



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:38 PM GMT

PDB ID : 1BSL  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

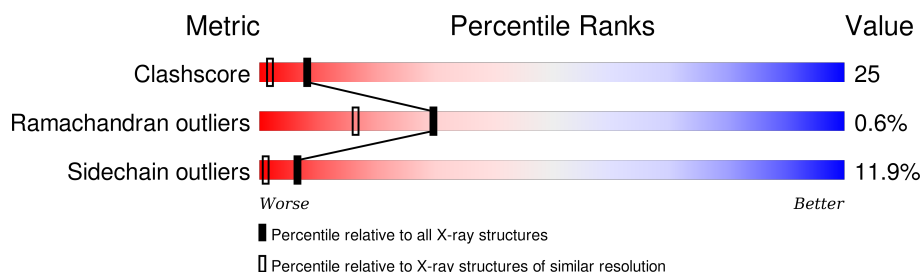
# 1 Overall quality at a glance

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	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	324	
1	B	324	

## 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.

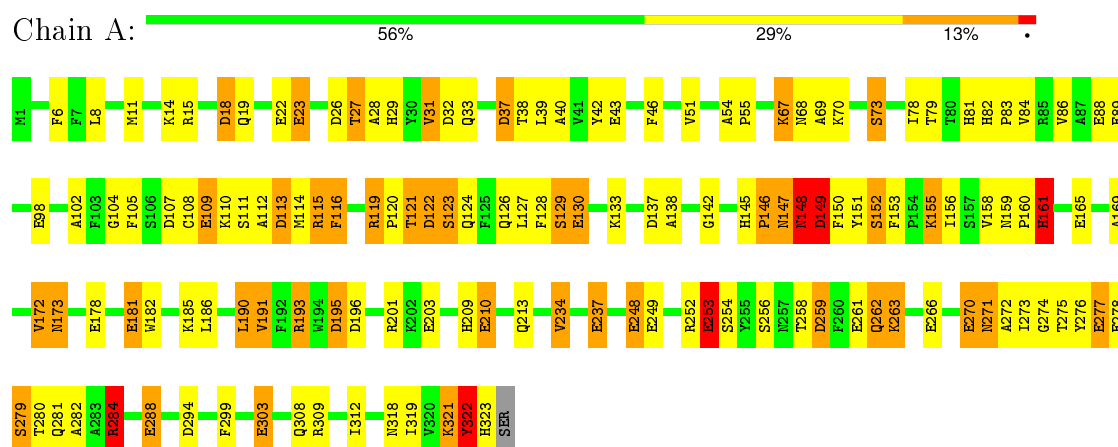
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	586	Total	O	0	0
			586	586		
2	B	403	Total	O	0	0
			403	403		

### 3 Residue-property plots

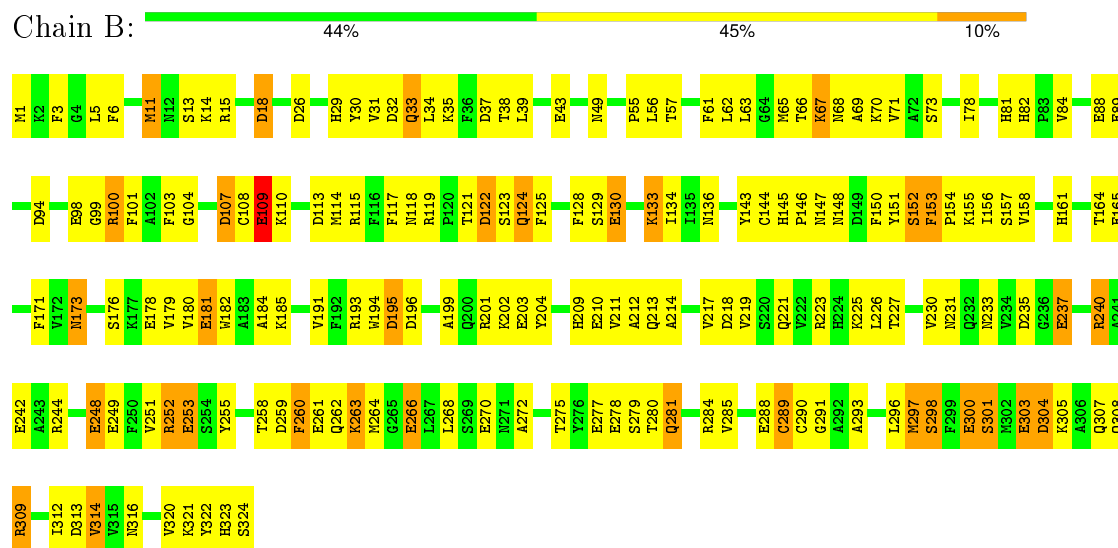
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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 will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	1.19	22/2629 (0.8%)	1.63	52/3556 (1.5%)
1	B	1.21	24/2640 (0.9%)	1.68	56/3570 (1.6%)
All	All	1.20	46/5269 (0.9%)	1.66	108/7126 (1.5%)

