



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 11:03 AM UTC

PDB ID : 1FUG / pdb_00001fug
Title : S-ADENOSYLMETHIONINE SYNTHETASE
Authors : Fu, Z.; Markham, G.D.; Takusagawa, F.
Deposited on : 1996-02-25
Resolution : 3.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

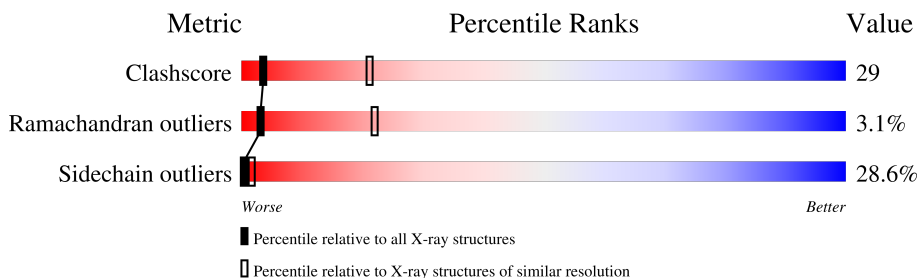
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	
1	B	383	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7170 atoms, of which 1286 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 S-ADENOSYLMETHIONINE SYNTHETASE.

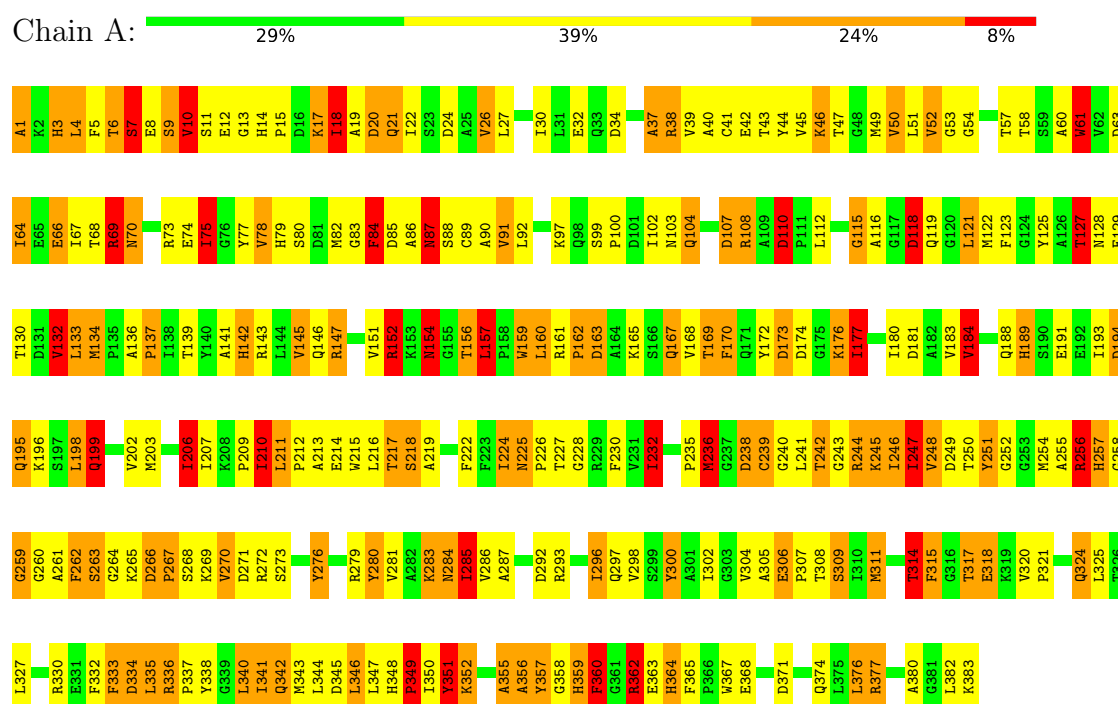
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	H	N	O	S	0	0	0
			3585	1856	643	503	570	13			
1	B	383	Total	C	H	N	O	S	0	0	0
			3585	1856	643	503	570	13			

3 Residue-property plots

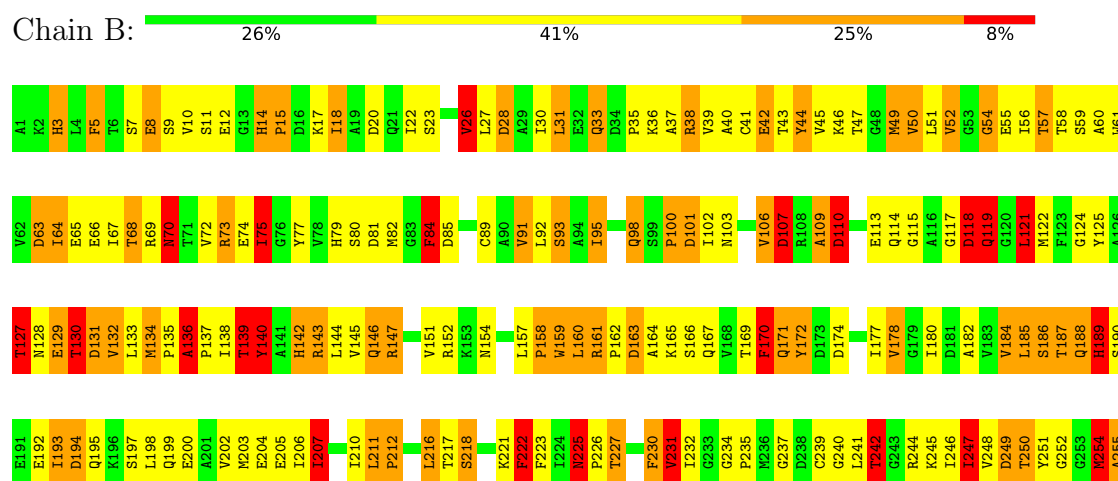
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: S-ADENOSYLMETHIONINE SYNTHETASE



• Molecule 1: S-ADENOSYLMETHIONINE SYNTHETASE



R256	H257	G258	G259	G260	A261	F262	S263	G264	P267	S268	D271	R272	S273	A274	A275	Y276	A277	A278	R279	Y280	V281	A282	R283	N284	I285	V286	A287	A288	G289	L290	C294	E295	I296	Q297	V298	S299	Y300	A301	I302	G303	V304	T308	S309	I310	M311	V312	E313	T314	F315	G316	T317	E318	K319	V320	P321
S322	L325	T326	L327	L328	V329	R330	E331	F332	F333	D334	L335	R336	P337	Y338	G339	L340	I341	Q342	M343	L344	D345	L346	L347	H348	P349	I350	Y351	K352	F353	T354	A355	A356	Y357	G358	H359	F360	G361	R362	E363	H364	F365	P366	W367	E368	D371	K372	A373	Q374	D378	A379	A380	G381	L382	K383	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.00Å 121.00Å 171.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.4 (8.00-3.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.210 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	1.23	15/3001 (0.5%)	2.31	167/4068 (4.1%)
1	B	1.22	14/3001 (0.5%)	2.35	168/4068 (4.1%)
All	All	1.23	29/6002 (0.5%)	2.33	335/8136 (4.1%)

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	19
1	B	0	18
All	All	0	37

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	ALA	CA-C	-8.79	1.42	1.53
1	B	359	HIS	CD2-NE2	-7.71	1.29	1.37
1	A	102	ILE	CA-CB	7.37	1.63	1.54
1	A	257	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	359	HIS	CD2-NE2	-6.99	1.30	1.37
1	B	3	HIS	CD2-NE2	-6.85	1.30	1.37
1	B	257	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	364	HIS	CD2-NE2	-6.62	1.30	1.37
1	B	142	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	142	HIS	CD2-NE2	-6.36	1.30	1.37
1	B	189	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	3	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	189	HIS	CD2-NE2	-5.91	1.31	1.37
1	B	260	GLY	CA-C	5.85	1.60	1.51
1	B	359	HIS	CG-ND1	-5.80	1.31	1.38
1	A	247	ILE	CA-CB	-5.74	1.49	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	14	HIS	CD2-NE2	-5.66	1.31	1.37
1	B	79	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	285	ILE	CA-CB	5.50	1.60	1.54
1	B	348	HIS	CD2-NE2	-5.39	1.31	1.37
1	A	359	HIS	CG-ND1	-5.26	1.32	1.38
1	A	50	VAL	CA-CB	-5.24	1.48	1.54
1	B	364	HIS	CD2-NE2	-5.23	1.32	1.37
