Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:56 PM GMT

PDB ID	:	1RBB
Title	:	THE CRYSTAL STRUCTURE OF RIBONUCLEASE B AT 2.5-ANGSTROMS RESOLUTION
Authors	:	Williams, R.L.; Greene, S.M.; McPherson, A.
Deposited on	:	1987-09-14
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

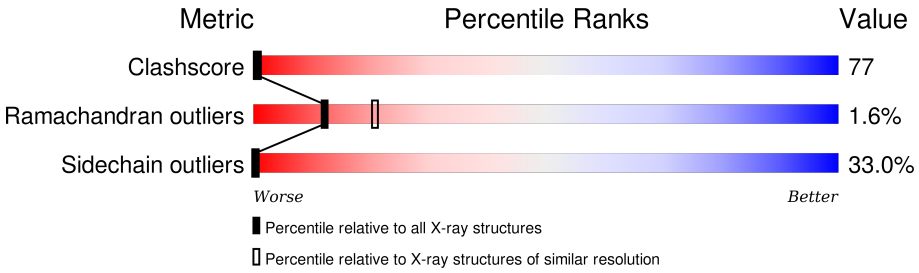
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 >=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 <=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	124	7% 29% 44% 20%
1	B	124	7% 26% 50% 17%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1900 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 RIBONUCLEASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			950	575	171	192	12			
1	B	124	Total	C	N	O	S	0	0	0
			950	575	171	192	12			

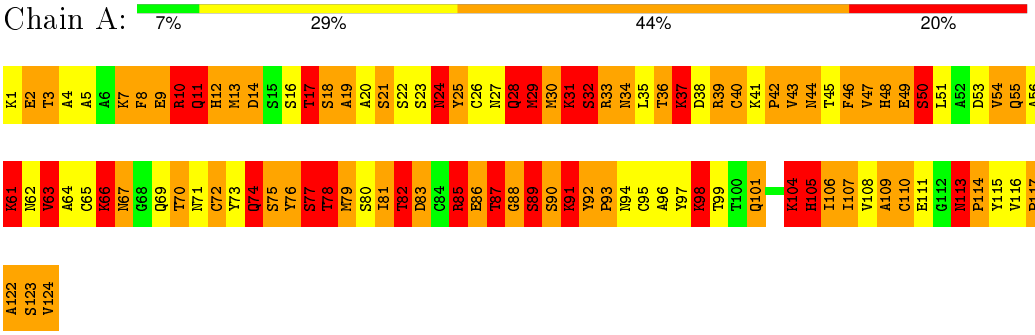
3 Residue-property plots (i)

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.

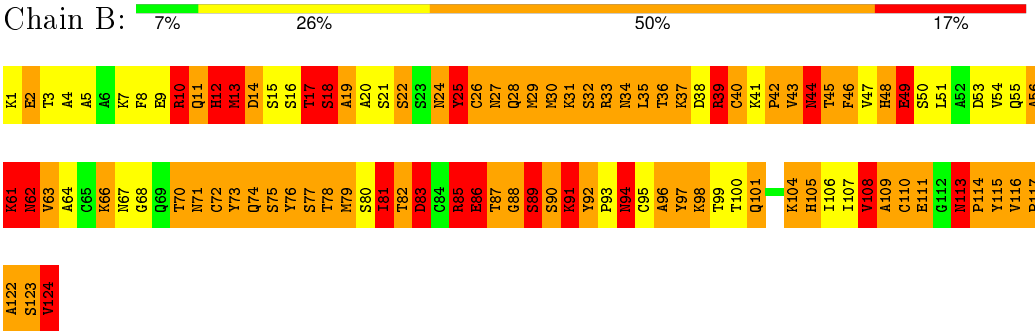
- Molecule 1: RIBONUCLEASE B

Chain A:



- Molecule 1: RIBONUCLEASE B

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.81Å 33.36Å 73.60Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CORELS	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1900	wwPDB-VP
Average B, all atoms (Å^2)	11.0	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	3.28	136/966 (14.1%)	3.17	106/1304 (8.1%)
1	B	3.20	133/966 (13.8%)	3.14	100/1304 (7.7%)
All	All	3.24	269/1932 (13.9%)	3.16	206/2608 (7.9%)

