Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:29 PM GMT

PDB ID	:	1B04
Title	:	STRUCTURE OF THE ADENYLATION DOMAIN OF AN NAD+ DEPENDENT LIGASE
Authors	:	Singleton, M.R.; Hakansson, K.; Timson, D.J.; Wigley, D.B.
Deposited on	:	1998-11-16
Resolution	:	2.80 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 (1)) were used in the production of this report:

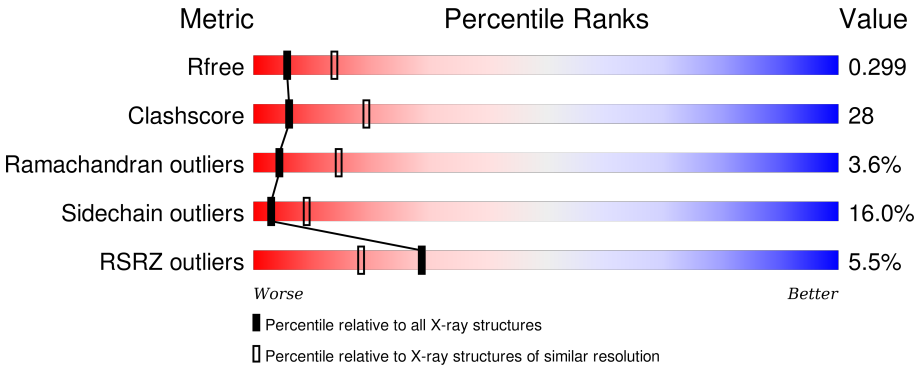
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	318	6% 42% 33% 18% 5% •
1	B	318	5% 43% 29% 21% 5% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5126 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 PROTEIN (DNA LIGASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2464	1547	444	467	6			
1	B	311	Total	C	N	O	S	0	0	0
			2472	1552	445	468	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ALA	LYS	ENGINEERED	UNP O87703
B	114	ALA	LYS	ENGINEERED	UNP O87703

- Molecule 2 is water.

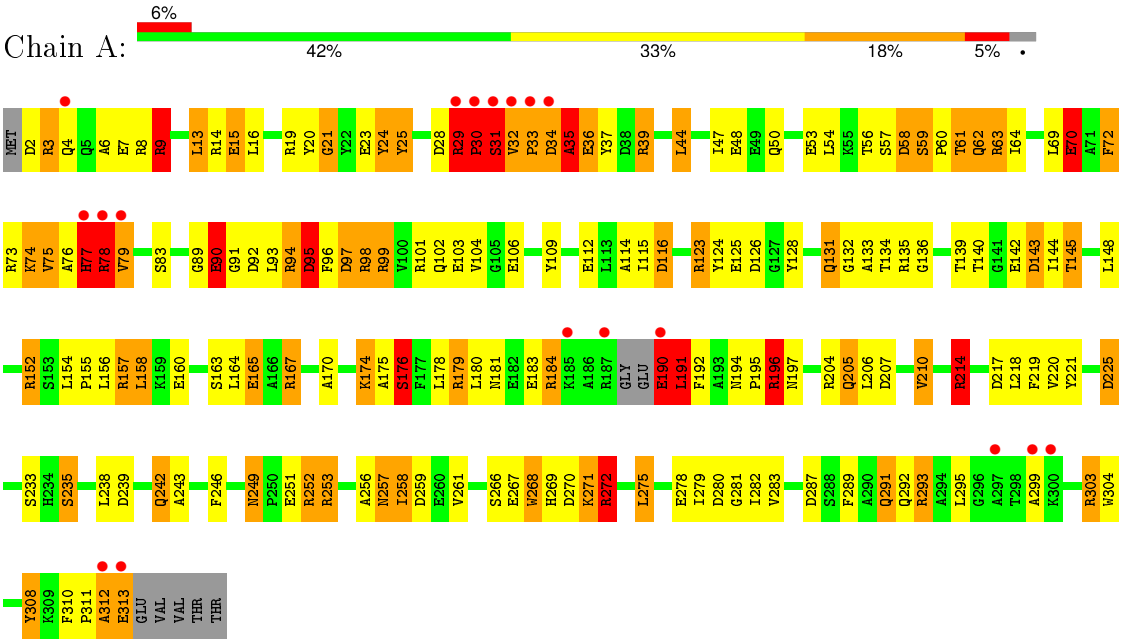
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	112	Total	O	0	0
			112	112		

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.

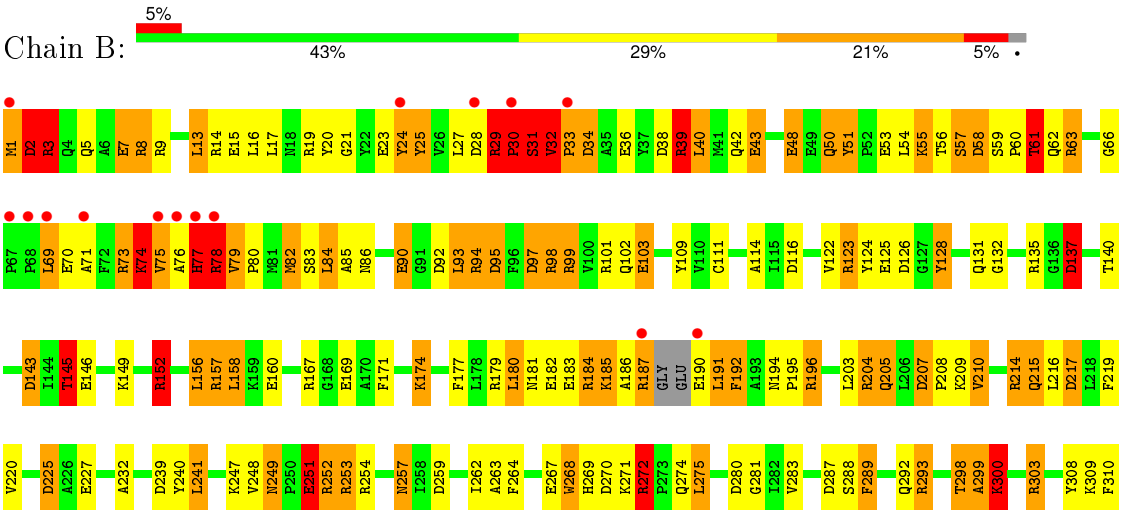
- Molecule 1: PROTEIN (DNA LIGASE)

Chain A:



- Molecule 1: PROTEIN (DNA LIGASE)

Chain B:




P311
A312
E313
GLU
VAL
VAL
THR
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	95.72Å 95.72Å 225.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.80) 97.6 (19.76-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.310 0.226 , 0.299	Depositor DCC
R_{free} test set	1301 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 79.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 25982 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5126	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.88	4/2511 (0.2%)	2.60	155/3393 (4.6%)
1	B	0.88	1/2519 (0.0%)	2.84	190/3403 (5.6%)
All	All	0.88	5/5030 (0.1%)	2.73	345/6796 (5.1%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	GLU	CD-OE1	14.15	1.41	1.25
1	A	313	GLU	CG-CD	10.33	1.67	1.51
1	A	313	GLU	CB-CG	6.76	1.65	1.52
1	B	78	ARG	NE-CZ	5.88	1.40	1.33
1	A	313	GLU	C-O	5.31	1.33	1.23