1	A	189	HIS	CG-ND1	-5.20	1.32	1.38
1	A	14	HIS	CG-ND1	-5.18	1.32	1.38
1	A	75	ILE	CA-CB	-5.11	1.48	1.54
1	B	336	ARG	NE-CZ	5.10	1.38	1.33
1	B	230	PHE	CA-CB	5.05	1.60	1.53

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ASP	CA-CB-CG	14.84	127.44	112.60
1	B	146	GLN	N-CA-C	-13.14	96.69	113.12
1	B	84	PHE	CA-CB-CG	12.90	126.70	113.80
1	B	286	VAL	N-CA-C	-12.43	99.89	111.45
1	B	261	ALA	O-C-N	10.84	135.36	122.46
1	A	356	ALA	N-CA-C	10.53	124.25	111.40
1	B	20	ASP	CA-CB-CG	10.32	122.92	112.60
1	B	373	ALA	N-CA-C	10.08	121.96	110.97
1	A	7	SER	CA-CB-OG	-9.89	91.32	111.10
1	A	181	ASP	N-CA-C	9.46	121.67	111.36
1	B	371	ASP	CA-CB-CG	9.38	121.98	112.60
1	B	230	PHE	CA-CB-CG	9.28	123.08	113.80
1	B	250	THR	N-CA-C	9.22	124.77	112.13
1	A	133	LEU	N-CA-CB	-9.12	99.41	110.53
1	B	271	ASP	CA-CB-CG	9.08	121.68	112.60
1	B	351	TYR	N-CA-C	9.02	123.39	112.38
1	A	269	LYS	N-CA-C	-9.02	95.45	109.25
1	B	107	ASP	CA-CB-CG	9.00	121.60	112.60
1	A	345	ASP	CA-CB-CG	8.91	121.51	112.60
1	A	232	ILE	N-CA-C	-8.83	97.24	108.89
1	A	285	ILE	N-CA-CB	8.78	120.19	110.62
1	A	20	ASP	CA-CB-CG	8.73	121.33	112.60
1	B	326	THR	CA-CB-OG1	-8.71	96.54	109.60
1	B	14	HIS	CA-CB-CG	8.69	122.49	113.80
1	A	314	THR	N-CA-C	-8.67	95.80	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	VAL	N-CA-C	-8.53	100.58	110.21
1	B	327	LEU	N-CA-C	-8.52	102.47	113.12
1	A	284	ASN	OD1-CG-ND2	-8.47	114.13	122.60
1	B	100	PRO	N-CA-C	8.44	129.85	112.47
1	B	225	ASN	CA-CB-CG	8.33	120.93	112.60
1	B	102	ILE	N-CA-C	8.25	119.61	106.32
1	A	332	PHE	N-CA-C	8.22	123.44	113.41
1	A	50	VAL	N-CA-C	-8.22	96.60	108.36
1	B	360	PHE	N-CA-C	-8.18	96.34	109.76
1	B	193	ILE	N-CA-C	8.14	119.64	108.89
1	B	59	SER	N-CA-C	-8.11	103.39	113.28
1	A	119	GLN	OE1-CD-NE2	-8.10	114.50	122.60
1	B	326	THR	CA-CB-CG2	8.08	124.24	110.50
1	A	142	HIS	CA-CB-CG	8.05	121.85	113.80
1	A	195	GLN	N-CA-C	7.96	119.96	111.28
1	A	163	ASP	CA-CB-CG	7.93	120.53	112.60
1	B	195	GLN	N-CA-C	7.89	120.58	111.11
1	B	85	ASP	CA-CB-CG	7.87	120.47	112.60
1	A	362	ARG	N-CA-C	-7.83	96.92	109.76
1	B	82	MET	CA-CB-CG	7.81	129.72	114.10
1	A	87	ASN	N-CA-C	7.80	122.46	111.30
1	B	143	ARG	N-CA-C	-7.75	102.91	111.36
1	A	90	ALA	CA-C-N	-7.67	113.27	122.93
1	A	90	ALA	C-N-CA	-7.67	113.27	122.93
1	B	314	THR	N-CA-C	-7.67	94.27	107.61
1	A	78	VAL	O-C-N	-7.66	112.99	122.57
1	A	103	ASN	N-CA-C	7.62	123.22	111.56
1	B	44	TYR	N-CA-C	-7.62	96.52	109.24
1	A	227	THR	N-CA-C	7.61	122.25	108.17
1	A	84	PHE	CA-CB-CG	7.58	121.38	113.80
1	A	242	THR	N-CA-C	7.56	121.64	110.30
1	B	297	GLN	OE1-CD-NE2	-7.56	115.04	122.60
1	A	270	VAL	CA-C-O	-7.55	112.85	120.85
1	B	61	TRP	N-CA-C	-7.47	96.24	108.41
1	B	136	ALA	N-CA-C	7.43	126.24	109.81
1	A	346	LEU	N-CA-C	7.38	119.12	111.14
1	B	313	GLU	N-CA-C	-7.38	101.34	110.41
1	A	227	THR	CA-C-O	7.37	130.29	121.66
1	B	286	VAL	N-CA-CB	7.36	122.09	110.31
1	B	129	GLU	N-CA-C	-7.33	101.49	112.04
1	A	70	ASN	CA-CB-CG	-7.31	105.29	112.60
1	A	176	LYS	N-CA-C	-7.30	98.26	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	PRO	N-CA-C	7.24	123.10	113.40
1	A	61	TRP	CB-CG-CD1	-7.23	116.06	126.90
1	A	357	TYR	N-CA-C	7.23	122.66	113.55