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	2
1	B	0	2
All	All	0	4

All (269) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	GLU	CD-OE2	13.92	1.41	1.25
1	A	2	GLU	CD-OE2	13.68	1.40	1.25
1	B	77	SER	CB-OG	12.62	1.58	1.42
1	A	77	SER	CB-OG	12.55	1.58	1.42
1	A	9	GLU	CD-OE2	11.08	1.37	1.25
1	A	85	ARG	CZ-NH2	11.00	1.47	1.33
1	A	18	SER	CA-CB	10.85	1.69	1.52
1	A	32	SER	CA-CB	10.82	1.69	1.52
1	B	85	ARG	CZ-NH2	10.79	1.47	1.33
1	B	9	GLU	CD-OE2	10.52	1.37	1.25
1	B	18	SER	CA-CB	10.44	1.68	1.52
1	A	33	ARG	CZ-NH2	10.43	1.46	1.33
1	A	49	GLU	CG-CD	10.37	1.67	1.51
1	A	117	PRO	N-CD	10.35	1.62	1.47
1	B	49	GLU	CG-CD	10.29	1.67	1.51
1	B	32	SER	CA-CB	10.20	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	SER	CB-OG	10.09	1.55	1.42
1	A	115	TYR	CG-CD1	10.08	1.52	1.39
1	A	97	TYR	CD2-CE2	9.98	1.54	1.39
1	B	97	TYR	CD2-CE2	9.88	1.54	1.39
1	A	22	SER	CB-OG	9.79	1.54	1.42
1	B	115	TYR	CG-CD1	9.64	1.51	1.39
1	B	33	ARG	CZ-NH2	9.62	1.45	1.33
1	B	117	PRO	N-CD	9.51	1.61	1.47
1	A	97	TYR	CB-CG	9.49	1.65	1.51
1	A	73	TYR	CE1-CZ	9.34	1.50	1.38
1	B	73	TYR	CE1-CZ	9.28	1.50	1.38
1	B	97	TYR	CB-CG	9.24	1.65	1.51
1	A	95	CYS	CB-SG	9.21	1.98	1.82
1	B	95	CYS	CB-SG	8.99	1.97	1.82
1	A	86	GLU	CG-CD	8.91	1.65	1.51
1	B	86	GLU	CG-CD	8.89	1.65	1.51
1	A	111	GLU	CD-OE2	8.88	1.35	1.25
1	A	94	ASN	N-CA	8.81	1.64	1.46
1	A	115	TYR	CE2-CZ	8.81	1.50	1.38
1	A	67	ASN	C-O	8.70	1.39	1.23
1	A	110	CYS	CB-SG	8.69	1.97	1.82
1	B	111	GLU	CD-OE2	8.67	1.35	1.25
1	A	86	GLU	CD-OE1	-8.65	1.16	1.25
1	B	88	GLY	N-CA	8.65	1.59	1.46
1	B	94	ASN	N-CA	8.52	1.63	1.46
1	B	110	CYS	CB-SG	8.51	1.96	1.82
1	B	8	PHE	CG-CD2	8.31	1.51	1.38
1	B	67	ASN	C-O	8.31	1.39	1.23
1	A	8	PHE	CG-CD2	8.29	1.51	1.38
1	A	48	HIS	C-O	8.20	1.39	1.23
1	A	73	TYR	CG-CD2	8.16	1.49	1.39
1	A	27	ASN	C-O	8.12	1.38	1.23
1	A	116	VAL	CB-CG2	8.09	1.69	1.52
1	B	73	TYR	CG-CD2	8.08	1.49	1.39
1	A	89	SER	CA-CB	8.07	1.65	1.52
1	A	42	PRO	N-CD	8.06	1.59	1.47
1	B	116	VAL	CB-CG2	8.01	1.69	1.52
1	A	120	PHE	CB-CG	8.01	1.65	1.51
1	B	48	HIS	C-O	7.99	1.38	1.23
1	B	27	ASN	C-O	7.98	1.38	1.23
1	A	88	GLY	N-CA	7.97	1.58	1.46
1	B	115	TYR	CE2-CZ	7.96	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	ALA	N-CA	7.93	1.62	1.46
1	B	120	PHE	CB-CG	7.93	1.64	1.51
1	A	120	PHE	CD2-CE2	7.90	1.55	1.39
1	A	85	ARG	CD-NE	7.88	1.59	1.46
1	B	85	ARG	CD-NE	7.86	1.59	1.46
1	B	105	HIS	CB-CG	7.84	1.64	1.50
1	B	120	PHE	CD2-CE2	7.82	1.54	1.39
1	B	89	SER	CA-CB	7.70	1.64	1.52
1	A	105	HIS	CB-CG	7.68	1.63	1.50
1	A	5	ALA	C-O	7.55	1.37	1.23
1	B	96	ALA	N-CA	7.55	1.61	1.46
1	A	2	GLU	CB-CG	7.51	1.66	1.52
1	B	5	ALA	C-O	7.47	1.37	1.23
1	B	42	PRO	N-CD	7.39	1.58	1.47
1	A	106	ILE	N-CA	7.35	1.61	1.46
1	B	106	ILE	N-CA	7.35	1.61	1.46
1	A	97	TYR	CD1-CE1	7.33	1.50	1.39
1	A	88	GLY	C-O	7.28	1.35	1.23
1	B	86	GLU	CD-OE1	-7.18	1.17	1.25
1	A	115	TYR	CE1-CZ	7.17	1.47	1.38
1	A	62	ASN	N-CA	7.16	1.60	1.46
1	B	2	GLU	CB-CG	7.16	1.65	1.52
1	A	123	SER	N-CA	7.11	1.60	1.46
1	B	49	GLU	CD-OE2	7.11	1.33	1.25
1	B	88	GLY	C-O	7.10	1.35	1.23
1	B	97	TYR	CD1-CE1	7.07	1.50	1.39
1	A	56	ALA	CA-CB	7.04	1.67	1.52
1	B	62	ASN	N-CA	7.00	1.60	1.46
1	A	26	CYS	N-CA	6.87	1.60	1.46
1	B	123	SER	N-CA	6.83	1.60	1.46
1	B	56	ALA	CA-CB	6.81	1.66	1.52
1	B	64	ALA	N-CA	6.80	1.59	1.46
1	A	64	ALA	N-CA	6.80	1.59	1.46
1	A	16	SER	CA-CB	6.78	1.63	1.52
1	B	115	TYR	CE1-CZ	6.71	1.47	1.38
1	A	34	ASN	CG-ND2	6.66	1.49	1.32
1	B	16	SER	CA-CB	6.63	1.62	1.52
1	B	8	PHE	CD1-CE1	6.62	1.52	1.39
1	A	12	HIS	CG-CD2	6.61	1.47	1.35
1	B	34	ASN	CG-ND2	6.60	1.49	1.32
1	A	8	PHE	CD1-CE1	6.60	1.52	1.39
1	A	33	ARG	CD-NE	6.59	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	SER	CB-OG	-6.59	1.33	1.42
1	A	86	GLU	CA-CB	6.57	1.68	1.53
1	B	12	HIS	CG-CD2	6.54	1.46	1.35
1	B	31	LYS	CD-CE	6.52	1.67	1.51
1	A	50	SER	CB-OG	-6.50	1.33	1.42
1	A	40	CYS	N-CA	6.50	1.59	1.46
1	A	90	SER	CA-C	6.47	1.69	1.52
1	A	115	TYR	CG-CD2	6.46	1.47	1.39
1	B	31	LYS	C-O	6.44	1.35	1.23
1	A	87	THR	C-O	6.43	1.35	1.23
1	A	31	LYS	C-O	6.42	1.35	1.23
1	A	62	ASN	CB-CG	6.42	1.65	1.51
1	A	97	TYR	CA-C	6.41	1.69	1.52
1	A	59	SER	CB-OG	6.40	1.50	1.42
1	A	12	HIS	CB-CG	6.37	1.61	1.50
1	A	21	SER	CB-OG	6.37	1.50	1.42
1	B	97	TYR	CA-C	6.34	1.69	1.52
1	A	49	GLU	CD-OE2	6.33	1.32	1.25
1	A	91	LYS	N-CA	6.32	1.58	1.46
1	B	90	SER	CA-C	6.30	1.69	1.52
1	B	92	TYR	CE1-CZ	6.30	1.46	1.38
1	B	26	CYS	N-CA	6.30	1.58	1.46
1	B	28	GLN	CD-OE1	6.27	1.37	1.24
1	A	5	ALA	N-CA	6.27	1.58	1.46
1	A	10	ARG	CZ-NH1	6.26	1.41	1.33
1	B	87	THR	C-O	6.25	1.35	1.23
1	B	40	CYS	N-CA	6.24	1.58	1.46
1	B	86	GLU	CA-CB	6.24	1.67	1.53
1	B	4	ALA	C-O	6.22	1.35	1.23
1	B	91	LYS	N-CA	6.21	1.58	1.46
1	B	115	TYR	CG-CD2	6.20	1.47	1.39