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	19	ARG	CD-NE-CZ	33.88	171.03	123.60
1	A	19	ARG	CD-NE-CZ	33.58	170.61	123.60
1	A	179	ARG	CD-NE-CZ	32.97	169.76	123.60
1	B	252	ARG	CD-NE-CZ	27.32	161.85	123.60
1	B	187	ARG	CD-NE-CZ	22.25	154.75	123.60
1	B	78	ARG	NE-CZ-NH2	-21.23	109.69	120.30
1	B	157	ARG	NE-CZ-NH1	-18.62	110.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	ARG	CD-NE-CZ	18.52	149.53	123.60
1	B	98	ARG	NE-CZ-NH1	18.24	129.42	120.30
1	A	73	ARG	NE-CZ-NH1	17.98	129.29	120.30
1	B	31	SER	C-N-CA	17.79	166.18	121.70
1	B	99	ARG	NE-CZ-NH1	-17.53	111.54	120.30
1	A	313	GLU	OE1-CD-OE2	16.13	142.66	123.30
1	B	123	ARG	NE-CZ-NH2	-15.75	112.42	120.30
1	A	179	ARG	NE-CZ-NH2	15.42	128.01	120.30
1	A	253	ARG	CD-NE-CZ	15.18	144.85	123.60
1	B	73	ARG	CD-NE-CZ	14.81	144.34	123.60
1	B	214	ARG	CD-NE-CZ	14.73	144.22	123.60
1	A	39	ARG	NE-CZ-NH2	-14.46	113.07	120.30
1	A	196	ARG	CD-NE-CZ	14.42	143.79	123.60
1	B	8	ARG	CD-NE-CZ	14.14	143.39	123.60
1	B	98	ARG	CD-NE-CZ	14.13	143.38	123.60
1	A	72	PHE	CB-CG-CD2	-14.09	110.94	120.80
1	B	97	ASP	CB-CG-OD1	14.04	130.94	118.30
1	A	225	ASP	CB-CG-OD2	-13.98	105.72	118.30
1	A	8	ARG	NE-CZ-NH2	13.96	127.28	120.30
1	A	72	PHE	CB-CG-CD1	13.87	130.51	120.80
1	B	252	ARG	NE-CZ-NH1	13.84	127.22	120.30
1	A	196	ARG	NE-CZ-NH1	-13.66	113.47	120.30
1	B	77	HIS	CA-CB-CG	13.62	136.76	113.60
1	A	39	ARG	NE-CZ-NH1	13.47	127.04	120.30
1	A	135	ARG	NE-CZ-NH1	13.46	127.03	120.30
1	A	63	ARG	NE-CZ-NH2	-13.34	113.63	120.30
1	A	78	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	A	98	ARG	NE-CZ-NH1	-13.19	113.70	120.30
1	B	204	ARG	NE-CZ-NH2	13.10	126.85	120.30
1	B	187	ARG	NE-CZ-NH1	13.06	126.83	120.30
1	B	32	VAL	CA-CB-CG1	13.00	130.40	110.90
1	B	252	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	B	214	ARG	NE-CZ-NH1	12.95	126.78	120.30
1	A	3	ARG	CD-NE-CZ	12.87	141.61	123.60
1	A	98	ARG	CD-NE-CZ	12.81	141.54	123.60
1	B	94	ARG	NE-CZ-NH2	12.67	126.64	120.30
1	B	101	ARG	NE-CZ-NH1	12.52	126.56	120.30
1	B	293	ARG	CD-NE-CZ	12.52	141.13	123.60
1	B	101	ARG	CD-NE-CZ	12.50	141.10	123.60
1	B	2	ASP	CB-CG-OD1	12.37	129.43	118.30
1	B	135	ARG	NE-CZ-NH2	11.94	126.27	120.30
1	B	272	ARG	CD-NE-CZ	11.88	140.23	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	303	ARG	NE-CZ-NH1	-11.75	114.42	120.30
1	B	78	ARG	C-N-CA	11.45	150.32	121.70
1	B	84	LEU	CA-CB-CG	11.40	141.51	115.30
1	B	99	ARG	NH1-CZ-NH2	11.22	131.74	119.40
1	B	152	ARG	CD-NE-CZ	11.03	139.04	123.60
1	B	73	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	167	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	A	157	ARG	CD-NE-CZ	10.78	138.68	123.60
1	B	3	ARG	CD-NE-CZ	10.75	138.66	123.60
1	B	78	ARG	CA-CB-CG	10.65	136.83	113.40
1	A	14	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	B	293	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	B	179	ARG	NE-CZ-NH1	-10.23	115.18	120.30
1	A	99	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	B	31	SER	O-C-N	-10.17	106.43	122.70
1	B	97	ASP	CB-CG-OD2	-9.98	109.32	118.30
1	A	25	TYR	CB-CG-CD1	-9.95	115.03	121.00
1	A	9	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	B	32	VAL	N-CA-C	9.88	137.67	111.00
1	A	272	ARG	NE-CZ-NH2	9.85	125.23	120.30
1	B	174	LYS	CA-CB-CG	9.84	135.06	113.40
1	B	109	TYR	CB-CG-CD1	-9.76	115.14	121.00
1	A	217	ASP	CB-CG-OD2	-9.62	109.64	118.30
1	A	311	PRO	C-N-CA	9.61	145.73	121.70
1	A	280	ASP	CB-CG-OD2	-9.50	109.75	118.30
1	B	101	ARG	NH1-CZ-NH2	-9.48	108.97	119.40
1	B	2	ASP	CA-C-N	9.28	137.62	117.20
1	A	135	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	B	39	ARG	CD-NE-CZ	9.01	136.22	123.60
1	A	167	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	B	32	VAL	CA-CB-CG2	-8.97	97.44	110.90
1	A	167	ARG	CD-NE-CZ	8.96	136.15	123.60
1	A	313	GLU	CB-CA-C	8.94	128.27	110.40
1	A	3	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	B	207	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	B	239	ASP	CB-CG-OD1	8.88	126.29	118.30
1	A	217	ASP	CB-CG-OD1	8.87	126.28	118.30
1	B	38	ASP	CB-CG-OD2	-8.86	110.32	118.30
1	B	253	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	B	38	ASP	CB-CG-OD1	8.79	126.22	118.30
1	B	58	ASP	CB-CG-OD1	8.77	126.19	118.30
1	A	76	ALA	C-N-CA	8.76	143.60	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	14	ARG	NE-CZ-NH1	-8.74	115.93	120.30
1	B	31	SER	CA-C-O	8.71	138.38	120.10
1	B	267	GLU	OE1-CD-OE2	-8.69	112.88	123.30
1	A	280	ASP	N-CA-CB	-8.64	95.04	110.60
1	B	303	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	B	253	ARG	CD-NE-CZ	-8.52	111.67	123.60
1	A	25	TYR	CB-CG-CD2	8.51	126.10	121.00
1	B	313	GLU	OE1-CD-OE2	-8.50	113.10	123.30
1	A	29	ARG	CG-CD-NE	8.49	129.63	111.80
1	A	90	GLU	CA-C-N	8.46	133.13	116.20
1	B	280	ASP	N-CA-CB	-8.46	95.38	110.60
1	A	78	ARG	CD-NE-CZ	8.46	135.44	123.60
1	B	98	ARG	NH1-CZ-NH2	-8.40	110.16	119.40
1	B	254	ARG	CD-NE-CZ	8.36	135.30	123.60
1	B	101	ARG	NE-CZ-NH2	8.35	124.47	120.30
1	A	9	ARG	CD-NE-CZ	8.33	135.26	123.60
1	B	251	GLU	OE1-CD-OE2	-8.33	113.31	123.30
1	B	78	ARG	NH1-CZ-NH2	8.32	128.55	119.40
1	B	71	ALA	CB-CA-C	8.29	122.54	110.10
1	A	44	LEU	N-CA-CB	8.24	126.87	110.40
1	A	256	ALA	N-CA-CB	8.19	121.57	110.10
1	B	7	GLU	OE1-CD-OE2	8.18	133.12	123.30
