Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:59 PM GMT

PDB ID	:	1RLR
Title	:	STRUCTURE OF RIBONUCLEOTIDE REDUCTASE PROTEIN R1
Authors	:	Uhlin, U.; Eklund, H.
Deposited on	:	1994-08-12
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:

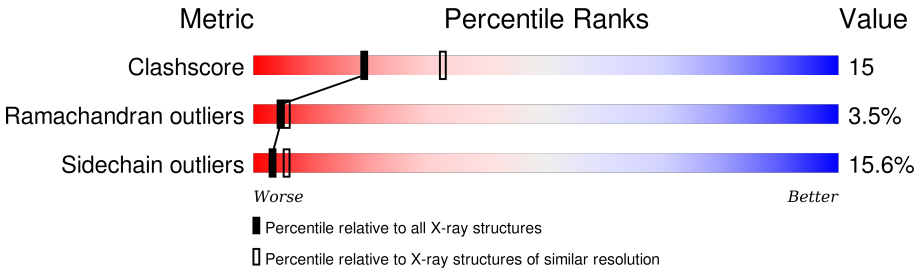
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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	761	55% 28% 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5875 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 RIBONUCLEOTIDE REDUCTASE PROTEIN R1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	737	5875	3729	1007	1115	24	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	479	ASP	GLU	CONFLICT	UNP P00452
A	526	LYS	ASN	CONFLICT	UNP P00452
A	527	HIS	ASP	CONFLICT	UNP P00452
A	739	ASP	GLY	CONFLICT	UNP P00452
A	740	ILE	ALA	CONFLICT	UNP P00452
A	741	ASP	GLU	CONFLICT	UNP P00452
A	743	LEU	ALA	CONFLICT	UNP P00452
A	744	SER	GLN	CONFLICT	UNP P00452
A	745	ASN	ASP	CONFLICT	UNP P00452
A	746	PHE	ASP	CONFLICT	UNP P00452
A	747	GLN	LEU	CONFLICT	UNP P00452
A	748	LEU	VAL	CONFLICT	UNP P00452

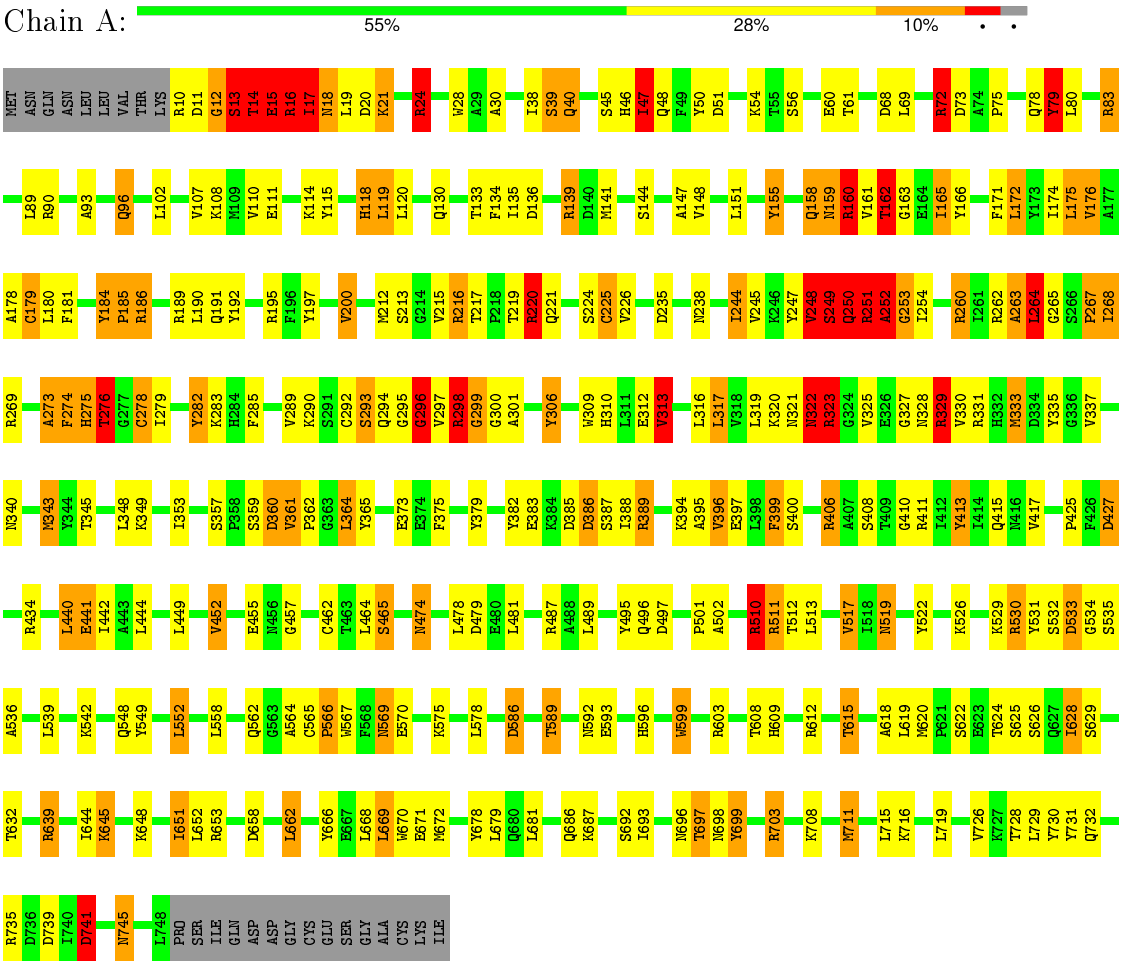
3 Residue-property plots (i)