1	A	112	LEU	CA-C-O	-7.21	113.23	120.80
1	B	26	VAL	N-CA-CB	7.19	121.37	110.58
1	A	309	SER	N-CA-C	7.18	120.11	108.76
1	A	61	TRP	CG-CD2-CE3	7.18	141.08	133.90
1	A	177	ILE	N-CA-CB	-7.17	103.01	111.83
1	A	380	ALA	N-CA-C	-7.16	102.66	111.40
1	B	261	ALA	CA-C-N	-7.16	110.70	120.44
1	B	261	ALA	C-N-CA	-7.16	110.70	120.44
1	A	254	MET	N-CA-C	7.12	121.42	112.87
1	A	5	PHE	CA-CB-CG	7.12	120.92	113.80
1	A	152	ARG	CA-CB-CG	7.06	128.22	114.10
1	B	163	ASP	N-CA-C	7.05	120.45	110.23
1	B	33	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	A	232	ILE	N-CA-CB	-7.03	102.87	110.53
1	B	157	LEU	N-CA-C	-7.02	98.37	109.04
1	A	154	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	A	78	VAL	N-CA-C	6.99	123.87	109.34
1	B	79	HIS	CA-CB-CG	6.97	120.77	113.80
1	A	85	ASP	CA-CB-CG	6.96	119.56	112.60
1	B	119	GLN	CA-CB-CG	6.96	128.02	114.10
1	A	255	ALA	CB-CA-C	-6.96	98.88	110.29
1	A	14	HIS	N-CA-C	-6.95	101.02	109.57
1	A	364	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	A	239	CYS	CA-CB-SG	-6.92	98.48	114.40
1	A	146	GLN	CA-CB-CG	-6.89	100.32	114.10
1	B	160	LEU	N-CA-C	-6.87	98.75	109.25
1	A	102	ILE	O-C-N	-6.86	114.63	122.17
1	B	142	HIS	CB-CG-CD2	-6.84	122.31	131.20
1	A	256	ARG	N-CA-C	-6.84	99.77	109.96
1	A	286	VAL	N-CA-C	6.84	116.98	110.42
1	B	42	GLU	CB-CA-C	-6.81	100.30	110.24
1	B	80	SER	N-CA-C	6.81	121.19	112.34
1	A	270	VAL	N-CA-CB	6.81	120.79	110.58
1	B	357	TYR	N-CA-C	6.81	119.79	110.06
1	B	222	PHE	N-CA-C	6.78	118.74	109.11
1	A	359	HIS	CB-CG-CD2	-6.77	122.39	131.20
1	B	232	ILE	O-C-N	6.76	129.69	122.45
1	A	194	ASP	CA-CB-CG	6.76	119.36	112.60
1	B	14	HIS	CB-CG-CD2	-6.75	122.42	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	TRP	CB-CG-CD1	-6.74	116.79	126.90
1	B	187	THR	CA-CB-OG1	-6.73	99.51	109.60
1	B	364	HIS	N-CA-CB	6.73	121.86	110.49
1	A	54	GLY	O-C-N	-6.71	116.35	123.00
1	A	13	GLY	CA-C-N	6.71	130.43	120.83
1	A	13	GLY	C-N-CA	6.71	130.43	120.83
1	B	326	THR	CB-CA-C	6.68	122.73	110.36
1	B	250	THR	O-C-N	-6.66	113.26	121.92
1	A	18	ILE	N-CA-CB	6.64	119.07	110.57
1	B	159	TRP	CG-CD2-CE3	6.64	140.54	133.90
1	B	128	ASN	N-CA-CB	6.63	120.61	110.60
1	B	260	GLY	N-CA-C	6.61	128.84	113.18
1	B	171	GLN	CA-C-O	6.59	129.06	121.28
1	A	371	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	216	LEU	N-CA-C	6.57	120.32	107.57
1	A	284	ASN	CB-CG-ND2	6.57	126.25	116.40
1	B	101	ASP	CA-C-O	-6.55	111.14	120.51
1	A	167	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	A	210	ILE	CB-CA-C	6.52	117.67	110.62
1	B	261	ALA	N-CA-C	6.52	119.91	108.56
1	B	66	GLU	N-CA-C	-6.52	104.10	111.14
1	B	346	LEU	N-CA-C	6.51	119.37	111.82
1	A	343	MET	N-CA-C	6.50	120.31	112.38
1	B	101	ASP	O-C-N	-6.50	113.95	122.59
1	A	26	VAL	N-CA-C	-6.46	104.19	110.72
1	A	134	MET	O-C-N	-6.46	116.24	121.80
1	A	169	THR	O-C-N	-6.45	115.63	123.30
1	A	9	SER	N-CA-C	-6.44	98.49	109.24
1	B	28	ASP	N-CA-C	-6.40	103.99	110.97
1	B	365	PHE	CA-CB-CG	6.40	120.20	113.80
1	B	101	ASP	N-CA-C	6.39	124.41	110.80
1	B	332	PHE	N-CA-C	6.36	118.56	110.61
1	B	232	ILE	N-CA-C	-6.34	98.37	107.37
1	B	374	GLN	CB-CG-CD	6.34	123.38	112.60
1	B	57	THR	CA-C-O	-6.34	113.47	120.38