1	B	62	ASN	CB-CG	6.19	1.65	1.51
1	A	67	ASN	N-CA	6.14	1.58	1.46
1	B	92	TYR	CG-CD2	6.13	1.47	1.39
1	A	24	ASN	CG-OD1	6.13	1.37	1.24
1	B	33	ARG	CD-NE	6.11	1.56	1.46
1	A	115	TYR	C-O	6.10	1.34	1.23
1	B	76	TYR	N-CA	6.06	1.58	1.46
1	A	30	MET	N-CA	6.05	1.58	1.46
1	B	111	GLU	CG-CD	6.03	1.60	1.51
1	B	2	GLU	N-CA	6.02	1.58	1.46
1	B	43	VAL	N-CA	6.01	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	GLU	N-CA	6.00	1.58	1.46
1	A	34	ASN	N-CA	5.99	1.58	1.46
1	A	82	THR	C-O	5.99	1.34	1.23
1	A	4	ALA	C-O	5.98	1.34	1.23
1	A	76	TYR	N-CA	5.98	1.58	1.46
1	A	31	LYS	CD-CE	5.97	1.66	1.51
1	A	13	MET	N-CA	5.94	1.58	1.46
1	A	120	PHE	N-CA	5.93	1.58	1.46
1	B	82	THR	C-O	5.93	1.34	1.23
1	A	93	PRO	CA-C	5.92	1.64	1.52
1	B	5	ALA	N-CA	5.91	1.58	1.46
1	B	115	TYR	C-O	5.91	1.34	1.23
1	B	21	SER	CB-OG	5.88	1.49	1.42
1	A	98	LYS	CE-NZ	5.87	1.63	1.49
1	A	89	SER	N-CA	5.86	1.58	1.46
1	A	21	SER	C-O	5.85	1.34	1.23
1	B	118	VAL	N-CA	5.85	1.58	1.46
1	B	120	PHE	N-CA	5.84	1.58	1.46
1	B	8	PHE	CD2-CE2	5.80	1.50	1.39
1	A	54	VAL	CB-CG1	5.80	1.65	1.52
1	B	14	ASP	C-O	5.80	1.34	1.23
1	A	28	GLN	CD-OE1	5.80	1.36	1.24
1	A	44	ASN	CA-C	5.79	1.68	1.52
1	B	64	ALA	C-O	5.79	1.34	1.23
1	A	92	TYR	CE1-CZ	5.79	1.46	1.38
1	A	33	ARG	CA-C	5.79	1.68	1.52
1	A	8	PHE	CD2-CE2	5.78	1.50	1.39
1	A	14	ASP	C-O	5.78	1.34	1.23
1	A	78	THR	CB-OG1	5.78	1.54	1.43
1	B	67	ASN	N-CA	5.76	1.57	1.46
1	A	92	TYR	CG-CD2	5.76	1.46	1.39
1	B	34	ASN	N-CA	5.75	1.57	1.46
1	B	14	ASP	CA-C	5.75	1.67	1.52
1	A	101	GLN	C-O	5.73	1.34	1.23
1	A	64	ALA	C-O	5.72	1.34	1.23
1	B	24	ASN	CG-OD1	5.72	1.36	1.24
1	A	85	ARG	CZ-NH1	5.71	1.40	1.33
1	A	14	ASP	CA-C	5.71	1.67	1.52
1	B	12	HIS	CB-CG	5.70	1.60	1.50
1	A	12	HIS	C-O	5.70	1.34	1.23
1	B	98	LYS	CE-NZ	5.67	1.63	1.49
1	B	44	ASN	CA-C	5.66	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	CYS	N-CA	5.65	1.57	1.46
1	B	13	MET	N-CA	5.65	1.57	1.46
1	B	21	SER	C-O	5.63	1.34	1.23
1	B	63	VAL	CA-C	5.62	1.67	1.52
1	A	4	ALA	CA-C	5.61	1.67	1.52
1	A	90	SER	CA-CB	-5.61	1.44	1.52
1	B	12	HIS	C-O	5.61	1.34	1.23
1	A	63	VAL	CA-C	5.60	1.67	1.52
1	A	34	ASN	C-O	5.60	1.33	1.23
1	B	93	PRO	CA-C	5.59	1.64	1.52
1	A	98	LYS	N-CA	5.59	1.57	1.46
1	B	101	GLN	C-O	5.59	1.33	1.23
1	A	118	VAL	N-CA	5.57	1.57	1.46
1	A	82	THR	CA-C	5.56	1.67	1.52
1	A	113	ASN	C-O	5.55	1.33	1.23
1	B	120	PHE	CE1-CZ	5.55	1.47	1.37
1	B	33	ARG	CA-C	5.53	1.67	1.52
1	A	120	PHE	CE1-CZ	5.52	1.47	1.37
1	B	98	LYS	N-CA	5.52	1.57	1.46
1	A	95	CYS	CA-C	5.51	1.67	1.52
1	B	30	MET	N-CA	5.50	1.57	1.46
1	A	43	VAL	N-CA	5.48	1.57	1.46
1	A	3	THR	CB-OG1	5.48	1.54	1.43
1	A	30	MET	C-O	5.46	1.33	1.23
1	A	39	ARG	CA-C	5.46	1.67	1.52
1	B	113	ASN	C-O	5.46	1.33	1.23
1	A	9	GLU	C-O	5.45	1.33	1.23
1	A	67	ASN	CG-ND2	5.43	1.46	1.32
1	A	24	ASN	N-CA	5.42	1.57	1.46
1	B	54	VAL	CB-CG1	5.41	1.64	1.52
1	A	23	SER	C-O	5.40	1.33	1.23
1	B	33	ARG	NE-CZ	5.40	1.40	1.33
1	B	30	MET	C-O	5.39	1.33	1.23
1	B	24	ASN	N-CA	5.38	1.57	1.46
1	B	4	ALA	CA-C	5.36	1.66	1.52
1	A	37	LYS	N-CA	5.34	1.57	1.46
1	A	19	ALA	CA-CB	5.34	1.63	1.52
1	B	39	ARG	CA-C	5.33	1.66	1.52
1	B	10	ARG	CG-CD	5.32	1.65	1.51
1	B	46	PHE	CB-CG	5.32	1.60	1.51
1	B	58	CYS	N-CA	5.32	1.56	1.46
1	A	29	MET	CA-C	5.30	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	GLN	N-CA	5.29	1.56	1.46
1	A	116	VAL	C-O	5.29	1.33	1.23
1	B	59	SER	CB-OG	5.28	1.49	1.42
1	B	42	PRO	CA-C	5.28	1.63	1.52
1	A	14	ASP	N-CA	5.28	1.56	1.46
1	B	78	THR	CB-OG1	5.28	1.53	1.43
1	B	11	GLN	CB-CG	5.27	1.66	1.52
1	B	67	ASN	CG-ND2	5.27	1.46	1.32
1	A	21	SER	N-CA	5.27	1.56	1.46
1	B	34	ASN	C-O	5.27	1.33	1.23
1	B	85	ARG	CZ-NH1	5.25	1.39	1.33
1	B	95	CYS	CA-C	5.25	1.66	1.52
1	A	79	MET	CA-CB	5.25	1.65	1.53
1	A	10	ARG	CA-CB	5.24	1.65	1.53
1	B	37	LYS	N-CA	5.22	1.56	1.46
1	B	10	ARG	CZ-NH1	5.20	1.39	1.33
1	B	105	HIS	CA-C	5.20	1.66	1.52
1	B	83	ASP	CG-OD2	5.18	1.37	1.25
1	B	117	PRO	CA-C	5.18	1.63	1.52
1	B	89	SER	N-CA	5.18	1.56	1.46
1	A	38	ASP	N-CA	5.17	1.56	1.46
1	B	9	GLU	C-O	5.17	1.33	1.23
1	B	10	ARG	CA-CB	5.17	1.65	1.53
1	B	19	ALA	CA-CB	5.17	1.63	1.52
1	B	82	THR	CA-C	5.16	1.66	1.52
1	B	79	MET	CA-CB	5.16	1.65	1.53
1	A	101	GLN	CD-OE1	5.15	1.35	1.24
1	A	108	VAL	N-CA	5.14	1.56	1.46
1	A	11	GLN	CB-CG	5.14	1.66	1.52
1	A	55	GLN	N-CA	5.13	1.56	1.46
1	A	10	ARG	CG-CD	5.12	1.64	1.51
1	B	1	LYS	N-CA	5.10	1.56	1.46
1	A	42	PRO	CA-C	5.07	1.62	1.52
1	A	45	THR	N-CA	5.07	1.56	1.46
1	A	111	GLU	CG-CD	5.05	1.59	1.51
1	A	46	PHE	CB-CG	5.04	1.59	1.51
1	A	105	HIS	CA-C	5.04	1.66	1.52
1	A	83	ASP	CG-OD2	5.03	1.36	1.25
1	B	108	VAL	N-CA	5.03	1.56	1.46
1	B	63	VAL	CB-CG1	5.01	1.63	1.52
1	B	101	GLN	CD-OE1	5.01	1.34	1.24
1	B	3	THR	CB-OG1	5.00	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	TYR	CD2-CE2	5.00	1.46	1.39

