542:HOH:O	2.14	0.47
1:A:73:SER:O	1:A:104:GLY:HA3	2.13	0.47
1:A:116:PHE:CE2	1:B:156:ILE:CG1	2.97	0.47
1:A:79:THR:HG21	1:A:108:CYS:H	1.79	0.47
1:B:173:ASN:ND2	1:B:193:ARG:HD3	2.30	0.47
1:A:43:GLU:HB2	1:A:55:PRO:HG3	1.97	0.47
1:A:116:PHE:HE2	1:B:156:ILE:CD1	2.24	0.47
1:B:82:HIS:CE1	1:B:84:VAL:CG2	2.97	0.47
1:B:109:GLU:HA	2:B:473:HOH:O	2.15	0.47
1:B:125:PHE:HZ	1:B:182:TRP:CB	2.28	0.47
1:A:68:ASN:ND2	2:A:388:HOH:O	2.29	0.47
1:B:56:LEU:HB2	2:B:338:HOH:O	2.14	0.47
1:B:33:GLN:HG2	1:B:34:LEU:CD2	2.41	0.46
1:B:43:GLU:HB2	1:B:55:PRO:HG3	1.96	0.46
1:B:62:LEU:O	1:B:66:THR:HG23	2.14	0.46
1:B:266:GLU:O	1:B:270:GLU:HG3	2.15	0.46
1:A:147:ASN:ND2	1:A:147:ASN:N	2.64	0.46
1:A:182:TRP:CE2	1:A:186:LEU:HD11	2.50	0.46
1:B:130[A]:GLU:OE2	1:B:134:ILE:HD11	2.15	0.46
1:A:146:PRO:HD3	1:A:153:PHE:CZ	2.47	0.45
1:B:226:LEU:HG	1:B:227:THR:N	2.31	0.45
1:B:146:PRO:CD	1:B:153:PHE:CE1	3.00	0.45
1:A:273:ILE:HG22	1:A:274:GLY:N	2.32	0.45
1:B:156:ILE:HD12	1:B:158:VAL:HG22	1.99	0.45
1:A:18:ASP:OD1	1:A:18:ASP:N	2.47	0.45
1:A:116:PHE:CE2	1:B:153:PHE:CZ	3.05	0.45
1:A:146:PRO:O	1:A:146:PRO:HG2	2.16	0.45
1:A:78:ILE:HD13	1:A:105:PHE:CD2	2.51	0.45
1:A:181:GLU:O	1:A:185:LYS:HE3	2.16	0.45
1:B:73:SER:O	1:B:104:GLY:HA3	2.17	0.44
1:B:251:VAL:CG1	1:B:260:PHE:CD1	2.97	0.44
1:A:323:HIS:NE2	2:A:892:HOH:O	2.35	0.44
1:B:125:PHE:CZ	1:B:182:TRP:HB2	2.52	0.44
1:B:38:THR:CG2	1:B:39:LEU:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASN:HA	1:B:191:VAL:HG13	2.00	0.44
1:B:194:TRP:CZ3	1:B:195:ASP:HB3	2.53	0.44
1:B:6:PHE:CE1	1:B:227:THR:HB	2.53	0.44
1:B:99:GLY:HA2	2:B:371:HOH:O	2.16	0.44
1:B:225:LYS:HE3	2:B:489:HOH:O	2.17	0.44
1:A:38:THR:CG2	1:A:39:LEU:N	2.79	0.44
1:A:172:VAL:O	1:A:190:LEU:HA	2.18	0.43
1:B:35:LYS:CA	1:B:316:ASN:HD21	2.31	0.43
1:A:273:ILE:CG2	1:A:274:GLY:N	2.81	0.43
1:B:148:ASN:ND2	1:B:150:PHE:CA	2.81	0.43
1:B:148:ASN:HD21	1:B:151:TYR:N	2.12	0.43
1:B:109:GLU:OE1	1:B:110:LYS:HG3	2.18	0.43
1:A:323:HIS:CD2	2:A:892:HOH:O	2.70	0.43
1:A:158:VAL:O	1:A:161[A]:HIS:ND1	2.51	0.43
1:A:123:SER:HA	2:A:543:HOH:O	2.18	0.43
1:A:195:ASP:N	1:A:195:ASP:OD1	2.39	0.43
1:A:19:GLN:O	1:A:23:GLU:HG3	2.19	0.43
1:B:236:GLY:C	1:B:240:ARG:NH2	2.77	0.42
1:B:82:HIS:CE1	1:B:84:VAL:CB	3.01	0.42
1:A:147:ASN:HA	2:A:431:HOH:O	2.18	0.42
1:B:204:TYR:HD1	1:B:204:TYR:HA	1.71	0.42
1:B:219:VAL:C	1:B:221:GLN:N	2.77	0.42
1:A:146:PRO:CG	1:A:153:PHE:CD2	2.96	0.42
1:B:63:LEU:CD2	1:B:71:VAL:CG2	2.98	0.42
1:B:148:ASN:ND2	1:B:150:PHE:CB	2.82	0.42
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.74	0.42
1:A:11:MET:HE3	1:A:11:MET:HB2	1.87	0.42
1:B:29:HIS:C	1:B:29:HIS:CD2	2.98	0.42
1:B:82:HIS:ND1	1:B:84:VAL:HB	2.34	0.42
1:B:211:VAL:O	1:B:214:ALA:HB3	2.20	0.42
1:B:173:ASN:HA	1:B:191:VAL:HG12	2.02	0.41
1:B:146:PRO:HD2	1:B:153:PHE:CD1	2.56	0.41
1:B:237:GLU:HA	1:B:240:ARG:NH2	2.36	0.41
1:A:15:ARG:O	1:A:15:ARG:HG2	2.20	0.41
1:B:34:LEU:N	1:B:34:LEU:CD2	2.73	0.41
1:A:37:ASP:OD1	1:A:70:LYS:HE3	2.21	0.41
1:B:82:HIS:CE1	1:B:84:VAL:HG23	2.55	0.41
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.75	0.41
1:B:152[A]:SER:OG	2:B:655:HOH:O	2.11	0.41
1:A:248:GLU:HB3	2:A:495:HOH:O	2.22	0.40
1:B:81:HIS:HD2	2:B:514:HOH:O	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASN:O	1:B:275:THR:HA	2.21	0.40
1:B:146:PRO:HD2	1:B:153:PHE:CE1	2.55	0.40
1:B:173:ASN:HD21	1:B:193:ARG:CD	2.34	0.40
1:B:218:ASP:CG	1:B:221:GLN:NE2	2.75	0.40
1:B:244:ARG:HG3	1:B:264:MET:HE3	2.03	0.40
1:B:153:PHE:HA	1:B:154:PRO:HD3	1.88	0.40
1:B:202:LYS:NZ	1:B:289:CYS:HB3	2.30	0.40
1:B:248:GLU:O	1:B:252:ARG:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:860:HOH:O	2:B:699:HOH:O[1_645]	0.36	1.84