1	B	167	GLN	CB-CA-C	-6.33	98.57	109.65
1	B	110	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	324	GLN	CB-CG-CD	6.32	123.34	112.60
1	A	236	MET	CG-SD-CE	-6.31	87.02	100.90
1	A	91	VAL	N-CA-CB	6.30	118.55	110.99
1	B	250	THR	CA-C-O	-6.29	110.80	120.16
1	A	108	ARG	N-CA-C	-6.28	98.38	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ASP	N-CA-C	-6.27	99.96	108.24
1	B	151	VAL	CB-CA-C	6.27	120.00	111.97
1	A	382	LEU	N-CA-C	-6.24	104.03	112.26
1	B	107	ASP	N-CA-C	6.23	118.34	110.24
1	A	360	PHE	CA-CB-CG	6.21	120.01	113.80
1	A	271	ASP	CB-CA-C	-6.20	98.43	110.46
1	A	63	ASP	CA-C-O	-6.20	113.68	120.81
1	B	207	ILE	N-CA-C	6.19	116.30	110.30
1	B	364	HIS	CB-CG-CD2	-6.18	123.17	131.20
1	A	133	LEU	N-CA-C	6.18	118.89	109.62
1	B	272	ARG	N-CA-C	-6.18	103.86	111.40
1	B	81	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	199	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	B	189	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	B	178	VAL	N-CA-C	6.13	122.09	109.34
1	B	167	GLN	N-CA-CB	6.10	121.06	110.81
1	A	348	HIS	CB-CG-CD2	-6.09	123.29	131.20
1	B	103	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	B	118	ASP	O-C-N	-6.00	114.77	122.20
1	B	247	ILE	CB-CA-C	6.00	119.87	112.02
1	B	8	GLU	CA-CB-CG	5.99	126.09	114.10
1	A	211	LEU	N-CA-C	5.99	119.18	108.47
1	A	132	VAL	N-CA-CB	5.98	119.15	112.34
1	B	119	GLN	N-CA-CB	-5.97	101.80	110.70
1	A	357	TYR	CA-CB-CG	-5.97	103.16	113.90
1	A	10	VAL	CA-CB-CG2	-5.96	100.27	110.40
1	A	118	ASP	N-CA-C	5.95	116.14	108.34
1	B	54	GLY	O-C-N	-5.94	116.79	123.62
1	B	302	ILE	N-CA-CB	5.93	116.99	110.53
1	B	336	ARG	CB-CG-CD	5.92	124.92	111.30
1	B	329	VAL	N-CA-C	-5.92	104.74	110.42
1	B	52	VAL	N-CA-CB	-5.91	104.50	111.60
1	B	262	PHE	CA-CB-CG	-5.89	107.91	113.80
1	A	32	GLU	CB-CG-CD	-5.88	102.59	112.60
1	B	20	ASP	N-CA-CB	-5.88	101.24	110.06
1	A	162	PRO	N-CA-C	5.87	124.56	112.47
1	B	259	GLY	CA-C-N	-5.86	109.92	121.41
1	B	259	GLY	C-N-CA	-5.86	109.92	121.41
1	A	134	MET	CG-SD-CE	-5.85	88.03	100.90
1	A	217	THR	CA-CB-CG2	5.84	120.44	110.50
1	B	345	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	304	VAL	N-CA-C	5.83	116.05	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	B	259	GLY	O-C-N	-5.81	115.15	122.70
1	A	66	GLU	N-CA-C	5.79	117.68	111.36
1	A	92	LEU	O-C-N	-5.79	116.13	122.84
1	A	110	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	130	THR	N-CA-C	5.76	123.07	110.80
1	A	238	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	306	GLU	CB-CA-C	5.75	121.49	110.17
1	B	79	HIS	N-CA-CB	5.74	119.23	109.87
1	B	279	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	A	64	ILE	CB-CG1-CD1	-5.72	101.78	113.80
1	A	263	SER	CB-CA-C	-5.72	99.86	109.53
1	B	381	GLY	N-CA-C	-5.72	101.91	112.62
1	A	147	ARG	N-CA-CB	5.71	119.13	110.28
1	B	114	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	8	GLU	CB-CG-CD	5.70	122.29	112.60
1	A	11	SER	CA-C-O	-5.69	115.40	121.94
1	A	157	LEU	N-CA-C	-5.67	101.39	109.62
1	A	84	PHE	N-CA-C	-5.67	98.58	107.93
1	B	70	ASN	CA-CB-CG	5.66	118.26	112.60
1	A	32	GLU	CA-C-O	5.66	126.47	119.97
1	B	170	PHE	CA-CB-CG	5.66	119.45	113.80