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	ARG	NE-CZ-NH1	36.85	138.72	120.30
1	B	10	ARG	NE-CZ-NH1	35.39	137.99	120.30
1	A	10	ARG	NE-CZ-NH2	-25.49	107.56	120.30
1	B	10	ARG	NE-CZ-NH2	-23.48	108.56	120.30
1	B	113	ASN	O-C-N	-17.87	87.14	121.10
1	A	113	ASN	O-C-N	-16.76	89.25	121.10
1	B	92	TYR	O-C-N	-15.42	91.81	121.10
1	A	92	TYR	O-C-N	-14.47	93.60	121.10
1	B	113	ASN	CA-C-N	13.62	155.24	117.10
1	A	113	ASN	CA-C-N	12.80	152.95	117.10
1	B	33	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	B	92	TYR	CA-C-N	12.35	151.68	117.10
1	A	92	TYR	CA-C-N	12.01	150.74	117.10
1	A	17	THR	N-CA-CB	-11.59	88.28	110.30
1	B	17	THR	N-CA-CB	-11.29	88.84	110.30
1	A	33	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	A	10	ARG	CD-NE-CZ	11.07	139.10	123.60
1	B	34	ASN	CB-CG-OD1	-10.82	99.95	121.60
1	A	34	ASN	CB-CG-OD1	-10.70	100.20	121.60
1	B	10	ARG	CD-NE-CZ	10.56	138.39	123.60
1	A	39	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	A	73	TYR	CG-CD2-CE2	10.43	129.65	121.30
1	A	70	THR	N-CA-CB	-10.39	90.56	110.30
1	B	73	TYR	CG-CD2-CE2	9.96	129.27	121.30
1	B	70	THR	N-CA-CB	-9.89	91.50	110.30
1	A	73	TYR	CZ-CE2-CD2	-9.64	111.12	119.80
1	B	1	LYS	O-C-N	9.46	137.84	122.70
1	B	95	CYS	O-C-N	9.42	137.77	122.70
1	B	73	TYR	CZ-CE2-CD2	-9.36	111.38	119.80
1	A	73	TYR	O-C-N	9.17	137.37	122.70
1	A	118	VAL	CG1-CB-CG2	9.11	125.48	110.90
1	B	83	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	B	118	VAL	CG1-CB-CG2	9.10	125.46	110.90
1	B	39	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	1	LYS	O-C-N	8.92	136.97	122.70
1	A	53	ASP	CB-CG-OD2	8.91	126.32	118.30
1	A	95	CYS	O-C-N	8.85	136.86	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	THR	CA-CB-CG2	8.69	124.56	112.40
1	B	61	LYS	O-C-N	8.59	136.44	122.70
1	B	9	GLU	OE1-CD-OE2	8.55	133.56	123.30
1	A	9	GLU	OE1-CD-OE2	8.53	133.53	123.30
1	A	70	THR	CA-CB-CG2	8.26	123.97	112.40
1	A	83	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	B	66	LYS	O-C-N	8.09	135.64	122.70
1	B	88	GLY	CA-C-O	-8.08	106.06	120.60
1	A	87	THR	N-CA-CB	-7.99	95.12	110.30
1	B	53	ASP	CB-CG-OD2	7.91	125.42	118.30
1	A	93	PRO	O-C-N	7.89	135.33	122.70
1	B	90	SER	O-C-N	7.77	135.13	122.70
1	B	73	TYR	O-C-N	7.75	135.09	122.70
1	B	85	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	93	PRO	O-C-N	7.72	135.05	122.70
1	B	87	THR	N-CA-CB	-7.71	95.64	110.30
1	A	85	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	A	53	ASP	O-C-N	7.56	134.79	122.70
1	A	88	GLY	CA-C-O	-7.47	107.15	120.60
1	A	61	LYS	O-C-N	7.36	134.48	122.70
1	B	115	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	A	12	HIS	O-C-N	7.21	134.24	122.70
1	A	105	HIS	O-C-N	7.20	134.22	122.70
1	A	70	THR	CA-CB-OG1	-7.13	94.02	109.00
1	A	90	SER	O-C-N	7.09	134.05	122.70
1	B	8	PHE	CG-CD2-CE2	7.08	128.59	120.80
1	A	8	PHE	CG-CD2-CE2	7.06	128.57	120.80
1	B	118	VAL	N-CA-CB	-7.03	96.04	111.50
1	A	124	VAL	CB-CA-C	7.00	124.71	111.40
1	B	70	THR	CA-CB-OG1	-6.92	94.46	109.00
1	A	73	TYR	CG-CD1-CE1	-6.92	115.77	121.30
1	A	11	GLN	O-C-N	6.92	133.76	122.70
1	A	115	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	104	LYS	CB-CA-C	-6.78	96.83	110.40
1	B	16	SER	N-CA-CB	-6.76	100.35	110.50
1	A	118	VAL	N-CA-CB	-6.74	96.67	111.50
1	A	66	LYS	O-C-N	6.73	133.47	122.70
1	A	46	PHE	CB-CG-CD2	-6.71	116.10	120.80
1	A	116	VAL	CA-CB-CG1	6.71	120.97	110.90
1	A	16	SER	N-CA-CB	-6.68	100.48	110.50
1	B	74	GLN	CG-CD-OE1	-6.66	108.27	121.60
1	B	124	VAL	CB-CA-C	6.62	123.99	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	SER	O-C-N	6.62	133.28	122.70
1	B	97	TYR	CA-C-N	-6.61	102.66	117.20
1	B	122	ALA	O-C-N	6.60	133.26	122.70
1	A	63	VAL	O-C-N	6.58	133.23	122.70
1	B	73	TYR	CG-CD1-CE1	-6.57	116.05	121.30
1	B	115	TYR	CD1-CE1-CZ	-6.57	113.89	119.80
1	A	74	GLN	CG-CD-OE1	-6.55	108.51	121.60
1	A	17	THR	OG1-CB-CG2	6.53	125.03	110.00
1	A	39	ARG	O-C-N	6.50	133.10	122.70
1	A	72	CYS	O-C-N	6.49	133.09	122.70
1	A	88	GLY	CA-C-N	6.47	131.44	117.20
1	A	75	SER	N-CA-CB	6.46	120.19	110.50
1	B	105	HIS	O-C-N	6.45	133.01	122.70
1	A	16	SER	CB-CA-C	6.42	122.29	110.10
1	A	97	TYR	CA-C-N	-6.41	103.09	117.20
1	B	115	TYR	CG-CD2-CE2	-6.41	116.18	121.30
1	A	109	ALA	N-CA-CB	6.40	119.06	110.10
1	A	17	THR	CA-CB-OG1	-6.38	95.59	109.00
1	B	58	CYS	N-CA-CB	6.34	122.01	110.60
1	B	25	TYR	CB-CG-CD2	-6.34	117.20	121.00
1	B	104	LYS	CB-CA-C	-6.33	97.73	110.40
1	B	34	ASN	OD1-CG-ND2	6.32	136.44	121.90
1	B	39	ARG	O-C-N	6.32	132.80	122.70
1	B	71	ASN	O-C-N	6.28	132.75	122.70
1	B	76	TYR	CZ-CE2-CD2	-6.27	114.16	119.80
1	A	115	TYR	CD1-CE1-CZ	-6.25	114.17	119.80
1	B	17	THR	OG1-CB-CG2	6.25	124.37	110.00
1	B	116	VAL	CA-CB-CG1	6.22	120.23	110.90
1	A	25	TYR	CB-CG-CD2	-6.21	117.27	121.00
1	A	58	CYS	N-CA-CB	6.19	121.74	110.60
1	A	73	TYR	CD1-CE1-CZ	6.18	125.36	119.80
1	A	34	ASN	OD1-CG-ND2	6.17	136.08	121.90
1	B	16	SER	CB-CA-C	6.15	121.79	110.10
1	B	83	ASP	OD1-CG-OD2	6.15	134.99	123.30
1	B	11	GLN	O-C-N	6.14	132.52	122.70
1	B	53	ASP	O-C-N	6.13	132.51	122.70
1	A	85	ARG	CG-CD-NE	-6.07	99.05	111.80
1	B	124	VAL	N-CA-CB	-6.07	98.14	111.50
1	B	57	VAL	O-C-N	6.05	132.39	122.70
1	B	50	SER	O-C-N	6.05	132.38	122.70
1	A	117	PRO	O-C-N	6.04	132.36	122.70
1	A	33	ARG	NE-CZ-NH2	-6.03	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	VAL	N-CA-CB	-5.97	98.36	111.50
1	A	115	TYR	CG-CD2-CE2	-5.97	116.52	121.30
1	B	17	THR	CA-CB-OG1	-5.95	96.51	109.00
1	A	39	ARG	NH1-CZ-NH2	-5.88	112.93	119.40
1	A	87	THR	OG1-CB-CG2	5.88	123.52	110.00
1	B	46	PHE	CB-CG-CD2	-5.88	116.69	120.80
1	B	63	VAL	O-C-N	5.87	132.09	122.70
1	B	73	TYR	CD1-CE1-CZ	5.83	125.05	119.80
1	B	87	THR	OG1-CB-CG2	5.80	123.34	110.00
1	B	75	SER	N-CA-CB	5.79	119.19	110.50
1	B	37	LYS	CD-CE-NZ	5.79	125.02	111.70
1	A	37	LYS	CD-CE-NZ	5.79	125.01	111.70
1	B	12	HIS	O-C-N	5.78	131.94	122.70
1	B	85	ARG	CG-CD-NE	-5.77	99.68	111.80
1	A	83	ASP	OD1-CG-OD2	5.77	134.26	123.30
1	B	36	THR	O-C-N	5.77	131.93	122.70
1	B	109	ALA	N-CA-CB	5.75	118.15	110.10
1	B	56	ALA	N-CA-CB	5.74	118.13	110.10
1	A	93	PRO	CA-C-N	-5.72	104.61	117.20
1	A	57	VAL	O-C-N	5.68	131.79	122.70
1	A	105	HIS	CA-C-N	-5.68	104.71	117.20
1	A	95	CYS	C-N-CA	-5.64	107.59	121.70
1	B	47	VAL	O-C-N	5.64	131.73	122.70
1	B	88	GLY	CA-C-N	5.62	129.55	117.20
1	B	92	TYR	CG-CD1-CE1	-5.57	116.84	121.30
1	A	33	ARG	O-C-N	5.57	131.61	122.70
1	B	39	ARG	NH1-CZ-NH2	-5.55	113.30	119.40
1	B	118	VAL	CB-CA-C	5.54	121.94	111.40
1	A	110	CYS	CA-C-N	-5.54	105.02	117.20
1	A	76	TYR	CZ-CE2-CD2	-5.53	114.83	119.80
1	B	10	ARG	NH1-CZ-NH2	-5.51	113.34	119.40
1	B	81	ILE	CA-CB-CG1	-5.50	100.55	111.00
1	B	18	SER	CA-CB-OG	-5.50	96.35	111.20
1	B	14	ASP	CA-C-N	-5.48	105.15	117.20
1	A	44	ASN	O-C-N	5.47	131.46	122.70
1	A	29	MET	CA-C-N	-5.45	105.22	117.20
1	A	56	ALA	N-CA-CB	5.44	117.71	110.10
1	B	93	PRO	CA-C-N	-5.44	105.24	117.20
1	B	108	VAL	O-C-N	5.43	131.38	122.70
1	B	33	ARG	O-C-N	5.42	131.37	122.70
1	A	49	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	B	115	TYR	CD1-CG-CD2	5.39	123.83	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	66	LYS	CB-CA-C	5.35	121.10	110.40
1	B	85	ARG	N-CA-CB	-5.34	100.98	110.60
1	A	93	PRO	C-N-CA	-5.34	108.35	121.70
1	A	18	SER	CA-CB-OG	-5.33	96.81	111.20
1	B	33	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	8	PHE	CZ-CE2-CD2	-5.32	113.71	120.10
1	A	78	THR	CA-CB-CG2	5.31	119.83	112.40
1	A	108	VAL	O-C-N	5.30	131.18	122.70
1	B	72	CYS	O-C-N	5.29	131.16	122.70
1	B	8	PHE	CZ-CE2-CD2	-5.28	113.77	120.10
1	A	10	ARG	NH1-CZ-NH2	-5.27	113.61	119.40
1	B	29	MET	CA-C-N	-5.24	105.66	117.20
1	A	85	ARG	N-CA-CB	-5.23	101.18	110.60
1	B	105	HIS	CA-C-N	-5.23	105.70	117.20
1	A	47	VAL	O-C-N	5.22	131.06	122.70
1	B	105	HIS	C-N-CA	-5.22	108.64	121.70
1	A	117	PRO	CA-C-N	-5.22	105.72	117.20
1	A	33	ARG	CA-C-N	-5.20	105.76	117.20
1	B	49	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	B	78	THR	CA-CB-CG2	5.19	119.66	112.40
1	B	19	ALA	N-CA-CB	-5.18	102.84	110.10
1	A	111	GLU	CG-CD-OE2	-5.18	107.94	118.30
1	A	92	TYR	CG-CD1-CE1	-5.17	117.16	121.30
1	A	105	HIS	C-N-CA	-5.16	108.81	121.70
1	A	29	MET	CG-SD-CE	-5.15	91.95	100.20
1	A	115	TYR	CD1-CG-CD2	5.15	123.56	117.90
1	B	121	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	81	ILE	CA-CB-CG1	-5.14	101.23	111.00
1	A	122	ALA	O-C-N	5.14	130.92	122.70
1	B	25	TYR	CA-C-N	-5.13	105.91	117.20
1	A	29	MET	O-C-N	5.10	130.87	122.70
1	B	97	TYR	O-C-N	5.09	130.84	122.70
1	A	66	LYS	N-CA-CB	-5.07	101.47	110.60
1	A	118	VAL	CB-CA-C	5.07	121.03	111.40
1	A	19	ALA	N-CA-CB	-5.06	103.02	110.10
1	B	12	HIS	C-N-CA	-5.06	109.06	121.70
1	B	74	GLN	CA-C-N	-5.05	106.08	117.20
1	B	95	CYS	C-N-CA	-5.05	109.07	121.70
1	A	44	ASN	CA-C-N	-5.05	106.10	117.20
1	A	88	GLY	N-CA-C	-5.04	100.50	113.10
1	B	66	LYS	CB-CA-C	5.03	120.46	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	PHE	N-CA-CB	5.00	119.60	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASN	Mainchain,Peptide
1	B	113	ASN	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	950	0	905	135	1
1	B	950	0	905	152	2
All	All	1900	0	1810	285	2