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 (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	LYS	CE-NZ	11.16	1.76	1.49
1	A	88	GLU	CD-OE1	11.10	1.37	1.25
1	B	261	GLU	CD-OE1	9.22	1.35	1.25
1	A	270	GLU	CD-OE1	8.89	1.35	1.25
1	A	109	GLU	CD-OE2	8.60	1.35	1.25
1	B	266	GLU	CD-OE2	-7.78	1.17	1.25
1	A	203	GLU	CD-OE1	7.67	1.34	1.25
1	B	277	GLU	CD-OE1	7.65	1.34	1.25
1	B	178	GLU	CD-OE1	7.59	1.33	1.25
1	A	89	GLU	CD-OE2	7.54	1.33	1.25
1	B	165	GLU	CD-OE1	7.51	1.33	1.25
1	A	288	GLU	CD-OE1	7.47	1.33	1.25
1	B	249	GLU	CD-OE2	7.40	1.33	1.25
1	A	253	GLU	CD-OE2	7.11	1.33	1.25
1	A	155	LYS	CE-NZ	-7.03	1.31	1.49
1	B	181	GLU	CD-OE1	6.95	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	GLU	CD-OE2	6.85	1.33	1.25
1	A	22	GLU	CD-OE1	6.76	1.33	1.25
1	B	303	GLU	CD-OE2	6.40	1.32	1.25
1	B	237	GLU	CD-OE2	6.39	1.32	1.25
1	A	303	GLU	CD-OE1	6.30	1.32	1.25
1	A	249	GLU	CD-OE1	6.29	1.32	1.25
1	A	237	GLU	CD-OE1	6.25	1.32	1.25
1	B	278	GLU	CD-OE1	6.05	1.32	1.25
1	B	210	GLU	CD-OE2	5.92	1.32	1.25
1	A	248	GLU	CD-OE1	5.89	1.32	1.25
1	A	178	GLU	CD-OE1	5.87	1.32	1.25
1	B	203	GLU	CD-OE2	5.87	1.32	1.25
1	A	181	GLU	CD-OE2	5.77	1.31	1.25
1	A	278	GLU	CD-OE1	5.74	1.31	1.25
1	B	98	GLU	CD-OE1	5.66	1.31	1.25
1	A	23	GLU	CD-OE1	5.66	1.31	1.25
1	B	242	GLU	CD-OE1	5.59	1.31	1.25
1	A	277	GLU	CD-OE1	5.57	1.31	1.25
1	A	98	GLU	CD-OE2	5.47	1.31	1.25
1	A	165	GLU	CD-OE2	5.40	1.31	1.25
1	B	130[A]	GLU	CD-OE2	-5.33	1.19	1.25
1	B	130[B]	GLU	CD-OE2	-5.33	1.19	1.25
1	B	109	GLU	CD-OE1	5.32	1.31	1.25
1	B	278	GLU	CD-OE2	-5.31	1.19	1.25
1	B	266	GLU	CD-OE1	5.30	1.31	1.25
1	A	109	GLU	CD-OE1	-5.22	1.20	1.25
1	B	32	ASP	CG-OD1	5.21	1.37	1.25
1	B	300	GLU	CD-OE1	5.21	1.31	1.25
1	B	88	GLU	CD-OE1	5.06	1.31	1.25
1	B	253	GLU	CD-OE2	5.00	1.31	1.25