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: RIBONUCLEOTIDE REDUCTASE PROTEIN R1

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	226.00Å 226.00Å 341.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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	1.26	33/6003 (0.5%)	2.08	233/8130 (2.9%)

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	5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	ALA	C-N	19.95	1.79	1.34
1	A	200	VAL	CA-CB	16.46	1.89	1.54
1	A	176	VAL	CA-CB	13.38	1.82	1.54
1	A	12	GLY	N-CA	10.42	1.61	1.46
1	A	17	ILE	N-CA	10.40	1.67	1.46
1	A	387	SER	C-N	-9.93	1.11	1.34
1	A	253	GLY	N-CA	8.73	1.59	1.46
1	A	275	HIS	N-CA	8.46	1.63	1.46
1	A	264	LEU	C-N	7.91	1.47	1.33
1	A	274	PHE	C-N	7.75	1.51	1.34
1	A	18	ASN	N-CA	7.47	1.61	1.46
1	A	298	ARG	N-CA	6.82	1.59	1.46
1	A	274	PHE	CA-C	6.62	1.70	1.52
1	A	275	HIS	CB-CG	6.53	1.61	1.50
1	A	17	ILE	C-N	6.50	1.49	1.34
1	A	296	GLY	CA-C	-6.37	1.41	1.51
1	A	299	GLY	N-CA	6.15	1.55	1.46
1	A	17	ILE	CA-CB	6.09	1.68	1.54
1	A	267	PRO	CA-C	5.88	1.64	1.52
1	A	213	SER	CA-CB	-5.78	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	GLY	C-N	-5.77	1.20	1.34
1	A	16	ARG	N-CA	-5.74	1.34	1.46
1	A	441	GLU	CD-OE2	-5.68	1.19	1.25
1	A	263	ALA	C-N	5.65	1.47	1.34
1	A	268	ILE	N-CA	5.46	1.57	1.46
1	A	300	GLY	N-CA	5.25	1.53	1.46
1	A	12	GLY	C-O	-5.19	1.15	1.23
1	A	17	ILE	CA-C	5.15	1.66	1.52
1	A	13	SER	C-N	5.12	1.45	1.34
1	A	532	SER	CA-CB	-5.11	1.45	1.52
1	A	56	SER	CA-CB	-5.07	1.45	1.52
1	A	155	TYR	CA-CB	-5.04	1.42	1.53
1	A	388	ILE	C-N	-5.01	1.22	1.34