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 77.

All (285) 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:10:ARG:O	1:B:33:ARG:HD2	1.26	1.29
1:B:108:VAL:CG1	1:B:117:PRO:HB3	1.67	1.24
1:B:17:THR:HG23	1:B:48:HIS:ND1	1.55	1.21
1:A:25:TYR:O	1:A:29:MET:HB2	1.43	1.19
1:A:20:ALA:HB2	1:A:82:THR:OG1	1.42	1.18
1:A:109:ALA:CB	1:A:119:HIS:CD2	2.27	1.17
1:B:60:GLN:HG2	1:B:76:TYR:CD2	1.80	1.17
1:A:109:ALA:CB	1:A:119:HIS:HD2	1.58	1.16
1:B:43:VAL:CG2	1:B:85:ARG:HH12	1.59	1.13
1:A:14:ASP:OD1	1:A:29:MET:HE1	1.48	1.13
1:A:106:ILE:C	1:A:107:ILE:HD12	1.69	1.12
1:B:17:THR:HG23	1:B:48:HIS:HD1	0.95	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LYS:C	1:B:91:LYS:HD3	1.71	1.11
1:A:109:ALA:HB2	1:A:119:HIS:CD2	1.83	1.10
1:B:78:THR:HG22	1:B:105:HIS:CD2	1.86	1.09
1:A:91:LYS:O	1:A:91:LYS:HG3	1.47	1.07
1:A:43:VAL:HG22	1:A:85:ARG:CD	1.84	1.07
1:A:85:ARG:NH1	1:A:85:ARG:HG2	1.62	1.07
1:A:19:ALA:HA	1:A:48:HIS:CD2	1.88	1.06
1:B:108:VAL:HG11	1:B:117:PRO:HB3	1.07	1.06
1:A:109:ALA:HB3	1:A:119:HIS:HD2	1.18	1.04
1:A:71:ASN:HD21	1:A:109:ALA:HB1	1.18	1.04
1:B:91:LYS:O	1:B:91:LYS:HD3	1.58	1.03
1:A:91:LYS:O	1:A:91:LYS:CG	2.07	1.02
1:B:14:ASP:OD2	1:B:17:THR:HG21	1.59	1.02
1:A:106:ILE:O	1:A:107:ILE:HD12	1.61	1.00
1:B:43:VAL:HG22	1:B:85:ARG:HH12	1.21	0.99
1:A:71:ASN:ND2	1:A:109:ALA:HB1	1.77	0.99
1:A:109:ALA:HB3	1:A:119:HIS:CD2	1.94	0.99
1:A:51:LEU:O	1:A:55:GLN:HG3	1.61	0.99
1:B:43:VAL:HG22	1:B:85:ARG:NH1	1.79	0.97
1:B:2:GLU:OE2	1:B:7:LYS:HA	1.64	0.97
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.25	0.95
1:A:31:LYS:HA	1:A:36:THR:HG23	1.46	0.93
1:A:87:THR:HG23	1:A:88:GLY:O	1.69	0.93
1:A:107:ILE:CD1	1:A:107:ILE:N	2.33	0.92
1:B:108:VAL:HG11	1:B:117:PRO:CB	2.00	0.92
1:A:67:ASN:ND2	1:A:69:GLN:HG3	1.86	0.91
1:B:41:LYS:HZ3	1:B:44:ASN:HB2	1.35	0.91
1:A:24:ASN:HB3	1:A:28:GLN:HE21	1.33	0.91
1:A:50:SER:O	1:A:54:VAL:HG23	1.71	0.90
1:A:106:ILE:C	1:A:107:ILE:CD1	2.40	0.90
1:A:60:GLN:HG2	1:A:76:TYR:CD2	2.09	0.88
1:B:43:VAL:CG2	1:B:85:ARG:NH1	2.34	0.88
1:B:109:ALA:HB3	1:B:119:HIS:HB3	1.56	0.87
1:B:10:ARG:O	1:B:33:ARG:CD	2.18	0.86
1:A:85:ARG:HH11	1:A:85:ARG:CG	1.86	0.86
1:B:90:SER:HB3	1:B:96:ALA:H	1.37	0.86
1:B:41:LYS:NZ	1:B:44:ASN:HB2	1.91	0.85
1:A:43:VAL:HG22	1:A:85:ARG:HD3	1.59	0.82
1:B:91:LYS:C	1:B:91:LYS:CD	2.48	0.81
1:B:40:CYS:SG	1:B:92:TYR:HA	2.20	0.81
1:B:30:MET:HG3	1:B:97:TYR:CD2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:HG2	1:A:90:SER:CB	2.10	0.81
1:A:24:ASN:HB3	1:A:28:GLN:NE2	1.95	0.81
1:B:33:ARG:HB2	1:B:35:LEU:HD11	1.62	0.81
1:A:78:THR:HG23	1:A:105:HIS:CE1	2.17	0.80
1:A:14:ASP:OD1	1:A:29:MET:CE	2.28	0.80
1:B:78:THR:HG22	1:B:105:HIS:HD2	1.41	0.80
1:B:90:SER:OG	1:B:96:ALA:HB3	1.82	0.80
1:B:24:ASN:ND2	1:B:28:GLN:HE22	1.81	0.78
1:B:44:ASN:HD22	1:B:44:ASN:C	1.88	0.77
1:A:87:THR:C	1:A:88:GLY:O	2.20	0.77
1:A:7:LYS:O	1:A:11:GLN:HG3	1.86	0.76
1:B:91:LYS:CD	1:B:92:TYR:O	2.34	0.75
1:B:2:GLU:OE2	1:B:7:LYS:CA	2.34	0.74
1:B:82:THR:CG2	1:B:99:THR:HG23	2.17	0.74
1:A:25:TYR:CZ	1:A:29:MET:HG3	2.23	0.74
1:A:107:ILE:HD13	1:A:107:ILE:N	2.01	0.74
1:A:78:THR:HG22	1:A:104:LYS:HA	1.70	0.73
1:A:10:ARG:O	1:A:33:ARG:HD2	1.89	0.73
1:B:42:PRO:HA	1:B:86:GLU:HB2	1.69	0.73
1:B:91:LYS:HD3	1:B:92:TYR:O	1.89	0.71
1:B:74:GLN:HG2	1:B:75:SER:N	2.05	0.71
1:B:60:GLN:CG	1:B:76:TYR:CD2	2.68	0.71
1:B:108:VAL:HG12	1:B:117:PRO:HB3	1.69	0.70
1:A:67:ASN:CG	1:A:69:GLN:HG3	2.11	0.70
1:B:90:SER:CB	1:B:96:ALA:H	2.03	0.70
1:A:75:SER:HG	1:A:105:HIS:HA	1.56	0.69
1:B:11:GLN:O	1:B:46:PHE:CE1	2.46	0.69
1:A:30:MET:SD	1:A:44:ASN:HB3	2.33	0.68
1:B:43:VAL:HG21	1:B:85:ARG:HH12	1.57	0.68
1:A:19:ALA:HA	1:A:48:HIS:HD2	1.53	0.67
1:A:86:GLU:HG2	1:A:90:SER:HB3	1.76	0.67
1:B:49:GLU:OE1	1:B:79:MET:HB3	1.94	0.67
1:A:7:LYS:O	1:A:11:GLN:CG	2.42	0.67
1:B:44:ASN:ND2	1:B:44:ASN:C	2.47	0.66
1:B:12:HIS:HA	1:B:46:PHE:CD1	2.29	0.66
1:A:61:LYS:HB2	1:A:76:TYR:HE1	1.60	0.66
1:B:30:MET:O	1:B:35:LEU:HD12	1.96	0.66
1:B:19:ALA:HB1	1:B:101:GLN:OE1	1.95	0.66
1:A:14:ASP:CG	1:A:29:MET:HE1	2.15	0.66