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ARG	NE-CZ-NH2	-13.51	113.54	120.30
1	B	100	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	A	201	ARG	NE-CZ-NH2	-12.43	114.09	120.30
1	A	201	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	A	318	ASN	CB-CA-C	10.50	131.41	110.40
1	B	15	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	B	196	ASP	CB-CG-OD2	-10.06	109.25	118.30
1	A	284	ARG	NE-CZ-NH1	10.02	125.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ASP	CB-CG-OD1	9.48	126.84	118.30
1	A	193	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	A	137	ASP	CB-CG-OD1	-9.24	109.98	118.30
1	B	26	ASP	CB-CG-OD1	-9.24	109.99	118.30
1	A	107	ASP	CB-CG-OD1	-8.44	110.71	118.30
1	A	18	ASP	CB-CG-OD1	-8.23	110.89	118.30
1	A	252	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	259	ASP	CB-CG-OD1	-8.00	111.10	118.30
1	A	113	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	B	107	ASP	CB-CG-OD1	-7.87	111.21	118.30
1	B	309	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	69	ALA	N-CA-CB	7.74	120.93	110.10
1	B	15	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	161[A]	HIS	CB-CA-C	7.67	125.75	110.40
1	A	161[B]	HIS	CB-CA-C	7.67	125.75	110.40
1	B	304	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	B	201	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	113	ASP	CB-CG-OD2	7.18	124.76	118.30
1	B	18	ASP	CB-CG-OD2	7.14	124.72	118.30
1	B	240	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	40	ALA	N-CA-CB	6.97	119.86	110.10
1	B	195	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	259	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	190	LEU	CB-CA-C	-6.91	97.07	110.20
1	B	100	ARG	CD-NE-CZ	6.89	133.25	123.60
1	B	70	LYS	N-CA-CB	-6.88	98.22	110.60
1	A	196	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	B	144	CYS	N-CA-CB	6.77	122.79	110.60
1	A	102	ALA	N-CA-CB	6.75	119.55	110.10
1	B	11	MET	N-CA-CB	-6.52	98.86	110.60
1	B	29	HIS	CA-CB-CG	-6.48	102.59	113.60
1	B	195	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	B	309	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	84	VAL	CG1-CB-CG2	-6.29	100.83	110.90
1	A	282	ALA	CB-CA-C	6.23	119.44	110.10
1	A	149	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	129	SER	N-CA-CB	6.19	119.79	110.50
1	A	119	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	152[A]	SER	N-CA-CB	6.18	119.77	110.50
1	B	152[B]	SER	N-CA-CB	6.18	119.77	110.50
1	B	297	MET	CG-SD-CE	6.17	110.08	100.20
1	B	259	ASP	CB-CG-OD1	6.10	123.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	201	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	18	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	240	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	196	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	27	THR	CA-CB-CG2	-6.01	103.99	112.40
1	A	73	SER	N-CA-CB	5.99	119.48	110.50
1	B	284	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	A	42	TYR	CB-CG-CD1	-5.96	117.43	121.00
1	B	26	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	322	TYR	CG-CD2-CE2	-5.85	116.62	121.30
1	B	37	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	294	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	26	ASP	CB-CA-C	-5.79	98.83	110.40
1	A	32	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	A	37	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	33	GLN	N-CA-CB	5.68	120.83	110.60
1	B	147	ASN	N-CA-CB	-5.67	100.39	110.60
1	A	258	THR	CA-CB-CG2	-5.67	104.47	112.40
1	A	29	HIS	CA-CB-CG	-5.65	104.00	113.60
1	A	26	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	223	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	113	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	322	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	A	271	ASN	N-CA-CB	5.58	120.64	110.60
1	B	136	ASN	N-CA-CB	-5.58	100.56	110.60
1	B	89	GLU	CG-CD-OE1	-5.57	107.16	118.30
1	B	244	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	161[A]	HIS	N-CA-CB	-5.54	100.63	110.60
1	A	161[B]	HIS	N-CA-CB	-5.54	100.63	110.60
1	B	298	SER	N-CA-CB	5.54	118.81	110.50
1	B	199	ALA	N-CA-CB	-5.53	102.36	110.10
1	A	319	ILE	CB-CA-C	-5.52	100.55	111.60
1	A	122	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	303	GLU	CB-CA-C	5.52	121.43	110.40
1	B	180	VAL	CA-CB-CG1	-5.50	102.65	110.90
1	B	89	GLU	CG-CD-OE2	5.50	129.29	118.30
1	B	235	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	296	LEU	N-CA-CB	5.37	121.15	110.40
1	A	149	ASP	CB-CG-OD1	5.34	123.10	118.30
1	B	184	ALA	N-CA-CB	-5.34	102.63	110.10
1	B	313	ASP	CB-CG-OD2	-5.32	113.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	PHE	CB-CG-CD1	5.32	124.52	120.80
1	B	195	ASP	N-CA-CB	5.31	120.16	110.60
1	B	171	PHE	N-CA-CB	5.27	120.09	110.60
1	A	6	PHE	N-CA-CB	5.21	119.98	110.60
1	A	195	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	B	57	THR	CA-CB-OG1	-5.20	98.08	109.00
1	B	30	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	B	280	THR	N-CA-CB	-5.13	100.55	110.30
1	A	234	VAL	CB-CA-C	-5.13	101.66	111.40
1	B	70	LYS	CA-CB-CG	-5.12	102.12	113.40
1	A	120	PRO	N-CA-CB	5.11	109.43	103.30
1	A	128	PHE	CB-CG-CD2	-5.09	117.23	120.80
1	B	109	GLU	N-CA-CB	-5.08	101.46	110.60
1	B	314	VAL	CG1-CB-CG2	5.03	118.95	110.90
1	A	191	VAL	N-CA-CB	5.02	122.55	111.50
1	A	130	GLU	CG-CD-OE1	5.01	128.32	118.30