1	A	8	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	A	99	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	272	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	B	95	ASP	CB-CG-OD1	8.09	125.58	118.30
1	B	137	ASP	CB-CG-OD2	8.08	125.57	118.30
1	A	308	TYR	CB-CG-CD1	8.06	125.84	121.00
1	B	300	LYS	CA-CB-CG	8.06	131.13	113.40
1	A	94	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	B	43	GLU	OE1-CD-OE2	-8.03	113.66	123.30
1	A	204	ARG	CD-NE-CZ	8.02	134.82	123.60
1	B	90	GLU	OE1-CD-OE2	-8.02	113.68	123.30
1	B	167	ARG	NE-CZ-NH1	-8.01	116.30	120.30
1	B	293	ARG	CG-CD-NE	7.98	128.55	111.80
1	B	82	MET	CA-CB-CG	7.96	126.84	113.30
1	A	299	ALA	C-N-CA	7.96	141.61	121.70
1	B	254	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	B	217	ASP	CB-CG-OD1	7.95	125.46	118.30
1	A	253	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	A	184	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	268	TRP	CA-CB-CG	-7.82	98.85	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	270	ASP	CB-CG-OD2	-7.79	111.28	118.30
1	A	279	ILE	C-N-CA	7.78	141.15	121.70
1	B	1	MET	CG-SD-CE	-7.76	87.78	100.20
1	B	99	ARG	CG-CD-NE	7.76	128.09	111.80
1	B	48	GLU	OE1-CD-OE2	-7.67	114.10	123.30
1	A	63	ARG	CD-NE-CZ	-7.67	112.87	123.60
1	A	30	PRO	CA-N-CD	-7.66	100.78	111.50
1	A	308	TYR	CB-CG-CD2	-7.59	116.44	121.00
1	A	30	PRO	CB-CA-C	7.58	130.96	112.00
1	B	280	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	A	39	ARG	CD-NE-CZ	7.55	134.17	123.60
1	A	313	GLU	CB-CG-CD	-7.54	93.85	114.20
1	A	97	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	90	GLU	CA-C-O	-7.49	104.38	120.10
1	A	184	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	58	ASP	CB-CA-C	7.42	125.23	110.40
1	B	39	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	A	123	ARG	NE-CZ-NH1	-7.41	116.60	120.30
1	B	146	GLU	OE1-CD-OE2	7.41	132.19	123.30
1	B	275	LEU	CA-CB-CG	7.33	132.16	115.30
1	B	56	THR	N-CA-CB	-7.32	96.40	110.30
1	B	53	GLU	CA-CB-CG	7.28	129.41	113.40
1	B	33	PRO	O-C-N	-7.21	111.17	122.70
1	A	252	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	A	135	ARG	CD-NE-CZ	7.17	133.65	123.60
1	B	99	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	311	PRO	CA-C-O	7.16	137.38	120.20
1	B	109	TYR	CB-CG-CD2	7.15	125.29	121.00
1	A	14	ARG	CD-NE-CZ	7.15	133.61	123.60
1	A	214	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	A	74	LYS	N-CA-CB	7.10	123.38	110.60
1	A	204	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	225	ASP	CA-CB-CG	-7.06	97.88	113.40
1	A	192	PHE	CB-CG-CD1	-7.04	115.87	120.80
1	B	29	ARG	NE-CZ-NH1	-6.99	116.81	120.30
1	B	169	GLU	OE1-CD-OE2	-6.97	114.94	123.30
1	B	270	ASP	OD1-CG-OD2	6.94	136.49	123.30
1	A	58	ASP	CB-CA-C	6.92	124.25	110.40
1	B	214	ARG	NH1-CZ-NH2	-6.88	111.83	119.40
1	A	24	TYR	N-CA-CB	6.87	122.96	110.60
1	B	292	GLN	CA-CB-CG	6.83	128.44	113.40
1	A	70	GLU	OE1-CD-OE2	6.80	131.46	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	73	ARG	NH1-CZ-NH2	-6.77	111.95	119.40
1	B	33	PRO	N-CA-C	-6.76	94.53	112.10
1	B	50	GLN	N-CA-CB	6.76	122.77	110.60
1	B	270	ASP	CB-CG-OD1	-6.75	112.23	118.30
1	A	35	ALA	O-C-N	-6.74	111.91	122.70
1	A	97	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	B	157	ARG	CG-CD-NE	-6.72	97.69	111.80
1	B	60	PRO	O-C-N	-6.72	111.95	122.70
1	B	239	ASP	OD1-CG-OD2	-6.71	110.54	123.30
1	B	157	ARG	NH1-CZ-NH2	6.68	126.75	119.40
1	B	293	ARG	C-N-CA	6.67	138.38	121.70
1	B	270	ASP	CB-CA-C	6.67	123.74	110.40
1	A	179	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	B	225	ASP	CA-CB-CG	-6.61	98.86	113.40
1	A	34	ASP	CA-CB-CG	6.61	127.93	113.40
1	A	280	ASP	OD1-CG-OD2	6.59	135.83	123.30
1	A	30	PRO	C-N-CA	6.55	138.07	121.70
1	B	152	ARG	CA-C-N	6.53	131.57	117.20
1	A	152	ARG	CD-NE-CZ	6.52	132.73	123.60
1	B	8	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	303	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	44	LEU	CA-CB-CG	6.45	130.12	115.30
1	A	190	GLU	CA-C-N	6.44	131.37	117.20
1	B	303	ARG	CD-NE-CZ	-6.43	114.59	123.60
1	A	72	PHE	CA-CB-CG	6.39	129.24	113.90
1	B	268	TRP	CA-CB-CG	-6.39	101.56	113.70
1	A	299	ALA	CA-C-O	6.36	133.45	120.10
1	B	30	PRO	N-CA-C	6.35	128.60	112.10
1	A	165	GLU	OE1-CD-OE2	6.34	130.90	123.30
1	B	29	ARG	CA-CB-CG	6.30	127.27	113.40
1	A	176	SER	N-CA-C	-6.28	94.05	111.00
1	B	280	ASP	OD1-CG-OD2	6.26	135.20	123.30
1	B	254	ARG	NH1-CZ-NH2	6.24	126.27	119.40
1	A	77	HIS	N-CA-C	6.23	127.83	111.00
1	A	291	GLN	CB-CA-C	6.22	122.84	110.40
1	A	311	PRO	O-C-N	-6.20	112.78	122.70
1	A	253	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	253	ARG	CB-CG-CD	6.19	127.70	111.60
1	B	73	ARG	O-C-N	-6.19	112.79	122.70
1	B	2	ASP	CA-C-O	-6.19	107.10	120.10
1	B	48	GLU	CG-CD-OE2	6.17	130.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	137	ASP	CB-CA-C	-6.17	98.06	110.40
1	B	24	TYR	CG-CD1-CE1	-6.15	116.38	121.30
1	A	63	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	35	ALA	CB-CA-C	6.11	119.26	110.10
1	A	97	ASP	N-CA-CB	6.08	121.55	110.60
1	B	76	ALA	CA-C-N	6.08	130.58	117.20
1	B	184	ARG	CD-NE-CZ	6.08	132.11	123.60
1	A	218	LEU	CA-CB-CG	6.08	129.28	115.30
1	B	84	LEU	CB-CG-CD1	6.04	121.28	111.00
1	B	70	GLU	CA-CB-CG	6.00	126.60	113.40
1	B	2	ASP	CB-CA-C	6.00	122.40	110.40
1	A	103	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	B	145	THR	CA-CB-CG2	5.98	120.78	112.40
1	B	25	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	B	32	VAL	N-CA-CB	-5.97	98.36	111.50