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	GLY	O-C-N	-27.57	78.59	122.70
1	A	12	GLY	C-N-CA	-16.06	81.56	121.70
1	A	12	GLY	CA-C-N	14.76	149.66	117.20
1	A	264	LEU	O-C-N	-14.18	99.09	123.20
1	A	406	ARG	NE-CZ-NH2	-13.65	113.48	120.30
1	A	189	ARG	NE-CZ-NH2	-13.35	113.62	120.30
1	A	262	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	A	155	TYR	CB-CG-CD2	-12.89	113.27	121.00
1	A	406	ARG	NE-CZ-NH1	12.41	126.51	120.30
1	A	615	THR	N-CA-CB	12.28	133.64	110.30
1	A	275	HIS	O-C-N	12.20	142.21	122.70
1	A	14	THR	O-C-N	-11.85	103.75	122.70
1	A	388	ILE	O-C-N	-11.56	104.21	122.70
1	A	248	VAL	CB-CA-C	-11.50	89.54	111.40
1	A	160	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	A	189	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	A	510	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	A	474	ASN	CA-CB-CG	10.49	136.48	113.40
1	A	155	TYR	CA-CB-CG	10.49	133.33	113.40
1	A	411	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	A	387	SER	O-C-N	-10.04	106.63	122.70
1	A	510	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	263	ALA	O-C-N	-9.91	106.84	122.70
1	A	251	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	A	15	GLU	C-N-CA	-9.88	97.01	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	13	SER	N-CA-C	9.84	137.56	111.00
1	A	434	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	A	530	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	A	10	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	670	TRP	CD1-CG-CD2	9.43	113.84	106.30
1	A	275	HIS	CA-C-N	-9.42	96.47	117.20
1	A	139	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	275	HIS	C-N-CA	9.16	144.61	121.70
1	A	172	LEU	CA-CB-CG	9.11	136.26	115.30
1	A	297	VAL	CB-CA-C	9.11	128.71	111.40
1	A	382	TYR	CB-CG-CD2	-9.09	115.54	121.00
1	A	387	SER	CA-C-N	9.06	137.14	117.20
1	A	16	ARG	N-CA-C	8.97	135.21	111.00
1	A	309	TRP	CD1-CG-CD2	8.75	113.30	106.30
1	A	323	ARG	CA-C-N	-8.75	98.69	116.20
1	A	599	TRP	CG-CD2-CE3	8.72	141.75	133.90
1	A	703	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	A	731	TYR	CB-CG-CD2	-8.50	115.90	121.00
1	A	225	CYS	CA-CB-SG	8.40	129.12	114.00
1	A	16	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	A	176	VAL	CB-CA-C	-8.25	95.72	111.40
1	A	14	THR	C-N-CA	-8.20	101.21	121.70
1	A	309	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	A	389	ARG	NE-CZ-NH2	8.07	124.34	120.30
1	A	434	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	A	200	VAL	N-CA-CB	7.96	129.01	111.50
1	A	603	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	252	ALA	O-C-N	7.92	136.66	123.20
1	A	276	THR	N-CA-C	7.88	132.28	111.00
1	A	322	ASN	CB-CG-ND2	7.87	135.58	116.70
1	A	17	ILE	N-CA-CB	7.82	128.79	110.80
1	A	269	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	599	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	A	189	ARG	CB-CG-CD	-7.68	91.64	111.60
1	A	670	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A	678	TYR	CB-CG-CD2	-7.66	116.41	121.00
1	A	13	SER	CB-CA-C	-7.64	95.58	110.10
1	A	252	ALA	C-N-CA	7.64	138.34	122.30
1	A	298	ARG	NE-CZ-NH2	7.63	124.12	120.30
1	A	530	ARG	CG-CD-NE	-7.59	95.85	111.80
1	A	452	VAL	CB-CA-C	-7.57	97.02	111.40
1	A	609	HIS	CA-CB-CG	-7.55	100.76	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	ARG	CD-NE-CZ	7.54	134.15	123.60
1	A	220	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	526	LYS	CB-CG-CD	-7.49	92.12	111.60
1	A	343	MET	CG-SD-CE	-7.48	88.24	100.20
1	A	28	TRP	CG-CD2-CE3	7.47	140.62	133.90
1	A	567	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	A	275	HIS	CA-CB-CG	7.47	126.30	113.60
1	A	599	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	A	711	MET	CG-SD-CE	-7.45	88.27	100.20
1	A	479	ASP	CA-CB-CG	7.25	129.35	113.40
1	A	671	GLU	CA-CB-CG	7.17	129.17	113.40
1	A	158	GLN	O-C-N	7.16	134.16	122.70
1	A	186	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	263	ALA	CA-C-N	7.13	132.88	117.20
1	A	260	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	306	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	A	264	LEU	CA-C-O	7.08	134.96	120.10
1	A	387	SER	C-N-CA	7.07	139.38	121.70
1	A	263	ALA	CB-CA-C	-7.01	99.58	110.10
1	A	273	ALA	O-C-N	-7.00	111.50	122.70
1	A	618	ALA	CA-C-N	6.93	132.46	117.20
1	A	136	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	252	ALA	CB-CA-C	-6.92	99.72	110.10
1	A	72	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	A	309	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	A	329	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	365	TYR	CB-CG-CD1	-6.69	116.99	121.00
1	A	323	ARG	O-C-N	6.67	134.53	123.20
1	A	282	TYR	CB-CG-CD1	6.66	125.00	121.00
1	A	313	VAL	CB-CA-C	-6.64	98.79	111.40
1	A	567	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	A	382	TYR	CB-CG-CD1	6.53	124.92	121.00
1	A	79	TYR	CB-CG-CD1	-6.50	117.10	121.00
1	A	479	ASP	CB-CG-OD1	6.47	124.13	118.30
1	A	191	GLN	CA-CB-CG	6.46	127.62	113.40
1	A	83	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	274	PHE	N-CA-C	6.43	128.36	111.00
1	A	244	ILE	O-C-N	-6.42	112.43	122.70
1	A	28	TRP	CD1-CG-CD2	6.39	111.41	106.30
1	A	599	TRP	CB-CG-CD1	-6.35	118.75	127.00
1	A	282	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	A	517	VAL	N-CA-CB	-6.24	97.78	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	322	ASN	OD1-CG-ND2	-6.24	107.56	121.90
1	A	119	LEU	CA-CB-CG	6.22	129.61	115.30
1	A	670	TRP	CG-CD1-NE1	-6.22	103.88	110.10
1	A	653	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	745	ASN	CB-CG-ND2	6.20	131.58	116.70