1	B	79	HIS	CB-CG-CD2	-5.65	123.85	131.20
1	A	100	PRO	N-CA-C	5.65	124.10	112.47
1	A	104	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	A	206	ILE	CA-CB-CG1	5.63	119.98	110.40
1	A	168	VAL	CG1-CB-CG2	-5.62	98.43	110.80
1	B	172	TYR	N-CA-C	-5.62	99.85	109.24
1	B	165	LYS	N-CA-C	-5.60	102.17	110.46
1	B	242	THR	CA-CB-OG1	-5.60	101.20	109.60
1	B	91	VAL	O-C-N	-5.60	117.27	123.03
1	B	139	THR	N-CA-C	-5.60	104.82	111.03
1	B	279	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	A	318	GLU	N-CA-C	5.59	118.09	110.55
1	B	383	LYS	N-CA-C	5.59	126.65	111.00
1	B	271	ASP	CB-CA-C	-5.58	101.58	110.84
1	A	225	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	355	ALA	O-C-N	5.58	128.05	122.03
1	B	217	THR	N-CA-CB	5.57	118.19	110.17
1	A	349	PRO	N-CA-C	5.57	123.94	112.47
1	B	49	MET	N-CA-C	5.56	118.51	109.06
1	A	211	LEU	CA-C-O	5.54	122.89	119.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ASP	O-C-N	-5.53	116.74	123.16
1	B	255	ALA	N-CA-C	5.53	118.55	109.76
1	A	173	ASP	CA-C-O	-5.53	115.00	120.80
1	A	243	GLY	CA-C-N	-5.52	112.39	122.38
1	A	243	GLY	C-N-CA	-5.52	112.39	122.38
1	A	176	LYS	CA-C-O	5.51	127.68	121.51
1	B	374	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	B	259	GLY	CA-C-O	-5.51	110.99	120.57
1	B	36	LYS	N-CA-C	5.49	119.85	113.20
1	B	200	GLU	CB-CG-CD	5.48	121.91	112.60
1	A	334	ASP	O-C-N	5.48	129.57	122.89
1	A	206	ILE	N-CA-CB	5.46	120.24	111.23
1	A	134	MET	CB-CA-C	-5.46	100.42	108.87
1	B	147	ARG	N-CA-C	5.45	117.98	111.71
1	A	102	ILE	CA-CB-CG1	5.44	119.65	110.40
1	B	231	VAL	CB-CA-C	5.44	120.21	111.29
1	A	51	LEU	CA-C-O	-5.44	114.89	120.54
1	B	109	ALA	CB-CA-C	-5.43	104.62	113.37
1	A	107	ASP	O-C-N	-5.43	116.48	122.72
1	B	359	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	B	212	PRO	N-CA-C	5.41	123.61	112.47
1	B	137	PRO	O-C-N	-5.41	116.06	122.17
1	A	266	ASP	CA-C-N	5.40	126.59	119.84
1	A	266	ASP	C-N-CA	5.40	126.59	119.84
1	B	339	GLY	N-CA-C	-5.40	106.24	112.50
1	A	244	ARG	CA-C-O	5.40	125.81	119.28
1	A	318	GLU	CB-CG-CD	5.39	121.77	112.60
1	A	145	VAL	O-C-N	-5.39	116.43	121.87
1	A	37	ALA	CB-CA-C	-5.38	100.80	109.72
1	A	66	GLU	CA-C-O	-5.37	114.72	120.42
1	B	363	GLU	O-C-N	-5.37	115.44	122.59
1	A	19	ALA	O-C-N	5.36	127.66	122.09
1	A	283	LYS	O-C-N	5.34	127.86	122.09
1	B	367	TRP	CG-CD2-CE3	5.33	139.23	133.90
1	A	351	TYR	CA-C-O	-5.32	112.34	119.47
1	A	246	ILE	N-CA-CB	-5.32	106.36	112.21
1	A	1	ALA	N-CA-C	-5.31	96.13	111.00
1	A	351	TYR	N-CA-C	5.30	120.23	113.18
1	B	260	GLY	CA-C-O	5.30	129.79	120.57
1	A	133	LEU	CB-CA-C	5.29	120.06	112.12
1	A	6	THR	N-CA-CB	-5.29	103.06	111.62
1	A	348	HIS	CB-CG-ND1	5.29	130.63	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	LEU	O-C-N	-5.28	117.14	123.27
1	A	128	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	184	VAL	CB-CA-C	-5.28	103.86	111.19
1	B	351	TYR	CA-C-O	-5.28	113.11	119.49
1	A	61	TRP	CE2-CD2-CG	-5.27	100.87	107.20
1	B	140	TYR	CB-CA-C	5.27	120.38	110.63
1	A	84	PHE	CB-CA-C	5.26	117.71	110.34
1	A	89	CYS	N-CA-C	-5.26	100.33	108.90
1	B	356	ALA	CA-C-N	-5.26	114.05	122.62
1	B	356	ALA	C-N-CA	-5.26	114.05	122.62
1	B	151	VAL	N-CA-CB	-5.25	104.41	110.55
