



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:02 PM UTC

PDB ID : 2NVW / pdb_00002nvw
Title : Crystal structure of transcriptional regulator Gal80p from *Kluyveromyces fragilis*
Authors : Thoden, J.B.; Sellick, C.A.; Reece, R.J.; Holden, H.M.
Deposited on : 2006-11-13
Resolution : 2.10 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

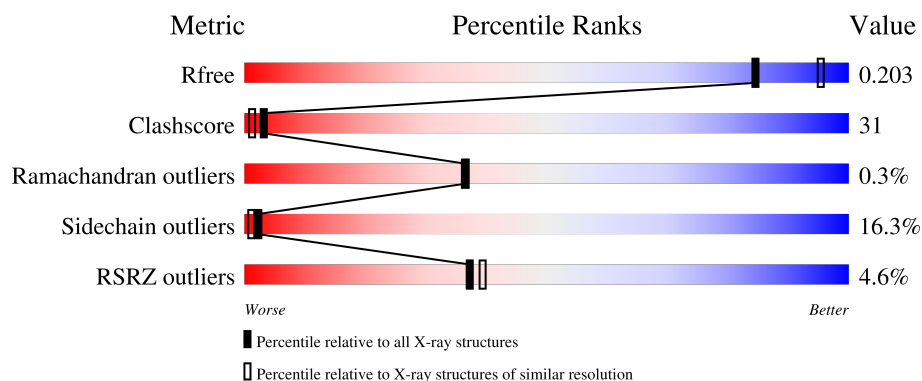
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	479	3% 37% 35% 12% • 14%
1	B	479	5% 32% 36% 14% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6895 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	1	0
			3310	2117	563	620	10			
1	B	405	Total	C	N	O	S	0	0	0
			3238	2072	547	609	10			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q06433
A	-20	GLY	-	cloning artifact	UNP Q06433
A	-19	SER	-	cloning artifact	UNP Q06433
A	-18	SER	-	cloning artifact	UNP Q06433
A	-17	HIS	-	expression tag	UNP Q06433
A	-16	HIS	-	expression tag	UNP Q06433
A	-15	HIS	-	expression tag	UNP Q06433
A	-14	HIS	-	expression tag	UNP Q06433
A	-13	HIS	-	expression tag	UNP Q06433
A	-12	HIS	-	expression tag	UNP Q06433
A	-11	SER	-	cloning artifact	UNP Q06433
A	-10	SER	-	cloning artifact	UNP Q06433
A	-9	GLU	-	cloning artifact	UNP Q06433
A	-8	ASN	-	cloning artifact	UNP Q06433
A	-7	LEU	-	cloning artifact	UNP Q06433
A	-6	TYR	-	cloning artifact	UNP Q06433
A	-5	PHE	-	cloning artifact	UNP Q06433
A	-4	GLN	-	cloning artifact	UNP Q06433
A	-3	GLY	-	cloning artifact	UNP Q06433
A	-2	HIS	-	cloning artifact	UNP Q06433
A	-1	MET	-	cloning artifact	UNP Q06433
A	0	LEU	-	cloning artifact	UNP Q06433
A	1	ALA	-	cloning artifact	UNP Q06433
B	-21	MET	-	initiating methionine	UNP Q06433
B	-20	GLY	-	cloning artifact	UNP Q06433

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	cloning artifact	UNP Q06433
B	-18	SER	-	cloning artifact	UNP Q06433
B	-17	HIS	-	expression tag	UNP Q06433
B	-16	HIS	-	expression tag	UNP Q06433
B	-15	HIS	-	expression tag	UNP Q06433
B	-14	HIS	-	expression tag	UNP Q06433
B	-13	HIS	-	expression tag	UNP Q06433
B	-12	HIS	-	expression tag	UNP Q06433
B	-11	SER	-	cloning artifact	UNP Q06433
B	-10	SER	-	cloning artifact	UNP Q06433
B	-9	GLU	-	cloning artifact	UNP Q06433
B	-8	ASN	-	cloning artifact	UNP Q06433
B	-7	LEU	-	cloning artifact	UNP Q06433
B	-6	TYR	-	cloning artifact	UNP Q06433
B	-5	PHE	-	cloning artifact	UNP Q06433
B	-4	GLN	-	cloning artifact	UNP Q06433
B	-3	GLY	-	cloning artifact	UNP Q06433
B	-2	HIS	-	cloning artifact	UNP Q06433
B	-1	MET	-	cloning artifact	UNP Q06433
B	0	LEU	-	cloning artifact	UNP Q06433
B	1	ALA	-	cloning artifact	UNP Q06433

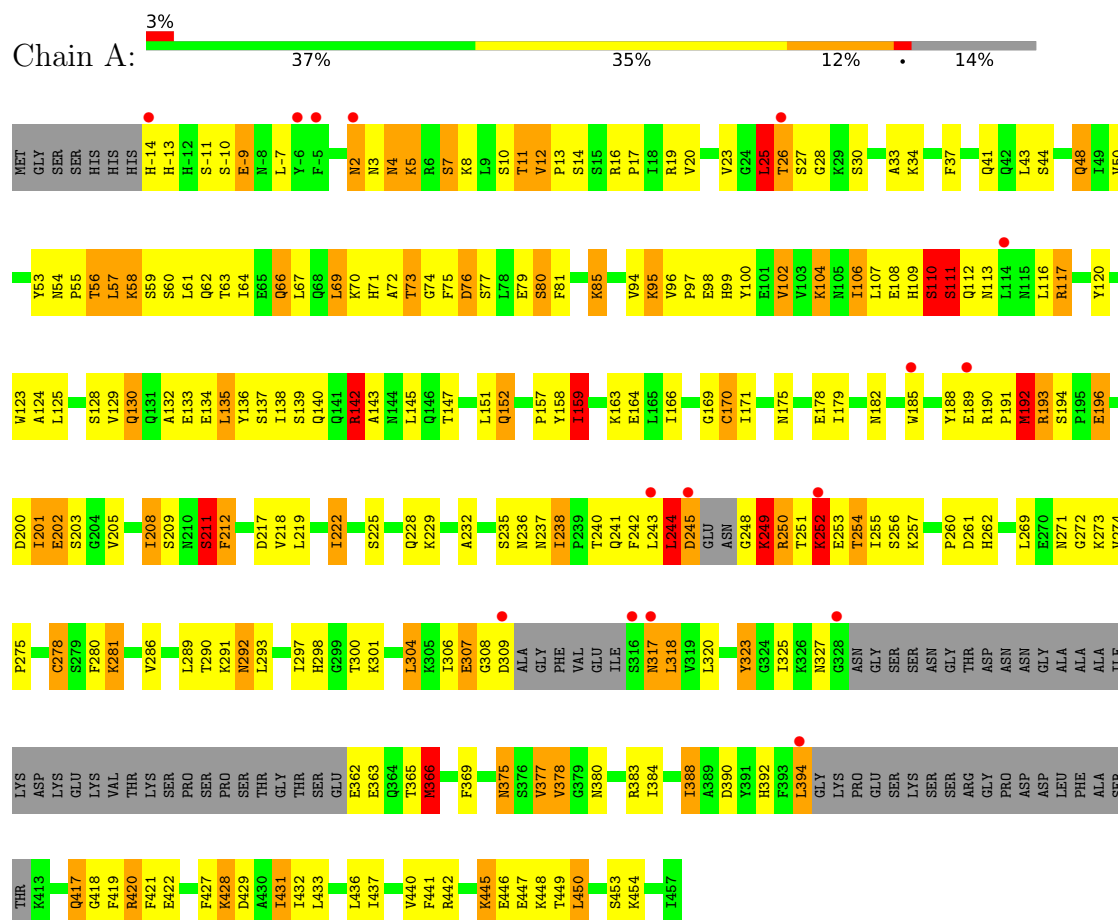
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	203	Total 203	O 203	0	0
2	B	144	Total 144	O 144	0	0