1	A	134	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	A	730	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	531	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	703	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	396	VAL	CB-CA-C	-6.14	99.73	111.40
1	A	220	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	111	GLU	CA-CB-CG	6.12	126.87	113.40
1	A	46	HIS	CA-C-N	6.12	130.67	117.20
1	A	726	VAL	CG1-CB-CG2	-6.10	101.14	110.90
1	A	28	TRP	CE2-CD2-CG	-6.08	102.43	107.30
1	A	178	ALA	O-C-N	-6.08	112.97	122.70
1	A	178	ALA	CA-C-N	6.06	130.53	117.20
1	A	522	TYR	CB-CG-CD2	-6.06	117.37	121.00
1	A	360	ASP	N-CA-CB	-6.05	99.70	110.60
1	A	238	ASN	O-C-N	-6.03	113.06	122.70
1	A	115	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	A	618	ALA	O-C-N	-6.01	113.08	122.70
1	A	13	SER	O-C-N	5.99	132.28	122.70
1	A	511	ARG	CD-NE-CZ	-5.98	115.22	123.60
1	A	589	THR	CA-CB-CG2	5.96	120.74	112.40
1	A	252	ALA	CA-C-N	-5.93	104.33	116.20
1	A	735	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	274	PHE	C-N-CA	5.91	136.47	121.70
1	A	653	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	274	PHE	CB-CA-C	-5.88	98.65	110.40
1	A	24	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	235	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	589	THR	CA-CB-OG1	-5.83	96.76	109.00
1	A	567	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	A	719	LEU	O-C-N	-5.74	113.51	122.70
1	A	534	GLY	O-C-N	-5.74	113.52	122.70
1	A	513	LEU	CA-C-N	5.72	127.65	116.20
1	A	511	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	78	GLN	CA-CB-CG	5.72	125.98	113.40
1	A	200	VAL	O-C-N	-5.70	113.58	122.70
1	A	158	GLN	CA-C-N	-5.67	104.71	117.20
1	A	687	LYS	CG-CD-CE	-5.67	94.89	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	309	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	A	730	TYR	N-CA-CB	-5.66	100.41	110.60
1	A	335	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	16	ARG	CG-CD-NE	-5.65	99.94	111.80
1	A	200	VAL	CB-CA-C	-5.62	100.72	111.40
1	A	699	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	A	671	GLU	N-CA-CB	-5.61	100.50	110.60
1	A	195	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	12	GLY	CA-C-O	5.58	130.64	120.60
1	A	263	ALA	N-CA-C	5.58	126.06	111.00
1	A	238	ASN	CA-C-N	5.58	129.47	117.20
1	A	730	TYR	CA-C-N	5.55	129.42	117.20
1	A	184	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	A	672	MET	CG-SD-CE	5.53	109.05	100.20
1	A	719	LEU	CA-C-N	5.53	129.38	117.20
1	A	158	GLN	C-N-CA	5.50	135.44	121.70
1	A	197	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	15	GLU	CB-CA-C	5.49	121.38	110.40
1	A	364	LEU	CA-CB-CG	5.49	127.93	115.30
1	A	309	TRP	CB-CG-CD1	-5.49	119.87	127.00
1	A	39	SER	CA-C-N	5.48	129.26	117.20
1	A	251	ARG	CD-NE-CZ	5.48	131.28	123.60
1	A	413	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	A	670	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	A	666	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	A	745	ASN	OD1-CG-ND2	-5.45	109.36	121.90
1	A	47	ILE	CB-CA-C	-5.45	100.71	111.60
1	A	268	ILE	CB-CA-C	-5.45	100.71	111.60
1	A	513	LEU	O-C-N	-5.45	113.94	123.20
1	A	245	VAL	CG1-CB-CG2	-5.41	102.24	110.90
1	A	68	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	406	ARG	CG-CD-NE	-5.41	100.44	111.80
1	A	427	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	408	SER	CB-CA-C	-5.37	99.89	110.10
1	A	399	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	A	741	ASP	CA-CB-CG	5.37	125.21	113.40
1	A	191	GLN	CB-CA-C	-5.36	99.69	110.40
1	A	50	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	A	411	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	221	GLN	OE1-CD-NE2	-5.33	109.64	121.90
1	A	17	ILE	CA-CB-CG1	5.32	121.11	111.00
1	A	16	ARG	CB-CA-C	-5.32	99.77	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	628	ILE	CG1-CB-CG2	-5.32	99.70	111.40
1	A	28	TRP	CB-CG-CD1	-5.29	120.13	127.00
1	A	562	GLN	OE1-CD-NE2	-5.28	109.75	121.90
1	A	40	GLN	CG-CD-NE2	5.27	129.35	116.70
1	A	333	MET	CA-C-N	5.26	128.78	117.20
1	A	651	ILE	O-C-N	-5.26	114.29	122.70
1	A	567	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	A	179	CYS	O-C-N	-5.24	114.32	122.70
1	A	542	LYS	CB-CG-CD	-5.24	97.99	111.60
1	A	279	ILE	CA-C-N	5.22	131.73	117.10
1	A	28	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	A	107	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	A	608	THR	N-CA-CB	-5.17	100.47	110.30
1	A	141	MET	CG-SD-CE	-5.17	91.93	100.20
1	A	80	LEU	CD1-CG-CD2	-5.16	95.01	110.50
1	A	10	ARG	NH1-CZ-NH2	-5.16	113.72	119.40
1	A	399	PHE	CG-CD1-CE1	-5.16	115.12	120.80
1	A	263	ALA	C-N-CA	5.16	134.59	121.70
1	A	155	TYR	N-CA-CB	5.15	119.87	110.60
1	A	269	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
1	A	179	CYS	CA-C-N	5.13	128.49	117.20
1	A	564	ALA	O-C-N	-5.13	114.50	122.70
1	A	331	ARG	CB-CG-CD	-5.11	98.31	111.60
1	A	362	PRO	CA-C-N	5.11	126.43	116.20
1	A	118	HIS	CA-CB-CG	-5.11	104.91	113.60
1	A	14	THR	N-CA-C	-5.08	97.29	111.00
1	A	249	SER	CB-CA-C	5.08	119.75	110.10
1	A	549	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	160	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
1	A	155	TYR	CB-CG-CD1	5.07	124.04	121.00
1	A	96	GLN	CB-CA-C	-5.06	100.29	110.40
1	A	15	GLU	N-CA-C	-5.05	97.37	111.00
1	A	13	SER	CA-C-N	-5.04	106.10	117.20
1	A	562	GLN	CG-CD-NE2	5.04	128.81	116.70
1	A	417	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	A	192	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	698	ASN	CB-CG-ND2	5.03	128.77	116.70
1	A	510	ARG	CB-CG-CD	5.02	124.64	111.60
1	A	599	TRP	CG-CD1-NE1	-5.01	105.08	110.10
1	A	19	LEU	O-C-N	-5.01	114.69	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLY	Mainchain
1	A	16	ARG	Peptide
1	A	264	LEU	Mainchain
1	A	361	VAL	Peptide
1	A	79	TYR	Sidechain