1	A	38	ARG	N-CA-CB	5.24	118.80	110.16
1	B	3	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	349	PRO	N-CA-C	-5.23	102.73	111.26
1	A	87	ASN	CA-CB-CG	5.22	117.82	112.60
1	B	139	THR	CA-C-O	-5.22	115.53	120.90
1	B	127	THR	O-C-N	-5.22	115.65	122.59
1	A	194	ASP	CA-C-O	-5.21	115.45	121.19
1	A	242	THR	CA-CB-OG1	-5.20	101.79	109.60
1	B	95	ILE	N-CA-CB	5.20	118.01	111.46
1	A	127	THR	CA-CB-CG2	5.19	119.33	110.50
1	B	267	PRO	N-CD-CG	-5.15	95.47	103.20
1	B	186	SER	N-CA-CB	5.15	118.78	110.65
1	B	279	ARG	N-CA-C	-5.14	107.56	113.88
1	B	336	ARG	CA-CB-CG	5.13	124.37	114.10
1	A	21	GLN	CA-CB-CG	-5.13	103.84	114.10
1	A	157	LEU	CA-C-N	5.13	126.25	119.84
1	A	157	LEU	C-N-CA	5.13	126.25	119.84
1	A	26	VAL	CG1-CB-CG2	-5.12	99.53	110.80
1	A	342	GLN	N-CA-CB	-5.12	102.58	110.16
1	B	63	ASP	CA-C-O	5.11	126.24	120.92
1	B	73	ARG	CA-CB-CG	5.11	124.31	114.10
1	A	244	ARG	NE-CZ-NH2	-5.11	114.61	119.20
1	A	346	LEU	O-C-N	-5.10	116.58	122.09
1	A	195	GLN	CA-C-O	-5.09	115.16	120.55
1	B	187	THR	N-CA-C	-5.08	101.98	110.17
1	B	285	ILE	CA-CB-CG2	5.08	119.14	110.50
1	A	100	PRO	O-C-N	-5.08	115.79	122.64
1	A	260	GLY	N-CA-C	5.07	125.21	113.18
1	A	209	PRO	CA-C-N	-5.07	116.51	122.14
1	A	209	PRO	C-N-CA	-5.07	116.51	122.14
1	B	358	GLY	O-C-N	-5.05	117.77	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	ARG	CB-CA-C	5.05	118.01	109.67
1	B	75	ILE	CA-CB-CG1	5.05	118.99	110.40
1	B	159	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	B	146	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	189	HIS	CB-CG-ND1	5.04	130.26	122.70
1	B	154	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	50	VAL	CB-CA-C	-5.03	102.98	110.33
1	B	320	VAL	N-CA-CB	5.03	118.26	111.21
1	B	237	GLY	CA-C-N	-5.03	115.10	122.19
1	B	237	GLY	C-N-CA	-5.03	115.10	122.19
1	A	42	GLU	CB-CG-CD	5.03	121.15	112.60
1	A	293	ARG	CA-C-O	-5.01	114.12	120.28
1	B	283	LYS	N-CA-C	-5.01	105.10	111.11
1	A	159	TRP	CB-CA-C	5.01	118.85	110.44
1	A	177	ILE	CA-CB-CG1	5.01	118.91	110.40
1	A	118	ASP	CA-CB-CG	-5.00	107.60	112.60

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ASP	Peptide
1	A	125	TYR	Sidechain
1	A	132	VAL	Mainchain
1	A	143	ARG	Sidechain
1	A	152	ARG	Mainchain
1	A	170	PHE	Sidechain
1	A	251	TYR	Sidechain
1	A	256	ARG	Sidechain
1	A	276	TYR	Sidechain
1	A	280	TYR	Sidechain
1	A	300	TYR	Sidechain
1	A	315	PHE	Sidechain
1	A	351	TYR	Sidechain
1	A	357	TYR	Sidechain
1	A	360	PHE	Sidechain
1	A	362	ARG	Sidechain
1	A	44	TYR	Sidechain
1	A	69	ARG	Sidechain
1	A	84	PHE	Sidechain
1	B	106	VAL	Peptide
1	B	107	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	140	TYR	Sidechain
1	B	170	PHE	Peptide
1	B	172	TYR	Sidechain
1	B	260	GLY	Peptide
1	B	272	ARG	Sidechain
1	B	276	TYR	Sidechain
1	B	280	TYR	Sidechain
1	B	294	CYS	Peptide
1	B	300	TYR	Sidechain
1	B	315	PHE	Sidechain
1	B	336	ARG	Sidechain
1	B	338	TYR	Sidechain
1	B	359	HIS	Sidechain
1	B	363	GLU	Mainchain
1	B	38	ARG	Sidechain
1	B	84	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2942	643	2908	171	0
1	B	2942	643	2908	187	0
All	All	5884	1286	5816	344	0

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 29.