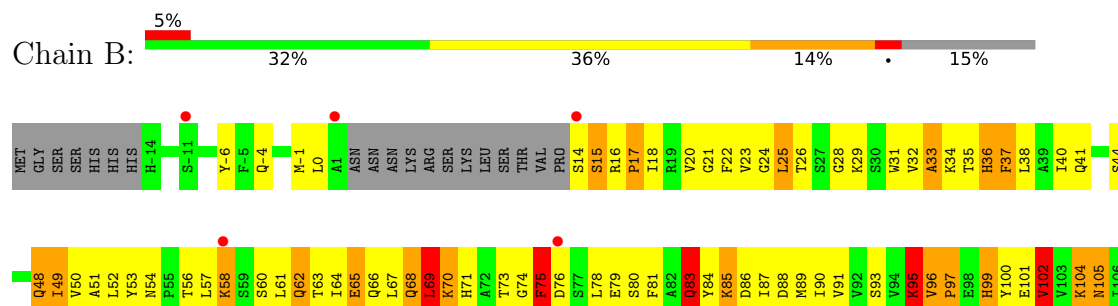
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Galactose/lactose metabolism regulatory protein GAL80



- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.20Å 137.10Å 72.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.10) 97.8 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.08Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.195 , 0.245 0.199 , 0.203	Depositor DCC
R_{free} test set	6589 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 112.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6895	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.97	4/3381 (0.1%)	1.95	100/4560 (2.2%)
1	B	0.96	4/3302 (0.1%)	1.97	122/4453 (2.7%)
All	All	0.96	8/6683 (0.1%)	1.96	222/9013 (2.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	VAL	CA-CB	-10.06	1.49	1.54
1	B	233	MET	SD-CE	6.67	1.96	1.79
1	A	306	ILE	CA-CB	-5.74	1.47	1.54
1	B	381	ILE	CA-CB	5.64	1.61	1.54
1	B	238	ILE	CA-CB	-5.54	1.47	1.54
1	B	297	ILE	CA-CB	-5.50	1.47	1.54
1	A	192	MET	SD-CE	5.41	1.93	1.79
1	A	366	MET	SD-CE	-5.24	1.66	1.79