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	5875	0	5774	178	1
All	All	5875	0	5774	178	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 15.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:VAL:CA	1:A:176:VAL:CB	1.82	1.57
1:A:200:VAL:CA	1:A:200:VAL:CB	1.89	1.50
1:A:273:ALA:C	1:A:274:PHE:N	1.79	1.35
1:A:264:LEU:HD23	1:A:389:ARG:NH1	1.66	1.09
1:A:249:SER:HB3	1:A:292:CYS:HB2	1.31	1.08
1:A:248:VAL:HG13	1:A:254:ILE:HG13	1.38	1.06
1:A:13:SER:HB2	1:A:15:GLU:H	1.22	1.04
1:A:248:VAL:HG13	1:A:254:ILE:CG1	1.90	1.00
1:A:328:ASN:O	1:A:329:ARG:NH1	1.97	0.97
1:A:329:ARG:HH11	1:A:329:ARG:HG3	1.28	0.96
1:A:250:GLN:NE2	1:A:251:ARG:HH11	1.65	0.93
1:A:14:THR:C	1:A:16:ARG:N	2.18	0.92
1:A:248:VAL:HG11	1:A:289:VAL:HB	1.53	0.91
1:A:249:SER:HB3	1:A:292:CYS:CB	2.00	0.90
1:A:155:TYR:HE2	1:A:628:ILE:HD13	1.36	0.90
1:A:250:GLN:NE2	1:A:251:ARG:NH1	2.19	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:HG22	1:A:54:LYS:HA	1.55	0.87
1:A:248:VAL:HG21	1:A:289:VAL:HA	1.55	0.86
1:A:155:TYR:CE2	1:A:628:ILE:HD13	2.09	0.86
1:A:250:GLN:HE22	1:A:251:ARG:NH1	1.74	0.84
1:A:160:ARG:O	1:A:162:THR:N	2.09	0.84
1:A:159:ASN:HB2	1:A:163:GLY:H	1.41	0.84
1:A:14:THR:C	1:A:16:ARG:H	1.78	0.83
1:A:276:THR:HG23	1:A:276:THR:O	1.77	0.83
1:A:249:SER:O	1:A:251:ARG:N	2.14	0.81
1:A:249:SER:CB	1:A:292:CYS:HB2	2.11	0.81
1:A:264:LEU:CD2	1:A:389:ARG:NH1	2.43	0.80
1:A:176:VAL:C	1:A:176:VAL:CB	2.50	0.79
1:A:329:ARG:HH11	1:A:329:ARG:CG	1.96	0.78
1:A:321:ASN:O	1:A:329:ARG:HD3	1.83	0.78
1:A:329:ARG:NH1	1:A:329:ARG:HG3	1.99	0.77
1:A:118:HIS:HD2	1:A:220:ARG:HH22	1.32	0.76
1:A:248:VAL:HG11	1:A:289:VAL:CB	2.16	0.75
1:A:13:SER:C	1:A:15:GLU:H	1.90	0.73
1:A:155:TYR:CE2	1:A:628:ILE:CD1	2.72	0.72
1:A:345:THR:O	1:A:349:LYS:HG2	1.89	0.72
1:A:248:VAL:HG13	1:A:254:ILE:HG12	1.70	0.72
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.71	0.72
1:A:118:HIS:CD2	1:A:220:ARG:HH22	2.08	0.71
1:A:13:SER:HB2	1:A:15:GLU:N	2.03	0.70
1:A:130:GLN:O	1:A:133:THR:HB	1.91	0.69
1:A:13:SER:CB	1:A:15:GLU:H	2.03	0.68
1:A:176:VAL:N	1:A:176:VAL:CB	2.55	0.68
1:A:425:PRO:HG2	1:A:615:THR:HG22	1.74	0.68
1:A:13:SER:C	1:A:15:GLU:N	2.44	0.68
1:A:519:ASN:ND2	1:A:632:THR:H	1.92	0.68
1:A:276:THR:CG2	1:A:276:THR:O	2.43	0.67
1:A:14:THR:HG21	1:A:54:LYS:HD2	1.75	0.67
1:A:30:ALA:HB2	1:A:38:ILE:HD11	1.74	0.67
1:A:251:ARG:O	1:A:252:ALA:HB2	1.94	0.67
1:A:110:VAL:HG11	1:A:120:LEU:HD12	1.76	0.66
1:A:200:VAL:C	1:A:200:VAL:CB	2.64	0.66
1:A:364:LEU:HD22	1:A:375:PHE:CE1	2.30	0.66
1:A:658:ASP:HB3	1:A:662:LEU:HD22	1.78	0.65
1:A:711:MET:HE3	1:A:715:LEU:HG	1.79	0.64
1:A:322:ASN:HD22	1:A:323:ARG:H	1.46	0.64
1:A:442:ILE:HD11	1:A:464:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ALA:HB1	1:A:312:GLU:HG3	1.78	0.64