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	323/324 (100%)	309 (96%)	13 (4%)	1 (0%)	36	28
1	B	325/324 (100%)	305 (94%)	17 (5%)	3 (1%)	14	6
All	All	648/648 (100%)	614 (95%)	30 (5%)	4 (1%)	21	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	B	260	PHE
1	B	68	ASN
1	B	320	VAL

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	275/274 (100%)	230 (84%)	45 (16%)	2	0
1	B	277/274 (101%)	250 (90%)	27 (10%)	8	2
All	All	552/548 (101%)	480 (87%)	72 (13%)	4	1

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	14	LYS
1	A	31	VAL
1	A	39	LEU
1	A	67	LYS
1	A	81	HIS
1	A	109	GLU
1	A	115	ARG
1	A	116	PHE
1	A	119	ARG
1	A	121	THR
1	A	123	SER
1	A	124	GLN
1	A	129	SER
1	A	130	GLU
1	A	146	PRO
1	A	147	ASN
1	A	148	ASN
1	A	149	ASP
1	A	152	SER
1	A	156	ILE
1	A	158	VAL
1	A	161[A]	HIS
1	A	161[B]	HIS
1	A	172	VAL
1	A	173	ASN
1	A	185	LYS

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Mol	Chain	Res	Type
1	A	193	ARG
1	A	202	LYS
1	A	210	GLU
1	A	226	LEU
1	A	234	VAL
1	A	237	GLU
1	A	248	GLU
1	A	252	ARG
1	A	253	GLU
1	A	256	SER
1	A	261	GLU
1	A	262	GLN
1	A	263	LYS
1	A	279	SER
1	A	284	ARG
1	A	303	GLU
1	A	320	VAL
1	A	321	LYS
1	B	5	LEU
1	B	11	MET
1	B	13	SER
1	B	14	LYS
1	B	33	GLN
1	B	34	LEU
1	B	109	GLU
1	B	118	ASN
1	B	121	THR
1	B	122	ASP
1	B	123	SER
1	B	124	GLN
1	B	129	SER
1	B	133	LYS
1	B	153	PHE
1	B	156	ILE
1	B	177	LYS
1	B	185	LYS
1	B	248	GLU
1	B	253	GLU
1	B	263	LYS
1	B	281	GLN
1	B	288	GLU
1	B	289	CYS

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Mol	Chain	Res	Type
1	B	301	SER
1	B	303	GLU
1	B	314	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	44	ASN
1	A	48	ASN
1	A	49	ASN
1	A	68	ASN
1	A	126	GLN
1	A	147	ASN
1	A	148	ASN
1	A	159	ASN
1	A	173	ASN
1	A	221	GLN
1	A	232	GLN
1	B	9	ASN
1	B	49	ASN
1	B	95	GLN
1	B	145	HIS
1	B	148	ASN
1	B	173	ASN
1	B	209	HIS
1	B	213	GLN
1	B	221	GLN
1	B	316	ASN
1	B	323	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.