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	LYS	N-CA-C	-13.20	96.56	113.72
1	B	452	VAL	N-CA-C	-12.07	99.08	111.88
1	A	72	ALA	N-CA-C	11.55	128.63	109.46
1	A	222	ILE	CB-CA-C	-10.70	97.70	112.14
1	B	215	THR	N-CA-C	10.51	122.31	111.07
1	A	250	ARG	N-CA-C	9.74	123.19	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	THR	N-CA-C	9.59	124.03	111.75
1	A	208	ILE	N-CA-C	9.47	119.44	110.53
1	B	186	TYR	N-CA-C	9.33	124.58	112.26
1	B	151	LEU	N-CA-C	-8.89	96.49	109.11
1	B	37	PHE	N-CA-C	8.86	120.55	111.07
1	B	309	ASP	N-CA-C	8.83	124.22	108.24
1	A	203	SER	N-CA-C	8.80	121.83	111.71
1	B	381	ILE	N-CA-C	-8.76	101.69	110.62
1	A	170	CYS	N-CA-C	8.73	123.03	112.38
1	A	244	LEU	N-CA-C	8.53	122.23	108.76
1	A	255	ILE	N-CA-C	8.39	120.87	108.45
1	A	238	ILE	CA-C-N	8.32	128.05	119.56
1	A	238	ILE	C-N-CA	8.32	128.05	119.56
1	A	237	ASN	N-CA-C	-8.31	102.86	113.16
1	A	254	THR	N-CA-C	8.14	122.89	109.95
1	B	447	GLU	CB-CA-C	-8.13	99.94	111.80
1	B	129	VAL	CB-CA-C	-8.05	101.27	112.14
1	A	421	PHE	N-CA-C	-8.05	101.79	111.69
1	B	18	ILE	N-CA-C	-8.04	98.28	108.89
1	B	104	LYS	N-CA-C	-7.95	102.56	111.07
1	A	274	VAL	N-CA-C	7.93	115.45	108.63
1	A	363	GLU	N-CA-C	-7.92	97.14	109.25
1	A	135	LEU	N-CA-C	-7.82	102.76	111.28
1	B	70	LYS	N-CA-C	7.81	119.79	111.28
1	A	249	LYS	N-CA-C	7.79	122.19	109.72
1	B	453	SER	CA-C-N	-7.79	111.65	122.87
1	B	453	SER	C-N-CA	-7.79	111.65	122.87
1	B	449	THR	N-CA-C	-7.65	96.25	108.73
1	A	58	LYS	N-CA-C	-7.64	101.94	111.11
1	A	20	VAL	N-CA-C	7.62	119.58	108.53
1	A	297	ILE	N-CA-C	7.60	118.82	107.80
1	A	5	LYS	N-CA-C	7.53	120.44	111.33
1	B	143	ALA	N-CA-C	7.46	120.36	111.33
1	A	112	GLN	CB-CA-C	7.37	122.27	109.15
1	B	76	ASP	N-CA-CB	-7.32	99.01	110.44
1	B	142	ARG	CB-CA-C	7.30	123.95	111.68
1	B	140	GLN	CA-C-N	7.18	129.91	120.28
1	B	140	GLN	C-N-CA	7.18	129.91	120.28
1	B	138	ILE	CB-CA-C	-7.17	102.33	112.22
1	A	292	ASN	N-CA-C	7.16	120.13	111.82
1	A	453	SER	CA-C-N	-7.10	110.79	122.08
1	A	453	SER	C-N-CA	-7.10	110.79	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	HIS	N-CA-C	7.08	120.03	111.40
1	B	62	GLN	N-CA-C	-7.04	103.30	110.97
1	B	49	ILE	CB-CA-C	-7.03	102.46	110.96
1	B	97	PRO	N-CA-C	-7.01	103.31	113.75
1	A	25	LEU	CA-C-N	6.95	130.45	120.79
1	A	25	LEU	C-N-CA	6.95	130.45	120.79
1	A	112	GLN	N-CA-CB	6.92	121.05	110.81
1	B	83	GLN	N-CA-C	6.91	121.73	113.16
1	B	33	ALA	N-CA-C	-6.87	103.72	111.07
1	A	375	ASN	N-CA-C	-6.87	97.35	108.41
1	B	69	LEU	N-CA-C	6.87	119.47	108.41
1	A	85	LYS	N-CA-C	6.85	120.89	112.54
1	B	36	HIS	N-CA-C	6.81	119.29	111.11
1	B	209	SER	CA-C-N	-6.79	112.37	122.56
1	B	209	SER	C-N-CA	-6.79	112.37	122.56
1	B	286	VAL	N-CA-C	6.78	117.87	110.21
1	A	417	GLN	N-CA-C	-6.78	104.02	112.90
1	B	194	SER	N-CA-C	-6.77	99.92	110.14
1	B	197	TYR	N-CA-C	6.75	119.47	111.71
1	B	372	ARG	CA-C-N	-6.67	108.79	121.54
1	B	372	ARG	C-N-CA	-6.67	108.79	121.54
1	A	95	LYS	CB-CA-C	-6.65	99.11	109.61
1	A	378	VAL	CB-CA-C	-6.63	103.59	111.94
1	A	110	SER	N-CA-C	-6.60	105.21	113.20
1	B	25	LEU	CA-C-N	6.52	129.90	120.38
1	B	25	LEU	C-N-CA	6.52	129.90	120.38
1	B	142	ARG	N-CA-C	6.50	120.21	107.98
1	B	258	THR	N-CA-CB	-6.47	100.61	110.12
1	A	317	ASN	CB-CA-C	-6.44	102.62	111.95
1	B	319	VAL	N-CA-C	-6.41	99.88	108.35
1	B	376	SER	N-CA-C	6.41	117.93	111.07
1	A	43	LEU	CA-C-N	6.38	129.11	120.38
1	A	43	LEU	C-N-CA	6.38	129.11	120.38
1	B	219	LEU	CA-CB-CG	-6.36	94.06	116.30
1	B	44	SER	N-CA-C	6.34	119.86	111.75
1	A	142	ARG	CA-CB-CG	-6.33	101.45	114.10
1	B	416	LYS	N-CA-CB	-6.30	101.76	111.46
1	B	23	VAL	N-CA-C	-6.30	99.29	108.11
1	A	185	TRP	CB-CA-C	-6.28	98.73	109.65
1	B	65	GLU	CA-CB-CG	6.27	126.63	114.10
1	A	306	ILE	N-CA-C	-6.26	99.35	108.11
1	A	307	GLU	N-CA-CB	-6.24	99.92	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	LYS	CA-C-N	6.22	128.61	120.28
1	B	257	LYS	C-N-CA	6.22	128.61	120.28
1	B	102	VAL	CA-C-N	-6.21	112.73	120.56
1	B	102	VAL	C-N-CA	-6.21	112.73	120.56
1	B	65	GLU	N-CA-C	-6.17	103.28	111.24
1	A	378	VAL	N-CA-C	-6.16	105.05	111.58
1	A	-14	HIS	N-CA-C	6.13	128.16	111.00
1	A	450	LEU	N-CA-C	6.13	119.69	109.95
1	B	96	VAL	O-C-N	6.13	124.34	120.42
1	B	391	TYR	N-CA-C	-6.12	104.53	111.14
1	B	-4	GLN	N-CA-C	-6.10	105.70	113.02
1	A	111	SER	N-CA-C	6.09	123.76	110.80
1	B	388	ILE	N-CA-C	-6.06	104.83	110.53
1	B	364	GLN	N-CA-C	6.05	119.43	110.48
1	A	377	VAL	N-CA-C	6.01	116.68	110.36
1	B	377	VAL	CB-CA-C	-6.01	104.30	111.81
1	B	222	ILE	CA-CB-CG2	6.00	120.69	110.50
1	A	151	LEU	N-CA-C	-5.97	96.98	107.73
1	A	164	GLU	CB-CA-C	-5.96	101.53	110.88
1	B	429	ASP	N-CA-C	-5.95	104.79	111.28
1	A	327	ASN	N-CA-C	5.92	118.21	109.69
1	A	130	GLN	N-CA-C	-5.91	104.76	111.14
1	A	81	PHE	N-CA-C	-5.91	104.02	111.11
1	A	318	LEU	N-CA-C	5.90	119.67	110.17
1	B	454	LYS	N-CA-C	5.90	117.62	109.54
1	B	-4	GLN	CA-C-O	5.89	126.56	119.43
1	A	102	VAL	N-CA-C	5.89	116.35	110.23
1	A	4	ASN	CA-C-N	5.88	128.44	120.38
1	A	4	ASN	C-N-CA	5.88	128.44	120.38
1	B	379	GLY	N-CA-C	5.87	119.77	112.73
1	A	-7	LEU	N-CA-C	5.85	118.13	111.11
1	A	4	ASN	N-CA-C	5.85	117.73	108.67
1	A	298	HIS	CA-C-N	-5.84	116.97	122.17
1	A	298	HIS	C-N-CA	-5.84	116.97	122.17
1	A	-10	SER	N-CA-C	-5.83	104.93	111.28
1	B	316	SER	CA-C-N	-5.79	114.38	123.13
1	B	316	SER	C-N-CA	-5.79	114.38	123.13
1	B	229	LYS	CB-CA-C	-5.79	96.70	109.56
1	A	99	HIS	N-CA-C	5.79	118.08	111.02
1	B	65	GLU	N-CA-CB	-5.78	101.57	110.07
1	B	183	GLY	N-CA-C	5.76	122.45	115.31
1	A	159	ILE	CB-CA-C	-5.74	104.30	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	THR	N-CA-C	-5.72	99.33	109.06
1	B	258	THR	CA-C-O	5.69	126.58	120.55
1	B	199	TYR	N-CA-C	5.67	120.19	113.16
1	B	424	PHE	CA-C-N	-5.67	114.13	120.14
1	B	424	PHE	C-N-CA	-5.67	114.13	120.14
1	A	158	TYR	N-CA-C	-5.66	105.10	112.23
1	A	274	VAL	CB-CA-C	-5.61	105.72	110.94
1	B	20	VAL	N-CA-C	5.61	117.42	108.89
1	A	11	THR	N-CA-C	5.61	118.71	109.85
1	A	125	LEU	N-CA-C	-5.58	105.11	111.07
1	B	200	ASP	N-CA-C	5.57	118.32	109.24
1	B	141	GLN	N-CA-C	-5.56	105.22	111.28
1	B	394	LEU	N-CA-C	5.56	120.17	112.45
1	A	17	PRO	CB-CA-C	-5.55	103.72	110.98
1	B	68	GLN	CB-CA-C	-5.54	103.55	112.09
1	A	388	ILE	N-CA-C	-5.53	105.13	110.72
1	B	393	PHE	N-CA-C	5.53	117.11	111.14
1	A	323	TYR	N-CA-C	-5.52	99.09	108.26
1	B	435	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	A	420	ARG	CG-CD-NE	-5.51	99.89	112.00
1	B	96	VAL	N-CA-C	5.50	119.55	112.67
1	B	214	HIS	N-CA-C	-5.49	105.30	111.28
1	B	304	LEU	CB-CG-CD1	-5.48	94.25	110.70
1	A	117	ARG	N-CA-CB	-5.47	103.62	110.90
1	A	317	ASN	N-CA-C	5.47	119.22	107.67
1	A	450	LEU	CA-C-N	-5.45	114.50	122.19
1	A	450	LEU	C-N-CA	-5.45	114.50	122.19
1	B	415	ASP	N-CA-C	5.45	122.42	110.80
1	A	436	LEU	N-CA-C	-5.45	105.03	110.97
1	B	185	TRP	CA-C-N	-5.45	114.53	122.86
1	B	185	TRP	C-N-CA	-5.45	114.53	122.86
1	B	268	ILE	CB-CA-C	-5.44	103.04	110.77
1	B	75	PHE	CA-C-N	5.43	131.22	121.66
1	B	75	PHE	C-N-CA	5.43	131.22	121.66
1	A	212	PHE	N-CA-C	-5.41	105.38	111.28
1	B	436	LEU	CB-CA-C	-5.41	102.38	110.88
1	A	171	ILE	N-CA-C	-5.40	107.46	112.43
1	A	145	LEU	CB-CG-CD2	-5.39	94.54	110.70
1	B	96	VAL	CA-C-O	5.38	122.80	118.71
1	A	143	ALA	N-CA-C	5.38	118.63	111.75
1	B	246	GLU	N-CA-C	-5.35	99.40	110.80
1	A	202	GLU	N-CA-C	5.35	118.91	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	PHE	CB-CA-C	-5.33	99.62	109.37
1	B	369	PHE	CA-C-O	5.32	126.08	120.33
1	B	17	PRO	O-C-N	5.32	129.35	122.91
1	B	142	ARG	CA-C-N	5.32	127.67	120.38
1	B	142	ARG	C-N-CA	5.32	127.67	120.38
1	A	417	GLN	CA-C-O	5.32	125.82	119.60
1	B	251	THR	CB-CA-C	-5.31	101.27	110.45
1	B	280	PHE	N-CA-C	5.30	117.29	108.02
1	B	118	TYR	N-CA-C	5.27	117.67	108.76
1	A	55	PRO	N-CA-C	-5.27	106.17	113.81
1	B	99	HIS	N-CA-C	5.26	117.02	111.28
1	B	22	PHE	N-CA-C	5.25	118.30	109.95
1	A	194	SER	N-CA-C	-5.25	101.45	109.64
1	A	235	SER	N-CA-C	5.23	118.25	110.14
1	B	371	LEU	N-CA-C	-5.23	101.94	110.20
1	B	456	MET	CA-C-O	5.23	125.40	119.18
1	A	429	ASP	N-CA-C	-5.22	105.70	111.71
1	B	224	GLY	CA-C-N	-5.22	114.39	122.59
1	B	224	GLY	C-N-CA	-5.22	114.39	122.59
1	B	85	LYS	N-CA-C	5.20	119.11	112.87
1	A	3	ASN	N-CA-C	-5.19	105.62	112.94
1	B	-1	MET	N-CA-CB	-5.18	102.63	110.77
1	A	208	ILE	CA-CB-CG1	-5.18	101.60	110.40
1	B	196	GLU	N-CA-C	-5.16	105.63	112.34
1	B	96	VAL	N-CA-CB	-5.15	107.07	110.52
1	B	73	THR	CB-CA-C	-5.15	98.92	109.38
1	B	442	ARG	N-CA-C	5.14	117.62	111.71
1	B	211	SER	N-CA-C	5.14	116.57	111.07
1	A	300	THR	N-CA-C	5.13	116.96	111.36
1	A	448	LYS	N-CA-CB	-5.13	102.77	111.69
1	B	443	SER	CB-CA-C	-5.12	102.15	110.85
1	A	59	SER	N-CA-C	5.10	116.53	111.07
1	A	73	THR	CB-CA-C	-5.10	100.91	109.48
1	B	-4	GLN	CA-C-N	-5.10	113.76	121.51
1	B	-4	GLN	C-N-CA	-5.10	113.76	121.51
1	A	191	PRO	CB-CA-C	-5.09	104.31	110.98
1	A	12	VAL	CB-CA-C	-5.09	107.34	114.00
1	A	102	VAL	CB-CA-C	-5.08	105.19	111.70
1	B	95	LYS	CG-CD-CE	-5.07	99.64	111.30
1	B	99	HIS	CB-CA-C	-5.05	102.41	110.79
1	B	254	THR	N-CA-C	5.04	118.24	110.42
1	B	108	GLU	N-CA-C	5.04	116.77	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	SER	CA-C-N	-5.02	113.55	120.28
1	A	211	SER	C-N-CA	-5.02	113.55	120.28
1	A	222	ILE	O-C-N	-5.02	117.00	121.87
1	B	305	LYS	CB-CA-C	-5.02	102.91	110.24
1	A	12	VAL	N-CA-C	5.01	118.37	112.35
1	B	57	LEU	N-CA-C	-5.00	106.02	111.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	112	GLN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ASN	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	3310	0	3309	182	1
1	B	3238	0	3218	225	0
2	A	203	0	0	15	0
2	B	144	0	0	7	1
All	All	6895	0	6527	405	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 31.