1:A:533:ASP:HB3	1:A:535:SER:H	1.62	0.64
1:A:244:ILE:HG22	1:A:248:VAL:CG2	2.30	0.62
1:A:176:VAL:CA	1:A:176:VAL:CG2	2.77	0.61
1:A:14:THR:CG2	1:A:54:LYS:HA	2.29	0.61
1:A:449:LEU:HD12	1:A:457:GLY:HA3	1.84	0.60
1:A:244:ILE:CG2	1:A:248:VAL:HG22	2.32	0.60
1:A:160:ARG:C	1:A:162:THR:N	2.55	0.60
1:A:686:GLN:HE22	1:A:692:SER:HA	1.67	0.59
1:A:159:ASN:ND2	1:A:162:THR:HG22	2.17	0.58
1:A:345:THR:CG2	1:A:349:LYS:HD3	2.34	0.58
1:A:406:ARG:HH21	1:A:413:TYR:HA	1.69	0.58
1:A:639:ARG:HG3	1:A:669:LEU:HD12	1.85	0.58
1:A:24:ARG:HG3	1:A:24:ARG:NH1	2.18	0.58
1:A:249:SER:HB3	1:A:292:CYS:SG	2.43	0.57
1:A:155:TYR:HE2	1:A:628:ILE:CD1	2.12	0.57
1:A:159:ASN:HD22	1:A:162:THR:HG22	1.69	0.57
1:A:343:MET:HE3	1:A:353:ILE:HD13	1.87	0.57
1:A:317:LEU:HD11	1:A:337:VAL:HG21	1.86	0.56
1:A:79:TYR:O	1:A:83:ARG:HG3	2.05	0.56
1:A:14:THR:O	1:A:16:ARG:N	2.36	0.56
1:A:18:ASN:O	1:A:21:LYS:HD3	2.05	0.56
1:A:114:LYS:HE3	1:A:166:TYR:CE2	2.41	0.56
1:A:711:MET:CE	1:A:715:LEU:HG	2.37	0.55
1:A:159:ASN:HB2	1:A:163:GLY:N	2.18	0.55
1:A:179:CYS:SG	1:A:216:ARG:HA	2.47	0.55
1:A:319:LEU:O	1:A:329:ARG:HG2	2.06	0.55
1:A:249:SER:O	1:A:250:GLN:C	2.44	0.55
1:A:322:ASN:HD22	1:A:323:ARG:N	2.05	0.54
1:A:345:THR:HG22	1:A:349:LYS:HD3	1.89	0.54
1:A:644:ILE:HG23	1:A:651:ILE:HG23	1.89	0.54
1:A:14:THR:O	1:A:15:GLU:C	2.26	0.53
1:A:519:ASN:HD22	1:A:632:THR:H	1.56	0.53
1:A:176:VAL:CA	1:A:176:VAL:CG1	2.80	0.53
1:A:15:GLU:C	1:A:16:ARG:CG	2.74	0.53
1:A:529:LYS:HB3	1:A:536:ALA:HB2	1.91	0.52
1:A:244:ILE:HG23	1:A:248:VAL:HG22	1.92	0.52
1:A:357:SER:O	1:A:360:ASP:HB3	2.08	0.52
1:A:273:ALA:HB1	1:A:274:PHE:N	2.25	0.52
1:A:510:ARG:HB2	1:A:512:THR:HG23	1.92	0.52
1:A:171:PHE:O	1:A:175:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:CG2	1:A:248:VAL:CG2	2.88	0.52
1:A:379:TYR:O	1:A:383:GLU:HG3	2.10	0.52
1:A:586:ASP:O	1:A:589:THR:HB	2.10	0.52
1:A:14:THR:CA	1:A:16:ARG:H	2.22	0.51
1:A:442:ILE:HG13	1:A:462:CYS:SG	2.50	0.51
1:A:310:HIS:O	1:A:313:VAL:HG22	2.10	0.51
1:A:148:VAL:HA	1:A:151:LEU:HD12	1.92	0.51
1:A:325:VAL:HG22	1:A:327:GLY:H	1.76	0.50
1:A:200:VAL:CG1	1:A:200:VAL:CA	2.84	0.50
1:A:294:GLN:HA	1:A:294:GLN:OE1	2.12	0.50
1:A:45:SER:HB2	1:A:61:THR:HG22	1.93	0.49
1:A:395:ALA:O	1:A:399:PHE:HD1	1.95	0.49
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.94	0.49
1:A:217:THR:OG1	1:A:219:THR:HG22	2.13	0.49
1:A:24:ARG:HH11	1:A:24:ARG:HG3	1.78	0.48
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.95	0.48
1:A:455:GLU:HG3	1:A:501:PRO:HB2	1.96	0.48
1:A:427:ASP:OD2	1:A:575:LYS:HE2	2.14	0.48
1:A:697:THR:HG22	1:A:732:GLN:HG3	1.95	0.48
1:A:248:VAL:CG1	1:A:254:ILE:HG12	2.41	0.48
1:A:321:ASN:O	1:A:329:ARG:CD	2.58	0.48