1	A	278	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	A	170	ALA	CB-CA-C	-5.93	101.21	110.10
1	B	126	ASP	N-CA-CB	5.92	121.26	110.60
1	A	253	ARG	CG-CD-NE	5.92	124.23	111.80
1	B	24	TYR	N-CA-CB	5.90	121.22	110.60
1	B	207	ASP	CB-CG-OD1	5.89	123.61	118.30
1	B	58	ASP	OD1-CG-OD2	-5.89	112.11	123.30
1	A	192	PHE	N-CA-CB	5.86	121.15	110.60
1	B	74	LYS	C-N-CA	5.86	136.35	121.70
1	B	99	ARG	CA-CB-CG	5.86	126.29	113.40
1	B	232	ALA	C-N-CA	5.86	136.34	121.70
1	A	95	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	313	GLU	CG-CD-OE1	-5.85	106.60	118.30
1	B	167	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	B	24	TYR	CB-CA-C	-5.82	98.75	110.40
1	B	219	PHE	CA-CB-CG	5.81	127.85	113.90
1	B	219	PHE	CB-CG-CD2	5.79	124.86	120.80
1	B	196	ARG	CD-NE-CZ	5.79	131.71	123.60
1	B	289	PHE	O-C-N	-5.78	113.45	122.70
1	B	254	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	59	SER	N-CA-CB	5.77	119.16	110.50
1	B	73	ARG	CA-C-O	5.77	132.22	120.10
1	B	192	PHE	CB-CG-CD1	5.77	124.84	120.80
1	B	76	ALA	CB-CA-C	5.74	118.71	110.10
1	A	44	LEU	CB-CA-C	-5.74	99.30	110.20
1	B	30	PRO	N-CA-CB	-5.73	96.30	102.60
1	A	158	LEU	N-CA-CB	-5.72	98.95	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	GLN	OE1-CD-NE2	5.71	135.04	121.90
1	A	94	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	A	192	PHE	CB-CG-CD2	5.70	124.79	120.80
1	B	143	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	A	303	ARG	N-CA-CB	5.68	120.82	110.60
1	B	73	ARG	CB-CA-C	-5.67	99.05	110.40
1	B	293	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
1	B	303	ARG	CA-CB-CG	5.65	125.83	113.40
1	B	90	GLU	CG-CD-OE2	5.64	129.58	118.30
1	B	34	ASP	CA-C-O	5.64	131.94	120.10
1	B	137	ASP	CA-CB-CG	5.63	125.78	113.40
1	A	126	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	270	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	B	24	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	A	61	THR	N-CA-CB	-5.58	99.69	110.30
1	A	31	SER	N-CA-CB	5.58	118.86	110.50
1	A	210	VAL	CA-CB-CG2	5.58	119.26	110.90
1	A	14	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	280	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	B	76	ALA	CA-C-O	-5.53	108.48	120.10
1	B	98	ARG	CA-C-O	-5.53	108.49	120.10
1	B	116	ASP	CA-C-N	5.52	127.25	116.20
1	B	241	LEU	CB-CG-CD2	5.52	120.38	111.00
1	A	225	ASP	OD1-CG-OD2	5.51	133.77	123.30
1	B	9	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	267	GLU	CG-CD-OE1	5.50	129.30	118.30
1	A	90	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	A	98	ARG	NH1-CZ-NH2	5.50	125.45	119.40
1	A	34	ASP	N-CA-CB	-5.50	100.71	110.60
1	A	135	ARG	N-CA-CB	5.48	120.47	110.60
1	B	2	ASP	O-C-N	-5.46	113.96	122.70
1	B	240	TYR	CA-CB-CG	5.46	123.77	113.40
1	B	249	ASN	N-CA-CB	-5.46	100.77	110.60
1	A	20	TYR	CB-CG-CD1	5.46	124.27	121.00
1	B	51	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	A	31	SER	C-N-CA	5.43	135.28	121.70
1	A	312	ALA	CB-CA-C	-5.43	101.95	110.10
1	B	288	SER	N-CA-CB	-5.42	102.36	110.50
1	B	78	ARG	CD-NE-CZ	-5.41	116.03	123.60
1	B	126	ASP	CB-CG-OD1	5.41	123.16	118.30
1	A	190	GLU	CA-C-O	-5.40	108.76	120.10
1	A	258	ILE	CA-CB-CG1	-5.38	100.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	ARG	N-CA-C	-5.36	96.54	111.00
1	A	62	GLN	O-C-N	-5.35	114.14	122.70
1	A	63	ARG	CG-CD-NE	5.35	123.03	111.80
1	A	221	TYR	CB-CG-CD1	5.34	124.20	121.00
1	A	256	ALA	CA-C-O	-5.34	108.88	120.10
1	B	75	VAL	CA-C-N	5.33	128.92	117.20
1	A	90	GLU	C-N-CA	-5.30	111.16	122.30
1	B	287	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	30	PRO	C-N-CA	5.29	134.93	121.70
1	B	248	VAL	CA-CB-CG1	5.27	118.81	110.90
1	A	157	ARG	CG-CD-NE	-5.27	100.74	111.80
1	B	28	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	55	LYS	CG-CD-CE	5.26	127.67	111.90
1	B	249	ASN	CB-CA-C	5.24	120.88	110.40
1	B	232	ALA	N-CA-C	5.24	125.14	111.00
1	B	137	ASP	N-CA-CB	5.23	120.02	110.60
1	B	28	ASP	CB-CA-C	5.23	120.86	110.40
1	A	92	ASP	N-CA-C	-5.22	96.90	111.00
1	A	253	ARG	N-CA-CB	-5.20	101.24	110.60
1	A	157	ARG	O-C-N	-5.20	114.39	122.70
1	A	143	ASP	CA-CB-CG	-5.17	102.03	113.40
1	B	56	THR	CA-CB-CG2	5.16	119.62	112.40
1	A	78	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	30	PRO	O-C-N	-5.14	114.47	122.70
1	A	289	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	B	293	ARG	O-C-N	-5.12	114.51	122.70
1	A	123	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	B	27	LEU	CB-CA-C	-5.11	100.48	110.20
1	A	197	ASN	CB-CG-OD1	5.09	131.79	121.60
1	B	152	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	21	GLY	CA-C-O	5.09	129.76	120.60
1	B	58	ASP	O-C-N	-5.09	114.56	122.70
1	B	239	ASP	CB-CG-OD2	5.07	122.87	118.30
1	B	128	TYR	CB-CG-CD2	5.05	124.03	121.00
1	A	131	GLN	CA-C-N	5.05	126.29	116.20
1	B	40	LEU	CB-CG-CD1	5.04	119.57	111.00
1	B	61	THR	CA-C-N	5.04	128.29	117.20
1	A	275	LEU	CA-CB-CG	5.03	126.87	115.30
1	B	53	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	A	106	GLU	OE1-CD-OE2	5.01	129.32	123.30
1	A	272	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	A	23	GLU	CA-C-N	5.00	128.21	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	GLU	N-CA-CB	5.00	119.60	110.60
1	B	184	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	GLN	Mainchain
1	A	29	ARG	Mainchain
1	B	32	VAL	Mainchain
1	B	69	LEU	Mainchain