All (405) 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:251:THR:HG22	1:A:253:GLU:H	1.06	1.15
1:B:25:LEU:HD23	1:B:52:LEU:HD21	1.36	1.07
1:B:159:ILE:HG23	1:B:222:ILE:HD11	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HG3	1:A:71:HIS:CD2	1.98	0.99
1:A:250:ARG:HG2	1:A:251:THR:H	1.26	0.98
1:B:152:GLN:H	1:B:152:GLN:HE21	1.15	0.94
1:B:152:GLN:H	1:B:152:GLN:NE2	1.66	0.94
1:B:136:TYR:HB2	1:B:431:ILE:HD13	1.48	0.93
1:A:152:GLN:H	1:A:152:GLN:HE21	1.01	0.93
1:B:251:THR:HG22	1:B:253:GLU:H	1.35	0.92
1:A:251:THR:CG2	1:A:253:GLU:H	1.83	0.91
1:B:152:GLN:HA	1:B:384:ILE:HD11	1.53	0.91
1:A:136:TYR:HB2	1:A:431:ILE:HD11	1.56	0.88
1:A:95:LYS:HB3	1:A:97:PRO:HD2	1.57	0.86
1:A:192:MET:SD	1:A:245:ASP:HB2	2.16	0.86
1:A:251:THR:HG22	1:A:253:GLU:N	1.89	0.86
1:B:159:ILE:HG23	1:B:222:ILE:CD1	2.06	0.85
1:A:26:THR:HB	1:A:30:SER:HB3	1.59	0.84
1:A:301:LYS:HD2	1:A:325:ILE:HD13	1.60	0.83
1:A:152:GLN:H	1:A:152:GLN:NE2	1.76	0.83
1:A:375:ASN:OD1	1:A:377:VAL:HG12	1.79	0.83
1:B:251:THR:HG21	1:B:253:GLU:HG3	1.62	0.81
1:B:138:ILE:O	1:B:141:GLN:HB2	1.81	0.80
1:B:123:TRP:CD2	1:B:124:ALA:HA	2.17	0.80
1:B:159:ILE:HG13	1:B:222:ILE:CD1	2.12	0.80
1:B:136:TYR:CB	1:B:431:ILE:HD13	2.12	0.79
1:B:152:GLN:HE21	1:B:152:GLN:N	1.79	0.79
1:B:159:ILE:CG2	1:B:222:ILE:HD11	2.11	0.79
1:B:192:MET:SD	1:B:245:ASP:HB2	2.23	0.78
1:A:309:ASP:HB3	2:A:633:HOH:O	1.83	0.78
1:A:309:ASP:OD1	1:A:317:ASN:HB2	1.84	0.78
1:B:251:THR:HG22	1:B:252:LYS:N	1.99	0.77
1:A:192:MET:CE	1:A:245:ASP:HB2	2.14	0.77
1:B:89:MET:HE3	1:B:91:VAL:CG2	2.15	0.77
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.20	0.77
1:B:54:ASN:HB2	1:B:60:SER:OG	1.84	0.76
1:B:128:SER:OG	1:B:130:GLN:HG2	1.85	0.76
1:A:152:GLN:HE21	1:A:152:GLN:N	1.81	0.75
1:B:185:TRP:NE1	2:B:530:HOH:O	2.19	0.75
1:A:251:THR:HG22	1:A:252:LYS:H	1.51	0.75
1:A:251:THR:HG22	1:A:252:LYS:N	2.01	0.75
1:B:201:ILE:HB	1:B:258:THR:HG22	1.68	0.75
1:B:428:LYS:HD2	1:B:428:LYS:O	1.87	0.75
1:B:451:ASP:OD1	1:B:453:SER:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LYS:HD2	1:A:428:LYS:O	1.87	0.74
1:B:84:TYR:CE1	1:B:86:ASP:HB2	2.22	0.74
1:B:79:GLU:O	1:B:83:GLN:NE2	2.20	0.74
1:B:455:ILE:HG12	1:B:456:MET:CE	2.17	0.73
1:B:159:ILE:HG13	1:B:222:ILE:HD11	1.69	0.73
1:A:250:ARG:HG2	1:A:251:THR:N	2.00	0.73
1:A:136:TYR:HB2	1:A:431:ILE:CD1	2.19	0.73
1:A:70:LYS:HG3	1:A:71:HIS:HD2	1.53	0.73
1:B:200:ASP:OD1	1:B:201:ILE:N	2.23	0.72
1:A:67:LEU:HB2	1:A:69:LEU:HD21	1.72	0.72
1:B:257:LYS:HD2	1:B:259:CYS:O	1.90	0.72
1:A:420:ARG:HD2	2:A:608:HOH:O	1.90	0.71
1:B:441:PHE:O	1:B:445:LYS:HG3	1.91	0.71
1:B:431:ILE:O	1:B:435:ARG:HG3	1.91	0.71
1:B:58:LYS:HD3	2:B:491:HOH:O	1.90	0.70
1:A:245:ASP:OD1	1:A:249:LYS:NZ	2.23	0.70
1:A:-11:SER:HB3	1:A:-9:GLU:HG3	1.73	0.70
1:B:130:GLN:CD	1:B:130:GLN:H	1.98	0.70
1:B:107:LEU:O	1:B:142:ARG:NH2	2.25	0.69
1:A:308:GLY:HA3	1:A:318:LEU:HD23	1.74	0.69
1:B:88:ASP:O	1:B:116:LEU:HD12	1.93	0.69
1:B:451:ASP:OD1	1:B:453:SER:N	2.26	0.69
1:A:192:MET:HE2	1:A:245:ASP:HB2	1.74	0.68
1:A:196:GLU:CD	1:A:196:GLU:H	1.98	0.68
1:A:249:LYS:HZ2	1:A:249:LYS:HB3	1.58	0.68
1:B:251:THR:CG2	1:B:253:GLU:H	2.07	0.68
1:A:201:ILE:HD12	1:A:201:ILE:O	1.93	0.68
1:A:2:ASN:HB3	1:A:4:ASN:H	1.57	0.67
1:A:380:ASN:HB2	2:A:655:HOH:O	1.93	0.67
1:A:4:ASN:O	1:A:10:SER:HB3	1.95	0.67
1:A:442:ARG:NH2	2:A:536:HOH:O	2.28	0.67
1:B:251:THR:HG22	1:B:252:LYS:H	1.60	0.67
1:A:377:VAL:HG13	1:A:378:VAL:N	2.10	0.66
1:A:286:VAL:HG13	1:A:292:ASN:ND2	2.11	0.66
2:A:612:HOH:O	1:B:448:LYS:HD3	1.95	0.66
1:A:12:VAL:HB	1:A:13:PRO:HD3	1.79	0.65
1:B:25:LEU:CD2	1:B:52:LEU:HD21	2.21	0.65
1:B:36:HIS:NE2	1:B:122:GLU:OE2	2.22	0.65
1:B:251:THR:CG2	1:B:253:GLU:HG3	2.26	0.65
1:B:31:TRP:CH2	1:B:35:THR:HG21	2.32	0.64
1:A:269:LEU:O	1:A:273:LYS:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:TRP:CZ2	1:B:35:THR:HG21	2.33	0.64
1:A:251:THR:HG21	1:A:253:GLU:HB2	1.79	0.64
1:A:106:ILE:O	1:A:110:SER:OG	2.16	0.64
1:B:136:TYR:HB2	1:B:431:ILE:CD1	2.23	0.63
1:B:251:THR:HG22	1:B:253:GLU:N	2.11	0.63
1:B:435:ARG:HD2	1:B:455:ILE:O	1.97	0.63
1:A:228:GLN:NE2	1:A:273:LYS:HE3	2.14	0.63
1:B:455:ILE:HG12	1:B:456:MET:HE1	1.80	0.63
1:B:200:ASP:OD1	1:B:200:ASP:C	2.39	0.63
1:A:249:LYS:NZ	1:A:249:LYS:HB3	2.14	0.63
1:A:290:THR:HA	2:A:511:HOH:O	1.97	0.63
1:A:241:GLN:HA	2:A:495:HOH:O	1.98	0.62
1:B:183:GLY:HA3	1:B:207:LEU:CD1	2.28	0.62
1:B:95:LYS:CG	1:B:97:PRO:HD2	2.29	0.62
1:A:26:THR:HG22	1:A:27:SER:N	2.13	0.62
1:A:57:LEU:HD23	1:A:61:LEU:CD1	2.29	0.62
1:B:80:SER:HA	1:B:83:GLN:NE2	2.15	0.62
1:B:163:LYS:HE3	1:B:221:TYR:CZ	2.34	0.62
1:B:192:MET:CE	1:B:245:ASP:HB2	2.30	0.62
1:A:317:ASN:HB3	2:A:660:HOH:O	2.00	0.62
1:B:201:ILE:CB	1:B:258:THR:HG22	2.30	0.61
1:A:110:SER:HB3	1:A:116:LEU:HD22	1.80	0.61
1:B:79:GLU:HG3	1:B:109:HIS:CE1	2.35	0.61
1:B:105:ASN:OD1	1:B:105:ASN:C	2.42	0.61
1:A:377:VAL:CG1	1:A:378:VAL:N	2.63	0.61
1:A:102:VAL:O	1:A:106:ILE:HD12	2.00	0.60
1:B:323:TYR:CD1	1:B:366:MET:HG2	2.36	0.60
1:B:85:LYS:O	1:B:115:ASN:ND2	2.34	0.60
1:B:123:TRP:HA	1:B:149:ILE:HD11	1.82	0.60
1:A:28:GLY:HA2	1:A:67:LEU:HD21	1.84	0.60
1:A:320:LEU:HD23	1:A:320:LEU:C	2.27	0.60
1:B:96:VAL:N	1:B:97:PRO:CD	2.65	0.60
1:B:16:ARG:HG2	1:B:17:PRO:O	2.02	0.60
1:B:195:PRO:HB2	1:B:197:TYR:CD2	2.37	0.60
1:B:201:ILE:HG22	1:B:258:THR:CG2	2.32	0.59
1:B:455:ILE:HG12	1:B:456:MET:HE3	1.82	0.59
1:B:159:ILE:CG1	1:B:222:ILE:HD11	2.33	0.59
1:B:284:THR:HB	1:B:285:PRO:HA	1.84	0.59
1:A:304:LEU:C	1:A:304:LEU:HD23	2.28	0.59
1:A:79:GLU:HG3	1:A:109:HIS:CG	2.38	0.58
1:B:84:TYR:CZ	1:B:86:ASP:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:TYR:HD1	1:B:285:PRO:HD3	1.67	0.58
1:A:377:VAL:HG13	1:A:378:VAL:HG23	1.85	0.58
1:B:251:THR:CG2	1:B:252:LYS:N	2.65	0.58
1:B:301:LYS:HB3	1:B:325:ILE:HD13	1.86	0.58
1:B:301:LYS:HD3	1:B:325:ILE:HD12	1.86	0.58
1:B:64:ILE:O	1:B:69:LEU:N	2.28	0.58
1:B:197:TYR:CZ	1:B:198:LEU:HD21	2.39	0.57