1:A:212:MET:O	1:A:216:ARG:NH2	2.46	0.48
1:A:244:ILE:HG22	1:A:248:VAL:HG21	1.96	0.48
1:A:215:VAL:O	1:A:216:ARG:HB3	2.14	0.47
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.95	0.47
1:A:72:ARG:O	1:A:75:PRO:HD3	2.15	0.47
1:A:283:LYS:HG2	1:A:330:VAL:HG22	1.96	0.47
1:A:200:VAL:CA	1:A:200:VAL:CG2	2.84	0.47
1:A:17:ILE:HD13	1:A:17:ILE:HG21	1.75	0.47
1:A:278:CYS:HB2	1:A:312:GLU:OE2	2.15	0.47
1:A:644:ILE:HG23	1:A:651:ILE:CG2	2.45	0.47
1:A:15:GLU:O	1:A:16:ARG:CB	2.46	0.47
1:A:144:SER:O	1:A:147:ALA:HB3	2.15	0.46
1:A:578:LEU:HD13	1:A:599:TRP:HE3	1.81	0.46
1:A:220:ARG:HG2	1:A:495:TYR:O	2.16	0.46
1:A:290:LYS:HB3	1:A:296:GLY:HA2	1.98	0.46
1:A:529:LYS:N	1:A:529:LYS:HD2	2.32	0.45
1:A:15:GLU:C	1:A:16:ARG:HG3	2.37	0.45
1:A:15:GLU:O	1:A:15:GLU:HG3	2.16	0.45
1:A:158:GLN:HB2	1:A:159:ASN:H	1.47	0.45
1:A:273:ALA:CA	1:A:274:PHE:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:HE3	1:A:333:MET:O	2.16	0.45
1:A:440:LEU:HD12	1:A:728:THR:HB	1.98	0.45
1:A:415:GLN:HG3	1:A:728:THR:HG22	1.98	0.45
1:A:697:THR:HG23	1:A:699:TYR:HE1	1.81	0.45
1:A:47:ILE:H	1:A:47:ILE:HG13	1.65	0.44
1:A:155:TYR:CE2	1:A:628:ILE:HD11	2.52	0.44
1:A:285:PHE:O	1:A:289:VAL:HG13	2.18	0.44
1:A:181:PHE:O	1:A:184:TYR:HB2	2.18	0.44
1:A:293:SER:HB2	1:A:294:GLN:H	1.73	0.44
1:A:47:ILE:HD12	1:A:48:GLN:HG3	1.99	0.43
1:A:593:GLU:OE2	1:A:596:HIS:HE1	2.01	0.43
1:A:548:GLN:O	1:A:552:LEU:HB2	2.18	0.43
1:A:457:GLY:O	1:A:502:ALA:HB1	2.19	0.43
1:A:708:LYS:HA	1:A:708:LYS:HD3	1.88	0.43
1:A:248:VAL:CG2	1:A:289:VAL:HA	2.38	0.43
1:A:282:TYR:CE2	1:A:316:LEU:HD22	2.53	0.43
1:A:329:ARG:NH1	1:A:329:ARG:CG	2.65	0.43
1:A:569:ASN:ND2	1:A:569:ASN:H	2.17	0.43
1:A:264:LEU:HD23	1:A:389:ARG:CZ	2.42	0.43
1:A:264:LEU:HD23	1:A:389:ARG:HH11	1.73	0.42
1:A:155:TYR:OH	1:A:624:THR:HG22	2.19	0.42
1:A:620:MET:SD	1:A:620:MET:N	2.86	0.42
1:A:668:LEU:O	1:A:669:LEU:C	2.57	0.42
1:A:226:VAL:HG21	1:A:247:TYR:CG	2.55	0.42
1:A:413:TYR:HB3	1:A:729:LEU:O	2.20	0.42
1:A:90:ARG:HH11	1:A:90:ARG:HD2	1.62	0.42
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.32	0.41
1:A:263:ALA:HB1	1:A:312:GLU:CG	2.48	0.41
1:A:15:GLU:HG2	1:A:16:ARG:HG2	2.02	0.41
1:A:93:ALA:HB2	1:A:165:ILE:HG22	2.02	0.41
1:A:160:ARG:HB2	1:A:166:TYR:OH	2.19	0.41
1:A:558:LEU:HD23	1:A:612:ARG:HG2	2.02	0.41
1:A:406:ARG:O	1:A:410:GLY:N	2.51	0.41
1:A:340:ASN:OD1	1:A:343:MET:HG2	2.21	0.41
1:A:264:LEU:CD2	1:A:389:ARG:HH11	2.31	0.41
1:A:645:LYS:HB2	1:A:652:LEU:HB2	2.03	0.41
1:A:244:ILE:HD13	1:A:244:ILE:HG21	1.77	0.40
1:A:306:TYR:OH	1:A:317:LEU:HD13	2.21	0.40
1:A:565:CYS:HA	1:A:566:PRO:HD3	1.95	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)
1:A:276:THR:OG1	1:A:293:SER:O[18_655]	1.19	1.01