1:A:20:ALA:CB	1:A:82:THR:OG1	2.34	0.66
1:A:17:THR:O	1:A:48:HIS:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASP:OD2	1:B:17:THR:CG2	2.39	0.65
1:A:75:SER:HB3	1:A:79:MET:HE3	1.78	0.65
1:B:83:ASP:N	1:B:100:THR:O	2.20	0.65
1:B:13:MET:O	1:B:33:ARG:NH1	2.29	0.64
1:B:107:ILE:HD11	1:B:124:VAL:HG11	1.79	0.64
1:B:24:ASN:HB3	1:B:28:GLN:OE1	1.98	0.64
1:B:82:THR:HG21	1:B:99:THR:HG23	1.80	0.63
1:A:7:LYS:CD	1:A:10:ARG:HH11	2.12	0.63
1:B:61:LYS:HZ2	1:B:76:TYR:HD1	1.42	0.63
1:A:57:VAL:CG2	1:A:79:MET:HE3	2.29	0.63
1:B:17:THR:HG23	1:B:48:HIS:CE1	2.33	0.62
1:A:107:ILE:N	1:A:122:ALA:O	2.30	0.62
1:B:25:TYR:C	1:B:25:TYR:CD2	2.74	0.61
1:B:20:ALA:HA	1:B:25:TYR:CD1	2.34	0.61
1:A:78:THR:HG22	1:A:104:LYS:CA	2.30	0.61
1:B:78:THR:CG2	1:B:105:HIS:CD2	2.76	0.61
1:A:24:ASN:O	1:A:28:GLN:HG3	2.01	0.61
1:B:26:CYS:HB2	1:B:99:THR:OG1	2.01	0.61
1:B:30:MET:HA	1:B:35:LEU:HD12	1.83	0.60
1:A:75:SER:O	1:A:105:HIS:CD2	2.54	0.60
1:B:27:ASN:H	1:B:27:ASN:ND2	1.98	0.60
1:B:17:THR:O	1:B:48:HIS:HB3	2.02	0.60
1:B:17:THR:CG2	1:B:48:HIS:ND1	2.48	0.60
1:A:107:ILE:HD12	1:A:107:ILE:N	2.01	0.59
1:B:24:ASN:O	1:B:28:GLN:OE1	2.18	0.59
1:B:20:ALA:HB2	1:B:82:THR:OG1	2.03	0.59
1:B:87:THR:C	1:B:88:GLY:O	2.37	0.59
1:A:25:TYR:CD2	1:A:82:THR:HG21	2.38	0.59
1:A:41:LYS:HD3	1:A:44:ASN:HB2	1.82	0.59
1:B:61:LYS:NZ	1:B:76:TYR:CD1	2.66	0.59
1:B:41:LYS:O	1:B:97:TYR:CE1	2.56	0.59
1:B:40:CYS:SG	1:B:92:TYR:CA	2.91	0.58
1:A:109:ALA:HB2	1:A:119:HIS:NE2	2.18	0.58
1:B:121:ASP:O	1:B:122:ALA:HB2	2.02	0.58
1:A:74:GLN:O	1:A:74:GLN:HG2	2.03	0.58
1:A:25:TYR:O	1:A:29:MET:CB	2.36	0.58
1:B:11:GLN:HB2	1:B:12:HIS:CD2	2.39	0.58
1:A:25:TYR:CZ	1:A:29:MET:HE2	2.39	0.58
1:A:43:VAL:HG22	1:A:85:ARG:NE	2.19	0.57
1:A:49:GLU:HG3	1:A:79:MET:HB3	1.85	0.57
1:A:57:VAL:HG21	1:A:79:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ASP:CG	1:A:29:MET:CE	2.71	0.56
1:A:42:PRO:C	1:A:43:VAL:HG23	2.25	0.56
1:B:12:HIS:HB3	1:B:45:THR:O	2.06	0.56
1:B:30:MET:CB	1:B:97:TYR:CE2	2.89	0.56
1:A:14:ASP:OD2	1:A:17:THR:HB	2.05	0.56
1:B:49:GLU:OE1	1:B:79:MET:HA	2.06	0.55
1:B:12:HIS:CD2	1:B:12:HIS:N	2.74	0.55
1:B:91:LYS:O	1:B:92:TYR:C	2.45	0.55
1:B:14:ASP:O	1:B:17:THR:HG22	2.06	0.55
1:A:75:SER:OG	1:A:105:HIS:HA	2.05	0.55
1:A:57:VAL:CG2	1:A:79:MET:CE	2.85	0.54
1:A:107:ILE:O	1:A:121:ASP:N	2.35	0.54
1:A:31:LYS:HA	1:A:36:THR:CG2	2.28	0.54
1:B:49:GLU:OE1	1:B:79:MET:CA	2.55	0.54
1:A:9:GLU:HA	1:A:13:MET:HG2	1.89	0.54
1:A:61:LYS:HB2	1:A:76:TYR:CE1	2.42	0.54
1:A:51:LEU:O	1:A:55:GLN:CG	2.48	0.54
1:A:19:ALA:HB1	1:A:101:GLN:CD	2.27	0.54
1:A:43:VAL:CG2	1:A:85:ARG:NE	2.70	0.54
1:A:25:TYR:CE1	1:A:29:MET:HE2	2.43	0.54
1:B:41:LYS:O	1:B:97:TYR:HE1	1.90	0.54
1:A:7:LYS:HD3	1:A:10:ARG:HH11	1.73	0.53
1:A:8:PHE:CD1	1:A:12:HIS:CD2	2.97	0.53
1:B:12:HIS:HA	1:B:46:PHE:HD1	1.70	0.53
1:B:61:LYS:NZ	1:B:76:TYR:HD1	2.02	0.53
1:A:32:SER:C	1:A:34:ASN:H	2.12	0.53
1:A:88:GLY:O	1:A:89:SER:CB	2.56	0.53
1:A:30:MET:O	1:A:35:LEU:HB2	2.09	0.53
1:A:19:ALA:CA	1:A:48:HIS:CD2	2.79	0.53
1:A:57:VAL:HG23	1:A:79:MET:HE1	1.91	0.53
1:A:11:GLN:O	1:A:46:PHE:CE1	2.62	0.52
1:B:60:GLN:HG2	1:B:76:TYR:CE2	2.38	0.52
1:B:91:LYS:N	1:B:94:ASN:O	2.36	0.52
1:A:10:ARG:HG3	1:B:76:TYR:CE1	2.45	0.52
1:A:29:MET:O	1:A:33:ARG:HG2	2.10	0.52
1:B:85:ARG:HB3	1:B:98:LYS:HB3	1.91	0.51
1:B:49:GLU:OE1	1:B:79:MET:CB	2.58	0.51
1:B:24:ASN:O	1:B:28:GLN:CD	2.48	0.51
1:B:91:LYS:O	1:B:91:LYS:CD	2.47	0.51
1:A:7:LYS:HD2	1:A:10:ARG:HH11	1.75	0.51
1:A:43:VAL:CG2	1:A:85:ARG:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:MET:HA	1:B:35:LEU:CD1	2.42	0.50
1:B:73:TYR:HD2	1:B:110:CYS:SG	2.35	0.50
1:B:32:SER:C	1:B:34:ASN:H	2.15	0.50
1:B:88:GLY:O	1:B:89:SER:HB3	2.12	0.50
1:A:113:ASN:C	1:A:114:PRO:O	2.50	0.49
1:B:73:TYR:CD2	1:B:110:CYS:SG	3.06	0.49
1:A:65:CYS:HB2	1:A:67:ASN:OD1	2.13	0.49
1:A:60:GLN:HG2	1:A:76:TYR:CG	2.47	0.49
1:B:104:LYS:HD3	1:B:123:SER:HB2	1.94	0.48
1:A:81:ILE:HD11	1:A:104:LYS:HG3	1.93	0.48
1:B:113:ASN:C	1:B:114:PRO:O	2.51	0.48
1:B:24:ASN:CG	1:B:28:GLN:HE22	2.16	0.48