1:A:242:PHE:CG	1:A:250:ARG:HD3	2.40	0.57
1:A:390:ASP:HA	1:A:394:LEU:HD12	1.86	0.57
1:B:433:LEU:O	1:B:437:ILE:HD12	2.05	0.57
1:A:244:LEU:HB3	1:A:249:LYS:O	2.05	0.57
1:B:33:ALA:O	1:B:37:PHE:HB3	2.05	0.57
1:B:428:LYS:HD2	1:B:428:LYS:C	2.27	0.57
1:A:134:GLU:HA	1:A:137:SER:OG	2.05	0.56
1:B:123:TRP:CG	1:B:124:ALA:HA	2.39	0.56
1:B:250:ARG:HG2	1:B:251:THR:N	2.20	0.56
1:A:200:ASP:OD1	1:A:202:GLU:HB2	2.05	0.56
1:B:89:MET:HE1	1:B:385:TYR:HE2	1.69	0.56
1:B:159:ILE:CB	1:B:222:ILE:HD11	2.35	0.56
1:A:236:ASN:ND2	1:A:260:PRO:HA	2.20	0.56
1:B:31:TRP:CE2	1:B:35:THR:HG21	2.41	0.56
1:B:432:ILE:HG12	1:B:456:MET:HA	1.88	0.56
1:A:26:THR:HB	1:A:30:SER:CB	2.35	0.56
1:A:325:ILE:O	1:A:325:ILE:HG13	2.06	0.55
1:B:25:LEU:HD13	1:B:32:VAL:HG12	1.89	0.55
1:B:127:ALA:HB1	1:B:203:SER:O	2.06	0.55
1:B:115:ASN:O	1:B:117:ARG:HG3	2.06	0.55
1:A:192:MET:HE2	1:A:245:ASP:HA	1.89	0.55
1:B:31:TRP:O	1:B:35:THR:N	2.39	0.55
1:A:13:PRO:HA	1:A:16:ARG:NH1	2.22	0.55
1:A:62:GLN:O	1:A:66:GLN:HG3	2.06	0.55
1:B:173:ASP:O	1:B:299:GLY:HA2	2.06	0.55
1:B:320:LEU:C	1:B:320:LEU:HD23	2.31	0.55
1:A:169:GLY:O	1:A:325:ILE:HD11	2.07	0.55
1:B:451:ASP:CG	1:B:453:SER:HB2	2.32	0.55
1:A:192:MET:HE2	1:A:245:ASP:CA	2.37	0.55
1:B:199:TYR:HD2	1:B:257:LYS:HG3	1.70	0.55
1:A:244:LEU:HB3	1:A:249:LYS:C	2.31	0.54
1:B:126:ALA:HB3	1:B:132:ALA:HB2	1.89	0.54
1:B:25:LEU:HD23	1:B:52:LEU:CD2	2.25	0.54
1:B:95:LYS:HG2	1:B:97:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LYS:HD3	1:B:325:ILE:CD1	2.38	0.54
1:A:209:SER:HA	1:A:437:ILE:HD13	1.89	0.54
1:B:187:GLY:HA3	1:B:284:THR:O	2.07	0.54
2:A:512:HOH:O	1:B:287:LYS:HG2	2.08	0.54
1:B:24:GLY:HA3	1:B:93:SER:O	2.07	0.54
1:B:384:ILE:O	1:B:387:SER:HB2	2.08	0.54
1:A:108:GLU:O	1:A:111:SER:OG	2.24	0.54
1:B:67:LEU:N	1:B:67:LEU:HD23	2.23	0.54
1:A:-13:HIS:HD2	1:A:-13:HIS:O	1.90	0.53
1:A:12:VAL:CB	1:A:13:PRO:HD3	2.37	0.53
1:A:192:MET:HE2	1:A:245:ASP:CB	2.38	0.53
1:B:325:ILE:C	1:B:327:ASN:H	2.15	0.53
1:B:189:GLU:HB3	1:B:244:LEU:HD21	1.89	0.53
1:B:89:MET:HE3	1:B:91:VAL:HG22	1.88	0.53
1:B:120:TYR:C	1:B:120:TYR:HD2	2.16	0.53
1:B:185:TRP:HB3	1:B:199:TYR:OH	2.07	0.53
1:A:2:ASN:HD22	1:A:7:SER:HG	1.54	0.53
1:A:133:GLU:O	1:A:136:TYR:HB3	2.08	0.53
1:B:149:ILE:HG13	1:B:430:ALA:HB2	1.90	0.53
1:B:323:TYR:HD1	1:B:366:MET:HG2	1.72	0.53
1:A:100:TYR:OH	1:A:104:LYS:HE3	2.08	0.53
1:B:455:ILE:CG1	1:B:456:MET:HE3	2.39	0.53
1:B:320:LEU:HB3	1:B:369:PHE:HB3	1.90	0.53
1:A:94:VAL:O	1:A:95:LYS:C	2.51	0.53
1:B:100:TYR:OH	1:B:134:GLU:OE1	2.23	0.53
1:B:244:LEU:HD23	1:B:250:ARG:HG3	1.91	0.52
1:A:262:HIS:CE1	1:A:281:LYS:HG3	2.44	0.52
1:B:14:SER:O	1:B:16:ARG:N	2.42	0.52
1:A:128:SER:HB2	1:A:130:GLN:OE1	2.09	0.52
1:B:120:TYR:C	1:B:120:TYR:CD2	2.87	0.52
1:B:128:SER:HG	1:B:130:GLN:HG2	1.74	0.52
1:B:201:ILE:CG2	1:B:258:THR:HG22	2.40	0.52
1:A:33:ALA:O	1:A:37:PHE:HB3	2.09	0.52
1:B:95:LYS:C	1:B:97:PRO:HD2	2.35	0.52
1:B:50:VAL:HA	1:B:71:HIS:O	2.10	0.52
1:B:201:ILE:HD12	1:B:201:ILE:O	2.10	0.52
1:B:325:ILE:C	1:B:327:ASN:N	2.65	0.51
1:B:67:LEU:O	1:B:68:GLN:HB2	2.09	0.51
1:B:14:SER:C	1:B:16:ARG:H	2.18	0.51
1:A:100:TYR:O	1:A:104:LYS:HB2	2.09	0.51
1:B:163:LYS:HE3	1:B:221:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:VAL:HG11	1:B:321:TYR:CZ	2.45	0.51
1:B:251:THR:CG2	1:B:252:LYS:H	2.22	0.51
1:A:102:VAL:HG12	1:A:106:ILE:HD12	1.92	0.51
1:A:79:GLU:HG3	1:A:109:HIS:CD2	2.46	0.50
1:A:188:TYR:CE1	1:B:300:THR:HG22	2.46	0.50
1:A:251:THR:HG21	1:A:253:GLU:CB	2.41	0.50
1:B:31:TRP:CZ3	1:B:35:THR:HG21	2.46	0.50
1:A:134:GLU:O	1:A:137:SER:OG	2.27	0.50
1:B:431:ILE:O	1:B:435:ARG:CG	2.59	0.50
1:B:192:MET:HE2	1:B:245:ASP:O	2.12	0.50
1:A:157:PRO:HG3	1:A:383:ARG:NH1	2.27	0.50
1:B:199:TYR:CD1	1:B:199:TYR:N	2.78	0.50
1:A:8:LYS:O	1:A:14:SER:OG	2.27	0.50
1:A:70:LYS:HE3	1:A:71:HIS:NE2	2.27	0.50
1:B:34:LYS:O	1:B:38:LEU:HD12	2.12	0.50
1:B:35:THR:OG1	1:B:36:HIS:N	2.39	0.50
1:B:37:PHE:O	1:B:41:GLN:HB2	2.11	0.50
1:B:228:GLN:HE21	1:B:229:LYS:HB2	1.76	0.50
1:B:236:ASN:HA	1:B:261:ASP:OD1	2.12	0.50
1:A:63:THR:HA	1:A:66:GLN:OE1	2.12	0.49
1:A:323:TYR:HA	1:A:365:THR:O	2.12	0.49
1:B:422:GLU:CD	1:B:422:GLU:H	2.19	0.49
1:A:25:LEU:HD12	1:A:25:LEU:C	2.29	0.49
1:B:130:GLN:CD	1:B:130:GLN:N	2.67	0.49
1:A:79:GLU:HB2	2:A:475:HOH:O	2.12	0.49
1:A:102:VAL:HG12	1:A:106:ILE:CD1	2.43	0.49
1:B:62:GLN:C	1:B:66:GLN:HE21	2.20	0.49
1:A:384:ILE:O	1:A:388:ILE:HG13	2.13	0.49
1:B:200:ASP:O	1:B:203:SER:OG	2.28	0.49
1:A:139:SER:O	1:A:140:GLN:C	2.51	0.49
1:A:159:ILE:N	1:A:159:ILE:CD1	2.75	0.49
1:B:14:SER:C	1:B:16:ARG:N	2.69	0.49
1:B:48:GLN:HB2	2:B:580:HOH:O	2.12	0.49
1:B:37:PHE:O	1:B:41:GLN:N	2.44	0.48
1:B:195:PRO:O	1:B:196:GLU:C	2.54	0.48
1:B:201:ILE:H	1:B:258:THR:CG2	2.26	0.48
1:A:57:LEU:CD2	1:A:61:LEU:HD11	2.44	0.48
1:B:96:VAL:N	1:B:97:PRO:HD3	2.27	0.48
1:A:375:ASN:HB2	2:A:607:HOH:O	2.13	0.48
1:A:48:GLN:OE1	1:A:71:HIS:CD2	2.66	0.48
1:B:88:ASP:C	1:B:116:LEU:HD12	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLN:O	1:B:418:GLY:C	2.55	0.48
1:A:26:THR:HG22	1:A:27:SER:CB	2.43	0.48
1:A:260:PRO:HD2	2:A:498:HOH:O	2.14	0.48
1:B:75:PHE:CD1	1:B:75:PHE:N	2.80	0.48
1:B:110:SER:HB2	1:B:142:ARG:HH12	1.79	0.48
1:A:365:THR:CG2	1:A:366:MET:N	2.77	0.48
1:B:129:VAL:HG21	1:B:438:ASP:OD1	2.14	0.48
1:B:227:PHE:HB2	2:B:535:HOH:O	2.14	0.48
1:A:175:ASN:O	1:A:275:PRO:HD2	2.14	0.48
1:A:232:ALA:CB	1:A:440:VAL:HG13	2.44	0.48
1:A:4:ASN:O	1:A:7:SER:HB3	2.14	0.48
1:A:107:LEU:HD13	1:A:138:ILE:CG2	2.43	0.48
1:A:428:LYS:HD2	1:A:428:LYS:C	2.38	0.48
1:B:112:GLN:HG2	2:B:581:HOH:O	2.14	0.48
1:B:188:TYR:CD1	1:B:285:PRO:HD3	2.48	0.48
1:A:96:VAL:N	1:A:97:PRO:CD	2.76	0.47
1:A:132:ALA:O	1:A:133:GLU:C	2.54	0.47
1:B:66:GLN:C	1:B:68:GLN:H	2.21	0.47
1:A:57:LEU:O	1:A:58:LYS:C	2.56	0.47
1:B:65:GLU:O	1:B:66:GLN:C	2.56	0.47
1:B:128:SER:CB	1:B:130:GLN:HG2	2.44	0.47
1:B:244:LEU:CD2	1:B:250:ARG:HG3	2.45	0.47