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	2464	0	2425	142	1
1	B	2472	0	2438	148	1
2	A	78	0	0	5	0
2	B	112	0	0	5	0
All	All	5126	0	4863	277	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 28.

All (277) 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:32:VAL:HB	1:A:33:PRO:HD2	1.36	1.06
1:A:205:GLN:NE2	1:A:207:ASP:H	1.59	1.01
1:A:205:GLN:HE22	1:A:207:ASP:H	1.05	0.95
1:A:58:ASP:HB3	1:A:156:LEU:HB3	1.48	0.95
1:B:77:HIS:O	1:B:78:ARG:HB2	1.67	0.95
1:B:1:MET:SD	1:B:5:GLN:HB2	2.06	0.94
1:B:66:GLY:H	1:B:208:PRO:HB2	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TYR:HB3	1:A:31:SER:HB3	1.54	0.87
1:A:91:GLY:O	1:A:95:ASP:OD1	1.93	0.86
1:B:257:ASN:HD22	1:B:259:ASP:H	1.22	0.85
1:B:58:ASP:HB3	1:B:156:LEU:HB3	1.56	0.85
1:A:205:GLN:HE22	1:A:207:ASP:N	1.75	0.84
1:B:257:ASN:HD21	1:B:259:ASP:HB2	1.45	0.81
1:A:3:ARG:HH21	1:A:53:GLU:HG3	1.44	0.81
1:B:180:LEU:HD23	1:B:181:ASN:N	1.96	0.80
1:A:32:VAL:HB	1:A:33:PRO:CD	2.12	0.79
1:A:77:HIS:NE2	1:B:86:ASN:N	2.30	0.78
1:A:75:VAL:HG23	1:A:77:HIS:HB2	1.66	0.78
1:B:182:GLU:HA	1:B:185:LYS:HD3	1.68	0.76
1:A:257:ASN:HD22	1:A:259:ASP:N	1.83	0.76
1:A:175:ALA:O	1:A:176:SER:HB2	1.84	0.76
1:A:257:ASN:HD22	1:A:259:ASP:H	1.31	0.75
1:B:24:TYR:OH	1:B:32:VAL:HG22	1.86	0.75
1:A:3:ARG:NH2	1:A:53:GLU:HG3	2.01	0.74
1:A:9:ARG:HG3	1:A:13:LEU:HD22	1.68	0.74
1:B:203:LEU:HD21	1:B:216:LEU:HD13	1.69	0.73
1:B:257:ASN:ND2	1:B:259:ASP:HB2	2.04	0.73
1:A:312:ALA:O	1:A:313:GLU:C	2.27	0.72
1:A:32:VAL:CB	1:A:33:PRO:HD2	2.17	0.71
1:B:132:GLY:H	1:B:145:THR:HG22	1.55	0.71
1:B:143:ASP:OD1	1:B:145:THR:HG23	1.89	0.71
1:B:32:VAL:HG12	1:B:32:VAL:O	1.91	0.70
1:B:207:ASP:HB3	1:B:210:VAL:HG13	1.74	0.70
1:B:103:GLU:HG3	2:B:595:HOH:O	1.91	0.70
1:A:77:HIS:CD2	1:B:86:ASN:H	2.10	0.69
1:A:132:GLY:H	1:A:145:THR:HG22	1.58	0.68
1:A:165:GLU:OE2	1:A:167:ARG:NH1	2.26	0.68
1:B:257:ASN:HD22	1:B:259:ASP:N	1.92	0.68
1:A:97:ASP:OD1	1:A:97:ASP:O	2.11	0.68
1:B:69:LEU:HD23	1:B:208:PRO:HD3	1.76	0.67
1:B:298:THR:HG23	1:B:303:ARG:NH1	2.09	0.67
1:B:298:THR:O	1:B:299:ALA:HB3	1.95	0.67
1:B:90:GLU:OE2	1:B:94:ARG:NH1	2.26	0.67
1:A:131:GLN:HE22	1:B:86:ASN:ND2	1.93	0.67
1:B:123:ARG:NH2	1:B:125:GLU:OE2	2.24	0.67
1:A:7:GLU:HG2	1:A:54:LEU:CD2	2.25	0.67
1:A:238:LEU:HD13	1:A:252:ARG:HD2	1.77	0.66
1:A:98:ARG:HD3	2:A:630:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:HD11	1:B:192:PHE:CE2	2.30	0.66
1:B:32:VAL:O	1:B:33:PRO:C	2.29	0.66
1:B:185:LYS:HG2	1:B:186:ALA:N	2.10	0.66
1:A:181:ASN:HA	1:A:184:ARG:HG3	1.78	0.66
1:B:32:VAL:O	1:B:32:VAL:CG1	2.45	0.65
1:B:77:HIS:O	1:B:78:ARG:CB	2.42	0.65
1:B:90:GLU:HG3	1:B:262:ILE:HD13	1.78	0.65
1:B:93:LEU:HD23	1:B:262:ILE:HG12	1.77	0.65
1:A:7:GLU:HG2	1:A:54:LEU:HD21	1.79	0.64
1:A:249:ASN:HD22	1:A:251:GLU:H	1.45	0.64
1:B:180:LEU:HD21	1:B:192:PHE:HD2	1.62	0.63
1:B:123:ARG:HD3	2:B:447:HOH:O	1.98	0.63
1:B:33:PRO:HB2	1:B:36:GLU:HG2	1.80	0.63
1:A:257:ASN:ND2	1:A:259:ASP:H	1.96	0.63
1:A:190:GLU:O	1:A:191:LEU:HB2	1.99	0.63
1:A:136:GLY:HA3	1:A:140:THR:O	1.98	0.63
1:A:194:ASN:HD21	1:A:196:ARG:HB3	1.64	0.63
1:A:249:ASN:ND2	1:A:251:GLU:H	1.95	0.62
1:B:180:LEU:HD12	1:B:214:ARG:HD2	1.80	0.62
1:B:31:SER:N	1:B:32:VAL:HG23	2.13	0.62
1:A:184:ARG:NH2	1:A:190:GLU:HB2	2.14	0.62
1:A:257:ASN:HD21	1:A:259:ASP:HB2	1.65	0.62
1:A:114:ALA:HB2	1:A:283:VAL:HG23	1.83	0.61
1:A:2:ASP:OD2	1:A:50:GLN:NE2	2.33	0.61
1:B:59:SER:OG	1:B:61:THR:HB	2.00	0.61
1:A:132:GLY:H	1:A:145:THR:CG2	2.13	0.61
1:B:132:GLY:H	1:B:145:THR:CG2	2.13	0.61
1:B:48:GLU:OE1	1:B:61:THR:HG21	2.00	0.61
1:B:73:ARG:O	1:B:74:LYS:HB2	2.00	0.61
1:B:251:GLU:HG3	1:B:268:TRP:CZ2	2.36	0.60
1:A:70:GLU:HB2	1:B:204:ARG:HH21	1.64	0.60
1:B:7:GLU:HG2	1:B:54:LEU:HD22	1.84	0.60
1:B:143:ASP:OD1	1:B:145:THR:CG2	2.50	0.60
1:A:268:TRP:O	1:A:272:ARG:HB3	2.02	0.60
1:A:132:GLY:HA3	1:A:148:LEU:HD12	1.83	0.59
1:B:220:VAL:CG1	1:B:241:LEU:HD13	2.32	0.59
1:A:131:GLN:HE22	1:B:86:ASN:HD22	1.49	0.59
1:B:24:TYR:CE1	1:B:32:VAL:HG21	2.37	0.59
1:A:74:LYS:HG2	1:B:137:ASP:HB3	1.84	0.58
1:B:299:ALA:O	1:B:300:LYS:HD3	2.04	0.58