1:A:60:GLN:HG2	1:A:76:TYR:CE2	2.47	0.48
1:B:72:CYS:HA	1:B:108:VAL:O	2.13	0.48
1:B:19:ALA:HA	1:B:48:HIS:CE1	2.48	0.48
1:B:14:ASP:O	1:B:48:HIS:HA	2.13	0.48
1:A:86:GLU:HG2	1:A:90:SER:OG	2.12	0.48
1:B:13:MET:CE	1:B:49:GLU:O	2.61	0.48
1:B:91:LYS:HD3	1:B:92:TYR:N	2.24	0.48
1:A:66:LYS:HE3	1:A:121:ASP:OD1	2.14	0.48
1:B:18:SER:O	1:B:19:ALA:HB2	2.14	0.47
1:B:57:VAL:HG21	1:B:79:MET:HE3	1.96	0.47
1:A:8:PHE:CD1	1:A:12:HIS:HD2	2.32	0.47
1:A:7:LYS:HD2	1:A:10:ARG:NH1	2.29	0.47
1:B:58:CYS:HB3	1:B:115:TYR:CD2	2.50	0.47
1:B:110:CYS:HB2	1:B:115:TYR:CE2	2.49	0.47
1:B:90:SER:HB3	1:B:96:ALA:N	2.17	0.47
1:A:105:HIS:O	1:A:124:VAL:N	2.45	0.47
1:B:60:GLN:CG	1:B:76:TYR:CE2	2.97	0.47
1:B:78:THR:HG22	1:B:105:HIS:NE2	2.27	0.47
1:A:72:CYS:HB3	1:A:107:ILE:CG2	2.46	0.47
1:B:71:ASN:ND2	1:B:110:CYS:O	2.48	0.47
1:A:63:VAL:O	1:A:72:CYS:HB2	2.15	0.46
1:A:37:LYS:HE2	1:A:37:LYS:HA	1.95	0.46
1:A:85:ARG:HH11	1:A:85:ARG:CB	2.27	0.46
1:A:78:THR:HG23	1:A:105:HIS:ND1	2.30	0.46
1:B:33:ARG:HB2	1:B:35:LEU:CD1	2.39	0.46
1:B:90:SER:OG	1:B:96:ALA:CB	2.59	0.46
1:A:43:VAL:HG22	1:A:85:ARG:HD2	1.88	0.46
1:B:88:GLY:O	1:B:89:SER:CB	2.64	0.46
1:B:73:TYR:CE2	1:B:115:TYR:HE2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:SER:CB	1:B:96:ALA:N	2.76	0.46
1:B:36:THR:HA	1:B:39:ARG:O	2.16	0.46
1:B:45:THR:HG22	1:B:81:ILE:HB	1.97	0.46
1:A:13:MET:O	1:A:33:ARG:NH1	2.49	0.45
1:A:67:ASN:HD21	1:A:69:GLN:HG3	1.78	0.45
1:B:62:ASN:ND2	1:B:70:THR:O	2.40	0.45
1:B:60:GLN:HG2	1:B:76:TYR:CG	2.44	0.45
1:B:105:HIS:O	1:B:123:SER:HA	2.17	0.45
1:A:105:HIS:O	1:A:123:SER:HA	2.17	0.45
1:B:36:THR:HG22	1:B:97:TYR:OH	2.16	0.45
1:A:78:THR:HG23	1:A:105:HIS:HE1	1.76	0.45
1:B:87:THR:HG22	1:B:88:GLY:O	2.17	0.45
1:A:98:LYS:HA	1:A:98:LYS:HD3	1.48	0.45
1:B:56:ALA:O	1:B:60:GLN:NE2	2.50	0.45
1:B:33:ARG:O	1:B:34:ASN:HB2	2.18	0.44
1:A:17:THR:HG22	1:A:48:HIS:ND1	2.31	0.44
1:B:43:VAL:HG22	1:B:85:ARG:CZ	2.45	0.44
1:A:7:LYS:O	1:A:11:GLN:HG2	2.17	0.44
1:B:108:VAL:CG1	1:B:117:PRO:CB	2.63	0.44
1:B:109:ALA:CB	1:B:119:HIS:HB3	2.38	0.44
1:A:31:LYS:CA	1:A:36:THR:HG23	2.33	0.44
1:A:61:LYS:HG2	1:A:63:VAL:CG1	2.48	0.44
1:B:110:CYS:HA	1:B:116:VAL:O	2.17	0.44
1:A:91:LYS:O	1:A:92:TYR:C	2.55	0.44
1:B:30:MET:HB3	1:B:97:TYR:CE2	2.53	0.44
1:B:39:ARG:HA	1:B:92:TYR:CD1	2.52	0.44
1:A:71:ASN:HD22	1:A:110:CYS:H	1.66	0.43
1:A:25:TYR:OH	1:A:29:MET:CE	2.66	0.43
1:A:10:ARG:HG3	1:B:76:TYR:CD1	2.53	0.43
1:A:34:ASN:N	1:A:34:ASN:OD1	2.50	0.43
1:B:24:ASN:OD1	1:B:27:ASN:ND2	2.52	0.43
1:B:44:ASN:ND2	1:B:45:THR:N	2.67	0.43
1:B:57:VAL:CG2	1:B:79:MET:CE	2.97	0.43
1:A:2:GLU:OE1	1:A:7:LYS:HD3	2.18	0.43
1:A:61:LYS:O	1:A:63:VAL:HG13	2.19	0.43
1:A:25:TYR:CE1	1:A:29:MET:HG3	2.52	0.43
1:B:61:LYS:HG2	1:B:63:VAL:HG13	2.01	0.43
1:B:7:LYS:HZ2	1:B:10:ARG:HH11	1.67	0.42
1:B:11:GLN:HE21	1:B:35:LEU:HD23	1.84	0.42
1:B:13:MET:HE1	1:B:49:GLU:O	2.19	0.42
1:A:25:TYR:OH	1:A:29:MET:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ALA:HB1	1:A:99:THR:HG21	2.01	0.42
1:B:58:CYS:HB3	1:B:115:TYR:HD2	1.85	0.42
1:B:57:VAL:CG2	1:B:79:MET:HE3	2.49	0.42
1:B:85:ARG:O	1:B:97:TYR:HA	2.19	0.42
1:A:123:SER:C	1:A:124:VAL:HG23	2.39	0.42
1:A:8:PHE:CD2	1:A:117:PRO:HB2	2.55	0.42
1:B:26:CYS:HB3	1:B:97:TYR:HB2	2.01	0.42
1:A:78:THR:CG2	1:A:104:LYS:HA	2.46	0.42
1:B:82:THR:CG2	1:B:99:THR:CG2	2.93	0.41
1:B:91:LYS:HE2	1:B:92:TYR:N	2.35	0.41
1:B:105:HIS:O	1:B:124:VAL:N	2.43	0.41
1:A:47:VAL:HG22	1:A:81:ILE:HG22	2.02	0.41
1:B:2:GLU:OE2	1:B:7:LYS:N	2.54	0.41
1:A:106:ILE:C	1:A:107:ILE:HD13	2.34	0.41
1:B:91:LYS:HD3	1:B:92:TYR:C	2.41	0.41
1:B:73:TYR:O	1:B:107:ILE:HA	2.21	0.41
1:B:11:GLN:NE2	1:B:35:LEU:HD23	2.35	0.41
1:B:7:LYS:NZ	1:B:10:ARG:HH11	2.19	0.41
1:B:78:THR:CG2	1:B:105:HIS:HD2	2.23	0.41
1:A:42:PRO:C	1:A:43:VAL:CG2	2.89	0.41
1:B:70:THR:C	1:B:72:CYS:H	2.25	0.41
1:A:75:SER:OG	1:A:105:HIS:CA	2.70	0.41
1:B:30:MET:C	1:B:35:LEU:HD12	2.41	0.40
1:B:39:ARG:HD2	1:B:39:ARG:C	2.42	0.40
1:B:29:MET:HB3	1:B:46:PHE:CE2	2.57	0.40
1:A:19:ALA:O	1:A:20:ALA:C	2.60	0.40
1:A:91:LYS:O	1:A:91:LYS:HG2	2.10	0.40