1:A:129:VAL:O	1:A:133:GLU:HG2	2.15	0.47
1:A:286:VAL:HG13	1:A:292:ASN:CG	2.39	0.47
1:A:245:ASP:C	1:A:248:GLY:N	2.73	0.47
1:B:66:GLN:C	1:B:68:GLN:N	2.72	0.47
1:B:155:LYS:O	1:B:383:ARG:NH1	2.40	0.47
1:B:100:TYR:HB2	1:B:131:GLN:OE1	2.15	0.47
1:B:195:PRO:C	1:B:197:TYR:N	2.70	0.47
1:A:272:GLY:O	1:A:273:LYS:C	2.56	0.47
1:B:116:LEU:HD12	1:B:116:LEU:HA	1.50	0.47
1:A:123:TRP:CE3	1:A:124:ALA:HA	2.50	0.46
1:B:375:ASN:OD1	1:B:375:ASN:C	2.58	0.46
1:A:286:VAL:HG13	1:A:292:ASN:HD21	1.80	0.46
1:B:284:THR:HA	1:B:285:PRO:C	2.40	0.46
1:A:238:ILE:O	1:A:238:ILE:HG22	2.14	0.46
1:A:257:LYS:HE3	1:A:257:LYS:HB3	1.62	0.46
1:B:177:ILE:HG12	1:B:297:ILE:HG12	1.97	0.46
1:A:27:SER:HA	1:A:63:THR:OG1	2.16	0.46
1:A:225:SER:HB2	1:A:271:ASN:ND2	2.31	0.46
1:B:28:GLY:HA3	1:B:66:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:PHE:O	1:B:445:LYS:CG	2.61	0.46
1:B:96:VAL:HA	1:B:99:HIS:CD2	2.51	0.46
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.67	0.46
1:A:95:LYS:HB2	1:A:98:GLU:OE1	2.16	0.46
1:A:200:ASP:O	1:A:201:ILE:C	2.58	0.46
1:B:21:GLY:HA2	1:B:51:ALA:O	2.16	0.46
1:B:454:LYS:NZ	2:B:563:HOH:O	2.42	0.46
1:A:193:ARG:HA	1:A:193:ARG:HD2	1.62	0.46
1:A:290:THR:HG23	2:A:510:HOH:O	2.15	0.45
1:B:89:MET:HE1	1:B:385:TYR:CE2	2.51	0.45
1:A:113:ASN:C	1:A:113:ASN:OD1	2.59	0.45
1:B:65:GLU:O	1:B:68:GLN:N	2.49	0.45
1:B:136:TYR:CB	1:B:431:ILE:CD1	2.91	0.45
1:B:152:GLN:CA	1:B:384:ILE:HD11	2.35	0.45
1:A:57:LEU:HD23	1:A:61:LEU:HD11	1.97	0.45
1:B:63:THR:HA	1:B:66:GLN:NE2	2.32	0.45
1:A:73:THR:HG22	1:A:74:GLY:N	2.27	0.45
1:A:417:GLN:O	1:A:418:GLY:C	2.60	0.45
1:B:53:TYR:CD2	1:B:53:TYR:C	2.89	0.45
1:A:-13:HIS:O	1:A:-13:HIS:CD2	2.70	0.45
1:A:289:LEU:HD21	1:B:323:TYR:HB2	1.98	0.45
1:A:229:LYS:HD2	1:A:449:THR:HG21	1.99	0.45
1:B:136:TYR:CG	1:B:431:ILE:HD13	2.52	0.44
1:B:201:ILE:HG22	1:B:258:THR:HG21	1.99	0.44
1:A:166:ILE:HD12	1:A:222:ILE:HG22	1.98	0.44
1:A:244:LEU:HA	1:A:249:LYS:O	2.18	0.44
1:A:441:PHE:O	1:A:445:LYS:N	2.47	0.44
1:A:229:LYS:HA	1:A:450:LEU:O	2.18	0.44
1:A:377:VAL:CG1	1:A:378:VAL:HG23	2.48	0.44
1:A:57:LEU:O	1:A:61:LEU:HD13	2.17	0.44
1:A:60:SER:O	1:A:64:ILE:HG13	2.18	0.44
1:B:325:ILE:O	1:B:325:ILE:HG12	2.17	0.44
1:B:101:GLU:O	1:B:102:VAL:C	2.57	0.44
1:B:259:CYS:HA	1:B:260:PRO:HD3	1.79	0.44
1:B:292:ASN:HB2	1:B:310:ALA:HB3	1.99	0.44
1:A:67:LEU:CB	1:A:69:LEU:HD21	2.46	0.43
1:B:165:LEU:HD21	1:B:326:LYS:HE3	2.01	0.43
1:B:195:PRO:CB	1:B:197:TYR:CD2	3.01	0.43
1:B:159:ILE:O	1:B:160:VAL:C	2.60	0.43
1:B:201:ILE:CG2	1:B:258:THR:CG2	2.96	0.43
1:A:365:THR:HG22	1:A:366:MET:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:SER:CB	1:B:142:ARG:HH12	2.31	0.43
1:B:257:LYS:HE3	1:B:257:LYS:HB3	1.78	0.43
1:B:95:LYS:C	1:B:97:PRO:CD	2.92	0.43
1:A:54:ASN:HB2	1:A:60:SER:OG	2.18	0.43
1:A:190:ARG:HD3	2:A:581:HOH:O	2.19	0.43
1:B:133:GLU:HA	1:B:431:ILE:HD11	2.00	0.43
1:B:309:ASP:HB2	1:B:316:SER:HA	2.01	0.43
1:A:13:PRO:O	1:A:16:ARG:HD3	2.19	0.43
1:A:57:LEU:CD2	1:A:61:LEU:CD1	2.96	0.43
1:A:179:ILE:HB	1:A:278:CYS:HB2	2.01	0.43
1:A:182:ASN:HA	1:A:281:LYS:O	2.18	0.43
1:A:211:SER:O	1:A:212:PHE:C	2.56	0.42
1:B:159:ILE:HG13	1:B:222:ILE:HD13	1.96	0.42
1:A:13:PRO:HA	1:A:16:ARG:HD3	2.00	0.42
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.78	0.42
1:B:163:LYS:O	1:B:167:SER:HB3	2.19	0.42
1:A:163:LYS:NZ	1:A:419:PHE:O	2.48	0.42
1:A:192:MET:SD	1:A:245:ASP:CB	2.97	0.42
1:A:201:ILE:HD12	1:A:201:ILE:C	2.42	0.42
1:B:152:GLN:HB2	1:B:380:ASN:HB3	2.01	0.42
1:B:232:ALA:HA	1:B:264:LEU:O	2.19	0.42
1:A:26:THR:HG22	1:A:27:SER:HB3	2.00	0.42
1:A:110:SER:CB	1:A:142:ARG:HH22	2.32	0.42
1:B:85:LYS:HD3	2:B:494:HOH:O	2.19	0.42
1:A:-13:HIS:CD2	1:A:-13:HIS:C	2.97	0.42
1:B:278:CYS:SG	1:B:280:PHE:HD1	2.42	0.42
1:B:53:TYR:CD2	1:B:53:TYR:O	2.73	0.42
1:B:79:GLU:C	1:B:83:GLN:NE2	2.77	0.42
1:B:183:GLY:HA3	1:B:207:LEU:HD12	2.02	0.42
1:B:95:LYS:HZ3	1:B:95:LYS:HG3	1.07	0.42
1:A:291:LYS:HA	1:A:291:LYS:HD3	1.69	0.42
1:A:320:LEU:HB3	1:A:369:PHE:HB3	2.02	0.42
1:B:301:LYS:CD	1:B:325:ILE:CD1	2.97	0.42
1:B:87:ILE:HG21	1:B:90:ILE:HG12	2.01	0.41
1:A:251:THR:CG2	1:A:252:LYS:N	2.74	0.41
1:A:53:TYR:CD2	1:A:53:TYR:C	2.98	0.41
1:A:107:LEU:O	1:A:142:ARG:NH2	2.53	0.41
1:A:217:ASP:HB2	1:A:433:LEU:HD22	2.02	0.41
1:A:196:GLU:CD	1:A:196:GLU:N	2.73	0.41
1:B:192:MET:SD	1:B:245:ASP:CB	3.02	0.41
1:A:428:LYS:HE2	1:A:432:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLU:HG3	1:B:109:HIS:CG	2.54	0.41
1:B:100:TYR:CZ	1:B:104:LYS:HD2	2.55	0.41
1:B:452:VAL:C	1:B:454:LYS:N	2.77	0.41
1:A:170:CYS:HB3	1:A:325:ILE:O	2.21	0.41
1:A:228:GLN:CD	1:A:273:LYS:HE3	2.45	0.41
1:A:325:ILE:HD11	2:A:577:HOH:O	2.20	0.41
1:B:74:GLY:C	1:B:75:PHE:CD1	2.99	0.41
1:B:102:VAL:H	1:B:102:VAL:HG23	1.65	0.41
1:A:54:ASN:C	1:A:56:THR:N	2.78	0.41
1:A:208:ILE:H	1:A:208:ILE:HG13	1.62	0.41
1:A:446:GLU:O	1:A:447:GLU:HB2	2.20	0.41
1:B:37:PHE:O	1:B:41:GLN:CB	2.68	0.41
1:B:160:VAL:O	1:B:164:GLU:HG3	2.21	0.41
1:B:179:ILE:HD13	1:B:179:ILE:HG21	1.83	0.41
1:A:2:ASN:O	1:A:10:SER:HA	2.21	0.41
1:A:23:VAL:HG12	1:A:94:VAL:CG1	2.51	0.41
1:B:61:LEU:HA	1:B:61:LEU:HD12	1.62	0.41
1:B:78:LEU:O	1:B:81:PHE:HB3	2.21	0.41
1:B:304:LEU:C	1:B:304:LEU:HD23	2.46	0.41
1:B:38:LEU:HA	1:B:38:LEU:HD23	1.77	0.40
1:A:120:TYR:CD2	1:A:120:TYR:C	3.00	0.40
1:B:-6:TYR:CE2	1:B:394:LEU:HD11	2.56	0.40
1:B:0:LEU:HD23	1:B:0:LEU:HA	1.67	0.40
1:B:192:MET:CE	1:B:245:ASP:O	2.69	0.40
1:A:19:ARG:HG2	1:A:50:VAL:HG11	2.03	0.40
1:A:179:ILE:HD11	1:A:219:LEU:HD22	2.04	0.40
1:B:38:LEU:O	1:B:41:GLN:HB3	2.21	0.40
1:A:147:THR:HB	1:A:427:PHE:CD1	2.56	0.40
1:B:257:LYS:HD2	1:B:259:CYS:C	2.47	0.40
1:A:57:LEU:HD23	1:A:61:LEU:HD13	2.01	0.40
1:A:75:PHE:HD2	1:A:80:SER:HB2	1.86	0.40
1:B:48:GLN:HE21	1:B:71:HIS:CD2	2.39	0.40
1:B:58:LYS:O	1:B:61:LEU:N	2.54	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:76:ASP:OD2	2:B:601:HOH:O[3_556]	2.16	0.04