1:A:154:LEU:HD12	1:A:155:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:PRO:HB3	1:B:32:VAL:CB	2.34	0.58
1:A:267:GLU:O	1:A:271:LYS:HB2	2.04	0.58
1:A:125:GLU:OE2	1:B:92:ASP:OD2	2.22	0.57
1:A:60:PRO:O	1:A:63:ARG:HG2	2.04	0.57
1:A:32:VAL:O	1:A:33:PRO:C	2.43	0.57
1:B:227:GLU:CD	1:B:293:ARG:HH11	2.08	0.57
1:B:131:GLN:HA	1:B:145:THR:HG21	1.85	0.57
1:B:217:ASP:OD2	1:B:247:LYS:NZ	2.37	0.57
1:B:114:ALA:HB2	1:B:283:VAL:HG23	1.87	0.57
1:B:180:LEU:HD12	1:B:214:ARG:CD	2.35	0.56
1:A:257:ASN:ND2	1:A:259:ASP:N	2.51	0.56
1:A:184:ARG:HB2	1:A:191:LEU:HD12	1.86	0.56
1:A:235:SER:OG	1:A:287:ASP:OD2	2.19	0.56
1:A:58:ASP:HB3	1:A:156:LEU:CB	2.30	0.56
1:A:207:ASP:HB3	1:A:210:VAL:HG13	1.88	0.56
1:A:78:ARG:HD2	1:A:123:ARG:CZ	2.36	0.56
1:B:50:GLN:HG3	1:B:51:TYR:CE1	2.41	0.55
1:B:69:LEU:CD2	1:B:208:PRO:HD3	2.35	0.55
1:B:171:PHE:CZ	1:B:217:ASP:HB3	2.41	0.55
1:A:258:ILE:HD12	1:A:261:VAL:HB	1.88	0.55
1:A:134:THR:HG23	1:A:144:ILE:HD13	1.87	0.55
1:B:271:LYS:O	1:B:274:GLN:HG2	2.06	0.55
1:B:5:GLN:HG2	2:B:495:HOH:O	2.07	0.54
1:B:215:GLN:N	1:B:215:GLN:HE21	2.05	0.54
1:A:95:ASP:OD1	1:A:95:ASP:N	2.41	0.54
1:B:55:LYS:HE3	1:B:61:THR:CG2	2.38	0.54
1:B:55:LYS:HG2	1:B:55:LYS:O	2.08	0.54
1:A:74:LYS:NZ	1:B:137:ASP:HB2	2.23	0.54
1:B:174:LYS:O	1:B:177:PHE:HB3	2.07	0.54
1:A:176:SER:HA	1:A:179:ARG:HH11	1.73	0.53
1:B:257:ASN:ND2	1:B:259:ASP:H	1.99	0.53
1:B:30:PRO:O	1:B:31:SER:HB2	2.08	0.53
1:B:298:THR:HG23	1:B:303:ARG:CZ	2.39	0.52
1:A:194:ASN:HD21	1:A:196:ARG:CB	2.22	0.52
1:A:131:GLN:NE2	1:B:86:ASN:HD22	2.07	0.52
1:A:34:ASP:O	1:A:37:TYR:HB3	2.10	0.52
1:B:63:ARG:NH1	1:B:156:LEU:HD13	2.23	0.52
1:B:66:GLY:N	1:B:208:PRO:HB2	2.17	0.52
1:A:143:ASP:HB3	2:A:576:HOH:O	2.08	0.52
1:B:128:TYR:CE2	1:B:157:ARG:HD2	2.45	0.52
1:B:160:GLU:HA	1:B:160:GLU:OE1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:HD23	1:B:181:ASN:H	1.72	0.51
1:A:44:LEU:HD22	1:A:48:GLU:OE2	2.09	0.51
1:A:32:VAL:O	1:A:34:ASP:N	2.43	0.51
1:B:24:TYR:HE1	1:B:32:VAL:CG1	2.23	0.51
1:B:16:LEU:HB3	1:B:20:TYR:CE2	2.46	0.51
1:A:69:LEU:O	1:A:206:LEU:HB3	2.11	0.51
1:B:181:ASN:OD1	1:B:191:LEU:HG	2.10	0.51
1:A:257:ASN:ND2	1:A:259:ASP:HB2	2.26	0.51
1:A:97:ASP:OD1	1:A:101:ARG:HG3	2.11	0.50
1:B:13:LEU:HD12	1:B:40:LEU:HD22	1.92	0.50
1:A:30:PRO:HB3	1:A:32:VAL:CG1	2.42	0.49
1:B:298:THR:O	1:B:299:ALA:CB	2.57	0.49
1:B:98:ARG:O	1:B:102:GLN:HG3	2.11	0.49
1:B:111:CYS:HB3	1:B:264:PHE:CE1	2.47	0.49
1:A:15:GLU:HG2	1:A:16:LEU:N	2.26	0.49
1:A:144:ILE:HG13	1:A:148:LEU:HG	1.94	0.49
1:B:24:TYR:HE1	1:B:32:VAL:HG11	1.76	0.49
1:A:194:ASN:ND2	1:A:196:ARG:N	2.61	0.49
1:A:142:GLU:OE2	1:B:137:ASP:OD2	2.30	0.49
1:A:128:TYR:OH	1:A:157:ARG:NH1	2.45	0.49
1:A:56:THR:HG22	1:A:58:ASP:H	1.77	0.49
1:B:185:LYS:HG2	1:B:186:ALA:H	1.78	0.49
1:B:90:GLU:HG3	1:B:262:ILE:CD1	2.43	0.49
1:B:21:GLY:O	1:B:25:TYR:HB2	2.13	0.48
1:B:1:MET:O	1:B:2:ASP:C	2.51	0.48
1:B:23:GLU:HB3	1:B:29:ARG:O	2.12	0.48
1:A:70:GLU:HB2	1:B:204:ARG:NH2	2.27	0.48
1:B:182:GLU:CA	1:B:185:LYS:HD3	2.42	0.48
1:A:133:ALA:HA	1:A:142:GLU:O	2.13	0.48
1:B:203:LEU:CD2	1:B:216:LEU:HD13	2.41	0.48
1:A:190:GLU:O	1:A:191:LEU:CB	2.61	0.48
1:B:269:HIS:HB2	1:B:310:PHE:CE1	2.48	0.48
1:B:31:SER:H	1:B:32:VAL:HG23	1.79	0.48
1:A:58:ASP:CB	1:A:156:LEU:HB3	2.32	0.48
1:A:115:ILE:HD13	1:A:219:PHE:HD2	1.78	0.48
1:A:295:LEU:O	1:A:303:ARG:HD2	2.14	0.48
1:B:30:PRO:HB3	1:B:32:VAL:CG2	2.44	0.48
1:A:112:GLU:O	1:A:282:ILE:HG23	2.13	0.48
1:A:48:GLU:OE1	1:A:61:THR:HG21	2.13	0.48
1:B:182:GLU:O	1:B:185:LYS:N	2.46	0.47
1:A:98:ARG:O	1:A:102:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:C	1:A:164:LEU:HD12	2.35	0.47
1:A:30:PRO:HB3	1:A:32:VAL:HG13	1.95	0.47
1:B:281:GLY:HA3	1:B:308:TYR:O	2.14	0.47
1:A:32:VAL:O	1:A:34:ASP:HB2	2.14	0.47
1:A:143:ASP:OD1	1:A:145:THR:HG23	2.14	0.47
1:A:30:PRO:HB2	2:A:640:HOH:O	2.14	0.47
1:A:77:HIS:O	1:A:78:ARG:HB2	2.15	0.47
1:B:17:LEU:HD21	1:B:40:LEU:HB2	1.96	0.47
1:A:293:ARG:HH11	1:A:293:ARG:HG3	1.79	0.47
1:A:131:GLN:HA	1:A:145:THR:HG21	1.96	0.47
1:A:91:GLY:O	1:A:95:ASP:CG	2.51	0.47
1:A:9:ARG:HG3	1:A:13:LEU:CD2	2.41	0.47
1:A:194:ASN:ND2	1:A:196:ARG:H	2.13	0.47