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	108	0
1	B	2568	0	2446	151	0
2	A	586	0	0	20	1
2	B	403	0	0	23	1
All	All	6116	0	4881	246	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 (246) 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:NZ	1:B:67:LYS:CE	1.76	1.46
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:114:MET:HE2	1:B:124:GLN:HG3	1.56	0.88
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:114:MET:CE	1:B:124:GLN:HG3	2.11	0.80
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:VAL:HG22	1:B:272:ALA:HB3	1.69	0.72
1:A:284:ARG:O	1:A:288:GLU:HG3	1.89	0.72
1:A:148:ASN:ND2	1:A:151:TYR:H	1.87	0.72
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:263:LYS:NZ	2:A:898:HOH:O	2.16	0.70
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: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:B:122:ASP:N	1:B:122:ASP:OD1	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:321:LYS:HD2	1:A:322:TYR:CE2	2.29	0.68
1:A:209:HIS:O	1:A:213:GLN:HG3	1.94	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:143:TYR:CE1	1:B:157:SER:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:HIS:HE1	1:B:84:VAL:CG2	2.12	0.62
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:B:248:GLU:OE2	1:B:252:ARG:NH1	2.35	0.60
1:B:61:PHE:O	1:B:65:MET:HG2	2.01	0.60
1:A:161[B]:HIS:HB3	2:A:525:HOH:O	2.01	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:B:67:LYS:CD	1:B:67:LYS:NZ	2.64	0.59
1:A:148:ASN:HD21	1:A:151:TYR:H	1.50	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:B:321:LYS:HE3	2:B:650:HOH:O	2.04	0.58
1:A:271:ASN:CB	1:A:273:ILE:HD12	2.34	0.58
1:B:148:ASN:ND2	1:B:151:TYR:N	2.48	0.58
1:B:218:ASP:CG	1:B:221:GLN:HE21	2.07	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:143:TYR:HE1	1:B:157:SER:HB2	1.69	0.57
1:B:63:LEU:HD23	1:B:71:VAL:HG23	1.87	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:253:GLU:HG2	1:A:254:SER:N	2.20	0.56
1:A:68:ASN:HA	2:A:388:HOH:O	2.04	0.56
1:B:148:ASN:ND2	1:B:150:PHE:HB2	2.21	0.56
1:B:125:PHE:CZ	1:B:182:TRP:CD1	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:63:LEU:CD2	1:B:71:VAL:HG23	2.36	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: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:A:266:GLU:O	1:A:270:GLU:HG3	2.09	0.52
1:B:78:ILE:HD11	1:B:128:PHE:CE1	2.45	0.51
1:A:259:ASP:OD2	1:A:262:GLN:HB2	2.10	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:28:ALA:HA	1:A:39:LEU:HD21	1.91	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:B:298:SER:OG	1:B:300:GLU:OE1	2.30	0.49
1:A:277:GLU:O	1:A:281:GLN:HG3	2.11	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
1:B:212:ALA:O	1:B:217:VAL:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:231:ASN:HD22	1:B:301:SER:HB2	1.78	0.48
1:B:101:PHE:HE2	1:B:103:PHE:HB2	1.78	0.48
1:A:67:LYS:NZ	2:A:608:HOH:O	2.41	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:116:PHE:CE2	1:B:156:ILE:CG1	2.97	0.47
1:A:73:SER:O	1:A:104:GLY:HA3	2.13	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:116:PHE:HE2	1:B:156:ILE:CD1	2.24	0.47
1:A:43:GLU:HB2	1:A:55:PRO:HG3	1.97	0.47
1:B:109:GLU:HA	2:B:473:HOH:O	2.15	0.47
1:B:82:HIS:CE1	1:B:84:VAL:CG2	2.97	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:62:LEU:O	1:B:66:THR:HG23	2.14	0.46
1:B:43:GLU:HB2	1:B:55:PRO:HG3	1.96	0.46
1:B:266:GLU:O	1:B:270:GLU:HG3	2.15	0.46
1:A:147:ASN:N	1:A:147:ASN:ND2	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:38:THR:CG2	1:A:39:LEU:N	2.79	0.45
1:A:146:PRO:O	1:A:146:PRO:HG2	2.16	0.45
1:A:116:PHE:CE2	1:B:153:PHE:CZ	3.05	0.45
1:A:18:ASP:N	1:A:18:ASP:OD1	2.47	0.45
1:A:181:GLU:O	1:A:185:LYS:HE3	2.16	0.45
1:A:78:ILE:HD13	1:A:105:PHE:CD2	2.51	0.45
1:B:251:VAL:CG1	1:B:260:PHE:CD1	2.97	0.44
1:B:73:SER:O	1:B:104:GLY:HA3	2.17	0.44
1:B:125:PHE:CZ	1:B:182:TRP:HB2	2.52	0.44
1:A:323:HIS:NE2	2:A:892:HOH:O	2.35	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:38:THR:CG2	1:B:39:LEU:N	2.81	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:B:35:LYS:CA	1:B:316:ASN:HD21	2.31	0.43
1:A:172:VAL:O	1:A:190:LEU:HA	2.18	0.43
1:B:148:ASN:ND2	1:B:150:PHE:CA	2.81	0.43
1:A:273:ILE:CG2	1:A:274:GLY:N	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:11:MET:HE3	2:A:338:HOH:O	2.18	0.43
1:A:195:ASP:OD1	1:A:195:ASP:N	2.39	0.43
1:A:123:SER:HA	2:A:543:HOH:O	2.18	0.43
1:A:19:GLN:O	1:A:23:GLU:HG3	2.19	0.43
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:HA	1:B:204:TYR:HD1	1.71	0.42
1:A:146:PRO:CG	1:A:153:PHE:CD2	2.96	0.42
1:B:148:ASN:ND2	1:B:150:PHE:CB	2.82	0.42
1:B:63:LEU:CD2	1:B:71:VAL:CG2	2.98	0.42
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.74	0.42
1:B:211:VAL:O	1:B:214:ALA:HB3	2.20	0.42
1:B:82:HIS:ND1	1:B:84:VAL:HB	2.34	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:CD2	1:B:34:LEU:N	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:B:233:ASN:O	1:B:275:THR:HA	2.21	0.40
1:B:81:HIS:HD2	2:B:514:HOH:O	2.05	0.40
1:A:248:GLU:HB3	2:A:495:HOH:O	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PHE:HA	1:B:154:PRO:HD3	1.88	0.40
1:B:248:GLU:O	1:B:252:ARG:HG3	2.22	0.40
1:B:202:LYS:NZ	1:B:289:CYS:HB3	2.30	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%)	46	35
1	B	325/324 (100%)	305 (94%)	17 (5%)	3 (1%)	21	9
All	All	648/648 (100%)	614 (95%)	30 (5%)	4 (1%)	30	16