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	404/479 (84%)	386 (96%)	18 (4%)	0	100	100
1	B	393/479 (82%)	361 (92%)	30 (8%)	2 (0%)	24	22
All	All	797/958 (83%)	747 (94%)	48 (6%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	SER
1	B	102	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/422 (88%)	312 (84%)	58 (16%)	2	1
1	B	359/422 (85%)	298 (83%)	61 (17%)	2	1
All	All	729/844 (86%)	610 (84%)	119 (16%)	2	1

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-9	GLU
1	A	5	LYS
1	A	7	SER
1	A	11	THR

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Mol	Chain	Res	Type
1	A	25	LEU
1	A	26	THR
1	A	34	LYS
1	A	41	GLN
1	A	44	SER
1	A	48	GLN
1	A	56	THR
1	A	57	LEU
1	A	66	GLN
1	A	69	LEU
1	A	76	ASP
1	A	77	SER
1	A	80	SER
1	A	85	LYS
1	A	104	LYS
1	A	106	ILE
1	A	110	SER
1	A	111	SER
1	A	117	ARG
1	A	142	ARG
1	A	152	GLN
1	A	159	ILE
1	A	178	GLU
1	A	189	GLU
1	A	192	MET
1	A	193	ARG
1	A	196	GLU
1	A	201	ILE
1	A	205	VAL
1	A	211	SER
1	A	218	VAL
1	A	240	THR
1	A	243	LEU
1	A	244	LEU
1	A	245	ASP
1	A	249	LYS
1	A	252	LYS
1	A	254	THR
1	A	256	SER
1	A	261	ASP
1	A	278	CYS
1	A	280	PHE