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	733/761 (96%)	661 (90%)	46 (6%)	26 (4%)	4 6

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	216	ARG
1	A	250	GLN
1	A	267	PRO
1	A	276	THR
1	A	298	ARG
1	A	385	ASP
1	A	386	ASP
1	A	161	VAL
1	A	253	GLY
1	A	295	GLY
1	A	296	GLY
1	A	299	GLY
1	A	301	ALA
1	A	322	ASN
1	A	511	ARG
1	A	185	PRO
1	A	252	ALA
1	A	741	ASP
1	A	162	THR
1	A	361	VAL
1	A	16	ARG
1	A	268	ILE

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Mol	Chain	Res	Type
1	A	17	ILE
1	A	248	VAL
1	A	265	GLY

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	633/654 (97%)	534 (84%)	99 (16%)	3 6

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	13	SER
1	A	14	THR
1	A	15	GLU
1	A	16	ARG
1	A	20	ASP
1	A	21	LYS
1	A	24	ARG
1	A	39	SER
1	A	40	GLN
1	A	47	ILE
1	A	51	ASP
1	A	60	GLU
1	A	69	LEU
1	A	72	ARG
1	A	73	ASP
1	A	89	LEU
1	A	96	GLN
1	A	102	LEU
1	A	108	LYS
1	A	119	LEU
1	A	139	ARG
1	A	159	ASN

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Mol	Chain	Res	Type
1	A	160	ARG
1	A	162	THR
1	A	165	ILE
1	A	172	LEU
1	A	175	LEU
1	A	180	LEU
1	A	185	PRO
1	A	186	ARG
1	A	190	LEU
1	A	220	ARG
1	A	224	SER
1	A	225	CYS
1	A	248	VAL
1	A	249	SER
1	A	250	GLN
1	A	251	ARG
1	A	260	ARG
1	A	264	LEU
1	A	275	HIS
1	A	276	THR
1	A	278	CYS
1	A	293	SER
1	A	298	ARG
1	A	313	VAL
1	A	317	LEU
1	A	322	ASN
1	A	323	ARG
1	A	329	ARG
1	A	348	LEU
1	A	359	SER
1	A	373	GLU
1	A	386	ASP
1	A	394	LYS
1	A	396	VAL
1	A	397	GLU
1	A	400	SER
1	A	440	LEU
1	A	441	GLU
1	A	452	VAL
1	A	465	SER
1	A	474	ASN
1	A	478	LEU

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Mol	Chain	Res	Type
1	A	481	LEU
1	A	487	ARG
1	A	496	GLN
1	A	497	ASP
1	A	510	ARG
1	A	517	VAL
1	A	519	ASN
1	A	530	ARG
1	A	533	ASP
1	A	539	LEU
1	A	552	LEU
1	A	566	PRO
1	A	569	ASN
1	A	570	GLU
1	A	586	ASP
1	A	592	ASN
1	A	622	SER
1	A	625	SER
1	A	626	SER
1	A	629	SER
1	A	639	ARG
1	A	645	LYS
1	A	648	LYS
1	A	662	LEU
1	A	669	LEU
1	A	679	LEU
1	A	681	LEU
1	A	696	ASN
1	A	697	THR
1	A	703	ARG
1	A	716	LYS
1	A	739	ASP
1	A	741	ASP
1	A	745	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	78	GLN
1	A	105	HIS
1	A	118	HIS

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Mol	Chain	Res	Type
1	A	159	ASN
1	A	221	GLN
1	A	250	GLN
1	A	321	ASN
1	A	322	ASN
1	A	415	GLN
1	A	519	ASN
1	A	548	GLN
1	A	569	ASN
1	A	596	HIS
1	A	686	GLN
1	A	698	ASN
1	A	733	ASN

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.