All (344) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:HG12	1:B:50:VAL:HG13	1.54	0.87
1:A:30:ILE:HG12	1:A:58:THR:HG21	1.59	0.85
1:B:251:TYR:HB2	1:B:255:ALA:HB2	1.60	0.84
1:B:203:MET:SD	1:B:222:PHE:HE2	2.01	0.83
1:B:134:MET:SD	1:B:279:ARG:NH2	2.51	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:TYR:HE1	1:B:359:HIS:HB3	1.45	0.81
1:B:45:VAL:HG22	1:B:240:GLY:HA3	1.64	0.80
1:B:152:ARG:HB3	1:B:160:LEU:HD11	1.64	0.80
1:A:121:LEU:HB2	1:A:297:GLN:HE22	1.47	0.79
1:A:134:MET:SD	1:A:279:ARG:NH2	2.55	0.79
1:A:15:PRO:HB2	1:A:240:GLY:HA3	1.64	0.78
1:A:177:ILE:HG13	1:A:215:TRP:CZ2	2.21	0.76
1:B:65:GLU:HG3	1:B:91:VAL:HG11	1.67	0.76
1:B:278:ALA:HA	1:B:281:VAL:HG23	1.69	0.75
1:B:134:MET:HG3	1:B:135:PRO:HD2	1.66	0.75
1:B:138:ILE:HB	1:B:252:GLY:HA2	1.69	0.74
1:A:292:ASP:HB2	1:A:317:THR:HG22	1.67	0.74
1:A:46:LYS:HB3	1:A:239:CYS:HG	1.50	0.74
1:B:203:MET:SD	1:B:222:PHE:CE2	2.81	0.72
1:B:130:THR:OG1	1:B:136:ALA:HB3	1.93	0.69
1:A:21:GLN:HE21	1:A:352:LYS:HE3	1.56	0.68
1:B:72:VAL:HG11	1:B:84:PHE:CE1	2.28	0.68
1:A:281:VAL:HG21	1:A:296:ILE:HD12	1.76	0.68
1:A:266:ASP:HB2	1:A:267:PRO:HD2	1.74	0.68
1:A:157:LEU:HD23	1:A:159:TRP:CZ2	2.30	0.67
1:B:11:SER:HA	1:B:357:TYR:HE1	1.60	0.66
1:B:134:MET:HA	1:B:279:ARG:HH22	1.60	0.66
1:B:5:PHE:CE2	1:B:254:MET:SD	2.88	0.66
1:A:161:ARG:O	1:A:188:GLN:HB3	1.96	0.66
1:B:122:MET:HG2	1:B:274:ALA:HB3	1.78	0.66
1:A:157:LEU:HD22	1:A:160:LEU:HD21	1.78	0.66
1:A:203:MET:SD	1:A:222:PHE:CD2	2.89	0.65
1:B:138:ILE:HB	1:B:252:GLY:CA	2.27	0.65
1:A:9:SER:HB2	1:A:141:ALA:HB1	1.78	0.65
1:A:10:VAL:HG23	1:A:165:LYS:HA	1.79	0.65
1:A:46:LYS:HB3	1:A:239:CYS:SG	2.37	0.65
1:B:129:GLU:HG2	1:B:135:PRO:HA	1.78	0.65
1:B:147:ARG:HD3	1:B:206:ILE:HA	1.78	0.64
1:A:261:ALA:HB3	1:A:265:LYS:NZ	2.13	0.64
1:A:297:GLN:HB3	1:A:311:MET:HB3	1.80	0.64
1:B:50:VAL:HG23	1:B:89:CYS:SG	2.37	0.64
1:A:30:ILE:HG21	1:A:39:VAL:HG11	1.79	0.64
1:A:262:PHE:O	1:A:272:ARG:HD3	1.99	0.63
1:B:145:VAL:HG12	1:B:206:ILE:HD11	1.80	0.63
1:A:245:LYS:HE3	1:A:245:LYS:HA	1.81	0.63
1:B:351:TYR:O	1:B:354:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:SER:HB3	1:B:164:ALA:HB3	1.81	0.62
1:A:308:THR:HG23	1:B:221:LYS:HZ2	1.64	0.62
1:B:42:GLU:HA	1:B:242:THR:HG21	1.82	0.62
1:B:109:ALA:HB2	1:B:115:GLY:HA2	1.82	0.62
1:B:134:MET:SD	1:B:279:ARG:CZ	2.87	0.62
1:A:83:GLY:HA3	1:A:236:MET:HB2	1.80	0.62
1:B:72:VAL:HG11	1:B:84:PHE:HE1	1.65	0.62
1:A:37:ALA:CB	1:A:58:THR:HG22	2.30	0.62
1:B:357:TYR:H	1:B:362:ARG:NH2	1.97	0.61
1:A:172:TYR:HE1	1:A:177:ILE:HG22	1.65	0.61
1:A:12:GLU:HB2	1:A:21:GLN:OE1	2.01	0.61
1:A:52:VAL:HG11	1:A:64:ILE:HG21	1.83	0.61
1:B:298:VAL:HG13	1:B:310:ILE:HG22	1.83	0.61
1:A:314:THR:HB	1:A:317:THR:OG1	2.01	0.60