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Mol	Chain	Res	Type
1	A	281	LYS
1	A	293	LEU
1	A	304	LEU
1	A	307	GLU
1	A	362	GLU
1	A	366	MET
1	A	394	LEU
1	A	422	GLU
1	A	428	LYS
1	A	431	ILE
1	A	445	LYS
1	A	454	LYS
1	B	15	SER
1	B	29	LYS
1	B	40	ILE
1	B	48	GLN
1	B	49	ILE
1	B	56	THR
1	B	58	LYS
1	B	69	LEU
1	B	70	LYS
1	B	75	PHE
1	B	83	GLN
1	B	95	LYS
1	B	105	ASN
1	B	110	SER
1	B	111	SER
1	B	112	GLN
1	B	120	TYR
1	B	129	VAL
1	B	130	GLN
1	B	139	SER
1	B	141	GLN
1	B	149	ILE
1	B	152	GLN
1	B	157	PRO
1	B	176	SER
1	B	178	GLU
1	B	194	SER
1	B	196	GLU
1	B	201	ILE
1	B	202	GLU

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Mol	Chain	Res	Type
1	B	203	SER
1	B	211	SER
1	B	218	VAL
1	B	219	LEU
1	B	222	ILE
1	B	228	GLN
1	B	230	ILE
1	B	236	ASN
1	B	244	LEU
1	B	254	THR
1	B	255	ILE
1	B	256	SER
1	B	257	LYS
1	B	261	ASP
1	B	281	LYS
1	B	287	LYS
1	B	316	SER
1	B	325	ILE
1	B	326	LYS
1	B	365	THR
1	B	366	MET
1	B	372	ARG
1	B	387	SER
1	B	415	ASP
1	B	422	GLU
1	B	428	LYS
1	B	431	ILE
1	B	435	ARG
1	B	437	ILE
1	B	453	SER
1	B	456	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-13	HIS
1	A	2	ASN
1	A	41	GLN
1	A	42	GLN
1	A	48	GLN
1	A	62	GLN
1	A	71	HIS

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Mol	Chain	Res	Type
1	A	83	GLN
1	A	140	GLN
1	A	152	GLN
1	A	175	ASN
1	A	228	GLN
1	A	236	ASN
1	A	271	ASN
1	A	380	ASN
1	B	-13	HIS
1	B	42	GLN
1	B	66	GLN
1	B	71	HIS
1	B	83	GLN
1	B	112	GLN
1	B	141	GLN
1	B	152	GLN
1	B	228	GLN
1	B	380	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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	413/479 (86%)	0.02	16 (3%) 43 45	19, 39, 81, 100	1 (0%)
1	B	405/479 (84%)	0.17	22 (5%) 31 33	22, 41, 79, 100	0
All	All	818/958 (85%)	0.09	38 (4%) 37 39	19, 40, 81, 100	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	328	GLY	5.1
1	A	328	GLY	3.8
1	A	2	ASN	3.7
1	B	327	ASN	3.6
1	A	243	LEU	3.3
1	B	316	SER	3.1
1	B	457	ILE	3.1
1	A	114	LEU	3.1
1	A	316	SER	3.1
1	B	311	GLY	3.0
1	B	247	ASN	2.9
1	B	1	ALA	2.8
1	B	14	SER	2.8
1	A	26	THR	2.8
1	B	395	GLY	2.8
1	A	394	LEU	2.6
1	B	246	GLU	2.5
1	A	-6	TYR	2.5
1	B	76	ASP	2.5
1	B	244	LEU	2.5
1	B	58	LYS	2.4
1	B	-11	SER	2.4
1	B	445	LYS	2.3
1	A	252	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	-5	PHE	2.3
1	A	309	ASP	2.3
1	B	310	ALA	2.3
1	B	204	GLY	2.2
1	A	189	GLU	2.2
1	B	253	GLU	2.2
1	A	317	ASN	2.2
1	B	254	THR	2.1
1	B	414	PHE	2.1
1	A	185	TRP	2.1
1	B	362	GLU	2.0
1	B	243	LEU	2.0
1	A	245	ASP	2.0
1	A	-14	HIS	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 oligosaccharides 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.