All (2) 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)
1:A:77:SER:OG	1:B:68:GLY:O[4_656]	1.82	0.38
1:B:92:TYR:CD2	1:B:92:TYR:CD2[2_657]	2.05	0.15

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	122/124 (98%)	109 (89%)	10 (8%)	3 (2%)	7 10
1	B	122/124 (98%)	110 (90%)	11 (9%)	1 (1%)	24 41
All	All	244/248 (98%)	219 (90%)	21 (9%)	4 (2%)	12 21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	B	114	PRO
1	A	89	SER
1	A	40	CYS

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	109/109 (100%)	71 (65%)	38 (35%)	0 0
1	B	109/109 (100%)	75 (69%)	34 (31%)	0 0
All	All	218/218 (100%)	146 (67%)	72 (33%)	0 0

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

Mol	Chain	Res	Type
1	A	3	THR
1	A	7	LYS

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Mol	Chain	Res	Type
1	A	10	ARG
1	A	11	GLN
1	A	17	THR
1	A	18	SER
1	A	21	SER
1	A	24	ASN
1	A	28	GLN
1	A	29	MET
1	A	31	LYS
1	A	32	SER
1	A	36	THR
1	A	37	LYS
1	A	39	ARG
1	A	50	SER
1	A	61	LYS
1	A	63	VAL
1	A	66	LYS
1	A	70	THR
1	A	74	GLN
1	A	77	SER
1	A	78	THR
1	A	80	SER
1	A	82	THR
1	A	83	ASP
1	A	85	ARG
1	A	87	THR
1	A	89	SER
1	A	91	LYS
1	A	93	PRO
1	A	98	LYS
1	A	104	LYS
1	A	105	HIS
1	A	107	ILE
1	A	113	ASN
1	A	118	VAL
1	A	119	HIS
1	B	10	ARG
1	B	12	HIS
1	B	13	MET
1	B	15	SER
1	B	17	THR
1	B	18	SER

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Mol	Chain	Res	Type
1	B	22	SER
1	B	25	TYR
1	B	31	LYS
1	B	35	LEU
1	B	37	LYS
1	B	38	ASP
1	B	39	ARG
1	B	44	ASN
1	B	45	THR
1	B	49	GLU
1	B	51	LEU
1	B	61	LYS
1	B	62	ASN
1	B	66	LYS
1	B	77	SER
1	B	80	SER
1	B	81	ILE
1	B	83	ASP
1	B	85	ARG
1	B	86	GLU
1	B	89	SER
1	B	91	LYS
1	B	94	ASN
1	B	108	VAL
1	B	111	GLU
1	B	118	VAL
1	B	119	HIS
1	B	124	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	28	GLN
1	A	71	ASN
1	A	113	ASN
1	A	119	HIS
1	B	11	GLN
1	B	12	HIS
1	B	24	ASN
1	B	27	ASN
1	B	69	GLN

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Mol	Chain	Res	Type
1	B	74	GLN
1	B	105	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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