1:B:124:TYR:CE2	1:B:158:LEU:HD13	2.50	0.47
1:A:292:GLN:HG2	1:A:304:TRP:CD2	2.50	0.47
1:A:24:TYR:O	1:A:28:ASP:HA	2.15	0.47
1:B:145:THR:O	1:B:149:LYS:HG3	2.16	0.47
1:B:55:LYS:HE3	1:B:61:THR:HG22	1.97	0.47
1:A:292:GLN:HG2	1:A:304:TRP:CG	2.49	0.46
1:A:9:ARG:O	1:A:13:LEU:HB2	2.15	0.46
1:A:205:GLN:HE22	1:A:207:ASP:CA	2.28	0.46
1:B:152:ARG:HD2	2:B:524:HOH:O	2.15	0.46
1:A:104:VAL:HG21	1:A:291:GLN:HB3	1.96	0.46
1:B:143:ASP:OD1	1:B:143:ASP:C	2.55	0.46
1:B:251:GLU:HG3	1:B:268:TRP:CH2	2.50	0.46
1:A:293:ARG:HA	1:A:293:ARG:HD3	1.81	0.46
1:B:268:TRP:O	1:B:272:ARG:HB3	2.15	0.46
1:B:29:ARG:O	1:B:29:ARG:HD2	2.16	0.46
1:B:182:GLU:O	1:B:183:GLU:C	2.54	0.45
1:B:73:ARG:HH21	1:B:74:LYS:HD3	1.81	0.45
1:B:39:ARG:O	1:B:43:GLU:HG3	2.15	0.45
1:B:194:ASN:HD21	1:B:196:ARG:HB3	1.81	0.45
1:B:1:MET:CG	1:B:5:GLN:HB2	2.46	0.45
1:B:7:GLU:HG2	1:B:54:LEU:CD2	2.45	0.45
1:B:195:PRO:HB2	2:B:637:HOH:O	2.15	0.45
1:B:215:GLN:HE21	1:B:215:GLN:CA	2.29	0.45
1:B:205:GLN:HE22	1:B:207:ASP:H	1.65	0.45
1:B:205:GLN:NE2	1:B:207:ASP:H	2.15	0.45
1:A:239:ASP:OD1	1:A:252:ARG:NH2	2.50	0.45
1:B:74:LYS:HD2	1:B:74:LYS:HA	1.68	0.45
1:B:252:ARG:O	1:B:252:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:TYR:CZ	1:B:32:VAL:CG2	3.00	0.44
1:A:56:THR:HG22	1:A:58:ASP:N	2.31	0.44
1:B:3:ARG:HH11	1:B:3:ARG:HG2	1.82	0.44
1:B:30:PRO:HB3	1:B:32:VAL:HB	1.99	0.44
1:B:32:VAL:O	1:B:34:ASP:N	2.50	0.44
1:B:95:ASP:OD1	1:B:98:ARG:NH1	2.50	0.44
1:B:180:LEU:HD11	1:B:192:PHE:HE2	1.79	0.44
1:A:143:ASP:OD1	1:A:143:ASP:C	2.55	0.44
1:A:195:PRO:O	1:A:196:ARG:C	2.55	0.44
1:A:7:GLU:HG2	1:A:54:LEU:HD22	2.00	0.44
1:A:238:LEU:CD1	1:A:252:ARG:HD2	2.47	0.44
1:A:59:SER:OG	1:A:61:THR:HB	2.18	0.44
1:A:35:ALA:O	1:A:36:GLU:C	2.56	0.44
1:A:2:ASP:O	1:A:6:ALA:N	2.45	0.44
1:A:98:ARG:HE	1:A:98:ARG:HB3	1.51	0.44
1:B:57:SER:O	1:B:62:GLN:HG3	2.17	0.44
1:B:214:ARG:O	1:B:215:GLN:HB2	2.17	0.43
1:B:215:GLN:HE21	1:B:215:GLN:H	1.65	0.43
1:A:132:GLY:HA3	1:A:148:LEU:CD1	2.47	0.43
1:A:249:ASN:HD22	1:A:249:ASN:C	2.21	0.43
1:A:258:ILE:HD12	1:A:258:ILE:HA	1.78	0.43
1:B:303:ARG:HD3	1:B:303:ARG:HH11	1.41	0.43
1:B:187:ARG:HD2	1:B:190:GLU:OE2	2.19	0.43
1:B:122:VAL:HG23	1:B:122:VAL:O	2.18	0.43
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.18	0.43
1:A:143:ASP:OD1	1:A:145:THR:CG2	2.66	0.43
1:A:233:SER:HB2	2:A:482:HOH:O	2.18	0.43
1:A:124:TYR:O	1:A:163:SER:HA	2.18	0.43
1:A:32:VAL:CB	1:A:33:PRO:CD	2.82	0.43
1:B:2:ASP:O	1:B:3:ARG:C	2.57	0.43
1:B:24:TYR:OH	1:B:32:VAL:CG2	2.62	0.42
1:B:262:ILE:O	1:B:263:ALA:C	2.56	0.42
1:A:74:LYS:HZ1	1:B:137:ASP:HB2	1.83	0.42
1:B:289:PHE:HB3	1:B:293:ARG:NH1	2.33	0.42
1:A:24:TYR:HD1	1:A:29:ARG:O	2.01	0.42
1:A:89:GLY:O	1:A:90:GLU:C	2.57	0.42
1:A:178:LEU:O	1:A:179:ARG:C	2.57	0.42
1:A:63:ARG:CZ	1:A:156:LEU:HG	2.50	0.42
1:B:79:VAL:HA	1:B:80:PRO:HD2	1.85	0.42
1:B:63:ARG:CZ	1:B:156:LEU:HD13	2.49	0.42
1:B:24:TYR:CZ	1:B:32:VAL:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:HG21	1:A:246:PHE:CD1	2.54	0.42
1:A:57:SER:HA	1:A:62:GLN:NE2	2.35	0.42
1:A:214:ARG:HD3	1:A:214:ARG:HH11	1.59	0.42
1:B:31:SER:H	1:B:32:VAL:CG2	2.33	0.42
1:A:174:LYS:HB2	2:A:610:HOH:O	2.20	0.42
1:B:257:ASN:ND2	1:B:259:ASP:N	2.61	0.42
1:A:97:ASP:CG	1:A:109:TYR:OH	2.59	0.42
1:A:242:GLN:O	1:A:243:ALA:C	2.58	0.41
1:B:39:ARG:HA	1:B:42:GLN:NE2	2.35	0.41
1:B:180:LEU:CD1	1:B:214:ARG:HD2	2.49	0.41
1:B:24:TYR:CD1	1:B:30:PRO:HG3	2.55	0.41
1:A:154:LEU:HD12	1:A:155:PRO:CD	2.50	0.41
1:A:269:HIS:HB2	1:A:310:PHE:CE1	2.54	0.41
1:B:312:ALA:O	1:B:313:GLU:HB2	2.21	0.41
1:A:268:TRP:HB2	1:A:282:ILE:HD11	2.03	0.41
1:A:281:GLY:HA3	1:A:308:TYR:O	2.21	0.41
1:B:253:ARG:HD2	1:B:253:ARG:HH11	1.55	0.41
1:A:257:ASN:C	1:A:257:ASN:HD22	2.23	0.40
1:A:13:LEU:HD12	1:A:13:LEU:HA	1.91	0.40
1:B:94:ARG:HD2	1:B:94:ARG:HH11	1.71	0.40
1:A:72:PHE:O	1:B:137:ASP:OD1	2.38	0.40
1:A:308:TYR:HE1	1:A:310:PHE:CD1	2.39	0.40
1:A:21:GLY:O	1:A:25:TYR:HB2	2.20	0.40
1:A:79:VAL:HG12	1:A:167:ARG:HH22	1.85	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:36:GLU:N	1:B:31:SER:OG[7_455]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