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/274 (100%)	237 (86%)	38 (14%)	4	1
1	B	277/274 (101%)	249 (90%)	28 (10%)	9	2
All	All	552/548 (101%)	486 (88%)	66 (12%)	6	1

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	31	VAL
1	A	46	PHE
1	A	67	LYS
1	A	81	HIS
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	155	LYS
1	A	156	ILE
1	A	160	PRO
1	A	161[A]	HIS
1	A	161[B]	HIS
1	A	172	VAL
1	A	173	ASN
1	A	193	ARG
1	A	210	GLU
1	A	234	VAL
1	A	237	GLU
1	A	253	GLU
1	A	256	SER
1	A	261	GLU
1	A	262	GLN

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Mol	Chain	Res	Type
1	A	263	LYS
1	A	279	SER
1	A	284	ARG
1	A	303	GLU
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	49	ASN
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	173	ASN
1	B	185	LYS
1	B	248	GLU
1	B	252	ARG
1	B	253	GLU
1	B	263	LYS
1	B	281	GLN
1	B	288	GLU
1	B	289	CYS
1	B	290	CYS
1	B	301	SER
1	B	303	GLU
1	B	314	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	33	GLN
1	A	68	ASN
1	A	126	GLN
1	A	147	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	148	ASN
1	A	173	ASN
1	A	232	GLN
1	B	9	ASN
1	B	33	GLN
1	B	145	HIS
1	B	148	ASN
1	B	173	ASN
1	B	221	GLN
1	B	316	ASN
1	B	323	HIS

### 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 carbohydrates 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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.