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	306/318 (96%)	270 (88%)	24 (8%)	12 (4%)	4 12
1	B	307/318 (96%)	282 (92%)	15 (5%)	10 (3%)	5 16
All	All	613/636 (96%)	552 (90%)	39 (6%)	22 (4%)	4 14

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	31	SER
1	A	32	VAL
1	A	77	HIS
1	A	78	ARG
1	A	176	SER
1	B	2	ASP
1	B	30	PRO
1	B	31	SER
1	B	75	VAL
1	B	78	ARG
1	A	35	ALA
1	A	191	LEU
1	B	74	LYS
1	B	299	ALA
1	B	32	VAL
1	A	33	PRO
1	A	79	VAL
1	A	174	LYS
1	A	180	LEU
1	B	85	ALA
1	B	300	LYS

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	252/259 (97%)	214 (85%)	38 (15%)	3 10
1	B	253/259 (98%)	210 (83%)	43 (17%)	2 7
All	All	505/518 (98%)	424 (84%)	81 (16%)	3 9

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	13	LEU
1	A	15	GLU
1	A	30	PRO
1	A	39	ARG
1	A	47	ILE
1	A	64	ILE
1	A	70	GLU
1	A	75	VAL
1	A	77	HIS
1	A	83	SER
1	A	90	GLU
1	A	93	LEU
1	A	94	ARG
1	A	95	ASP
1	A	96	PHE
1	A	99	ARG
1	A	116	ASP
1	A	139	THR
1	A	145	THR
1	A	152	ARG
1	A	158	LEU
1	A	183	GLU
1	A	190	GLU
1	A	191	LEU
1	A	196	ARG
1	A	205	GLN
1	A	214	ARG
1	A	225	ASP
1	A	235	SER
1	A	249	ASN
1	A	253	ARG
1	A	257	ASN
1	A	266	SER
1	A	271	LYS

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Mol	Chain	Res	Type
1	A	272	ARG
1	A	275	LEU
1	A	293	ARG
1	B	2	ASP
1	B	3	ARG
1	B	8	ARG
1	B	13	LEU
1	B	15	GLU
1	B	29	ARG
1	B	30	PRO
1	B	39	ARG
1	B	57	SER
1	B	61	THR
1	B	63	ARG
1	B	74	LYS
1	B	77	HIS
1	B	79	VAL
1	B	82	MET
1	B	83	SER
1	B	84	LEU
1	B	93	LEU
1	B	97	ASP
1	B	99	ARG
1	B	103	GLU
1	B	137	ASP
1	B	140	THR
1	B	145	THR
1	B	152	ARG
1	B	156	LEU
1	B	158	LEU
1	B	180	LEU
1	B	184	ARG
1	B	185	LYS
1	B	191	LEU
1	B	205	GLN
1	B	209	LYS
1	B	210	VAL
1	B	215	GLN
1	B	225	ASP
1	B	249	ASN
1	B	251	GLU
1	B	257	ASN

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Mol	Chain	Res	Type
1	B	272	ARG
1	B	275	LEU
1	B	298	THR
1	B	309	LYS

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	5	GLN
1	A	42	GLN
1	A	194	ASN
1	A	205	GLN
1	A	249	ASN
1	A	257	ASN
1	A	291	GLN
1	B	42	GLN
1	B	50	GLN
1	B	86	ASN
1	B	194	ASN
1	B	205	GLN
1	B	215	GLN
1	B	249	ASN
1	B	257	ASN
1	B	291	GLN

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	310/318 (97%)	-0.09	18 (5%)	26	16	6, 49, 85, 97	0
1	B	311/318 (97%)	-0.23	16 (5%)	32	21	22, 39, 80, 90	0
All	All	621/636 (97%)	-0.16	34 (5%)	29	18	6, 43, 82, 97	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	SER	6.1
1	A	312	ALA	4.9
1	A	313	GLU	4.8
1	B	67	PRO	4.5
1	A	32	VAL	3.8
1	B	68	PRO	3.8
1	B	1	MET	3.6
1	A	30	PRO	3.6
1	B	187	ARG	3.3
1	B	190	GLU	3.2
1	B	78	ARG	3.2
1	A	33	PRO	3.1
1	A	4	GLN	3.1
1	B	312	ALA	3.1
1	A	29	ARG	3.1
1	B	33	PRO	2.9
1	A	190	GLU	2.7
1	A	77	HIS	2.6
1	A	185	LYS	2.6
1	B	30	PRO	2.6
1	B	24	TYR	2.5
1	B	69	LEU	2.5
1	B	75	VAL	2.5
1	A	34	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	300	LYS	2.4
1	B	76	ALA	2.4
1	A	299	ALA	2.4
1	A	187	ARG	2.3
1	A	79	VAL	2.3
1	A	297	ALA	2.1
1	B	77	HIS	2.1
1	A	78	ARG	2.1
1	B	71	ALA	2.0
1	B	28	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.