1:A:167:GLN:NE2	1:B:119:GLN:HG2	2.17	0.60
1:B:15:PRO:HA	1:B:18:ILE:HG22	1.82	0.60
1:A:30:ILE:CG2	1:A:39:VAL:HG11	2.32	0.60
1:A:37:ALA:HB2	1:A:58:THR:HG22	1.83	0.60
1:A:261:ALA:HB3	1:A:265:LYS:HZ2	1.65	0.60
1:A:281:VAL:CG2	1:A:296:ILE:HD12	2.32	0.59
1:B:65:GLU:HA	1:B:91:VAL:HG21	1.83	0.59
1:A:9:SER:OG	1:A:142:HIS:HD2	1.86	0.59
1:A:247:ILE:HB	1:B:259:GLY:CA	2.33	0.59
1:A:263:SER:HA	1:A:272:ARG:NH1	2.18	0.59
1:A:320:VAL:HB	1:A:321:PRO:HD2	1.83	0.59
1:B:184:VAL:HB	1:B:223:PHE:HB2	1.84	0.59
1:B:295:GLU:HG2	1:B:315:PHE:HE1	1.68	0.59
1:B:319:LYS:N	1:B:319:LYS:HD2	2.18	0.59
1:B:185:LEU:HD21	1:B:206:ILE:HD13	1.84	0.58
1:A:272:ARG:HG2	1:A:276:TYR:CE2	2.38	0.58
1:A:256:ARG:HH12	1:B:256:ARG:HH22	1.51	0.58
1:B:23:SER:CB	1:B:41:CYS:SG	2.92	0.58
1:A:122:MET:SD	1:A:122:MET:N	2.77	0.57
1:A:239:CYS:SG	1:A:240:GLY:N	2.76	0.57
1:B:133:LEU:HD12	1:B:283:LYS:HG3	1.87	0.57
1:A:188:GLN:HA	1:A:230:PHE:HB3	1.85	0.57
1:A:250:THR:HG22	1:A:360:PHE:CE1	2.39	0.57
1:B:10:VAL:HA	1:B:164:ALA:O	2.03	0.57
1:B:164:ALA:HA	1:B:186:SER:O	2.05	0.57
1:A:159:TRP:O	1:A:189:HIS:HA	2.04	0.57
1:A:17:LYS:NZ	1:A:356:ALA:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLN:HA	1:A:224:ILE:HD11	1.87	0.57
1:A:242:THR:HG22	1:B:244:ARG:NH2	2.19	0.56
1:B:23:SER:HB3	1:B:41:CYS:SG	2.45	0.56
1:B:27:LEU:HD13	1:B:31:LEU:HD21	1.87	0.56
1:B:161:ARG:HE	1:B:190:SER:HA	1.70	0.56
1:A:159:TRP:CD2	1:A:193:ILE:HG13	2.40	0.56
1:B:122:MET:SD	1:B:122:MET:N	2.78	0.56
1:B:171:GLN:HG3	1:B:178:VAL:HG13	1.87	0.56
1:B:367:TRP:O	1:B:368:GLU:HG3	2.06	0.56
1:A:276:TYR:HE1	1:A:359:HIS:HD2	1.52	0.56
1:B:378:ASP:O	1:B:382:LEU:HD23	2.06	0.56
1:A:84:PHE:HD2	1:A:235:PRO:HD2	1.70	0.56
1:B:11:SER:HA	1:B:357:TYR:CE1	2.41	0.56
1:B:152:ARG:HH22	1:B:162:PRO:HG3	1.71	0.56
1:B:272:ARG:NH2	1:B:354:THR:HG21	2.21	0.56
1:A:118:ASP:HA	1:A:302:ILE:HA	1.87	0.55
1:A:37:ALA:HA	1:A:57:THR:O	2.06	0.55
1:A:285:ILE:HA	1:A:376:LEU:HD23	1.89	0.55
1:A:46:LYS:HA	1:A:235:PRO:HB3	1.89	0.55
1:B:127:THR:HB	1:B:129:GLU:HB2	1.89	0.55
1:B:335:LEU:HA	1:B:340:LEU:HD21	1.88	0.55
1:B:121:LEU:C	1:B:122:MET:SD	2.89	0.55
1:B:296:ILE:HA	1:B:311:MET:O	2.07	0.55
1:A:177:ILE:HG13	1:A:215:TRP:HZ2	1.71	0.55
1:A:121:LEU:HB2	1:A:297:GLN:NE2	2.18	0.54
1:A:276:TYR:HE1	1:A:359:HIS:CD2	2.24	0.54
1:B:18:ILE:HD11	1:B:72:VAL:HG22	1.88	0.54
1:A:320:VAL:HG23	1:A:321:PRO:O	2.07	0.54
1:A:159:TRP:CZ3	1:A:198:LEU:HG	2.42	0.54
1:A:259:GLY:N	1:B:247:ILE:HG21	2.22	0.54
1:B:140:TYR:O	1:B:144:LEU:HB2	2.08	0.54
1:A:259:GLY:HA2	1:B:247:ILE:HB	1.90	0.54
1:A:156:THR:HG22	1:A:157:LEU:HD12	1.90	0.53
1:A:40:ALA:HA	1:A:264:GLY:O	2.08	0.53
1:B:56:ILE:HG13	1:B:95:ILE:HD12	1.91	0.53
1:A:22:ILE:HD13	1:A:50:VAL:HG11	1.90	0.53
1:A:280:TYR:O	1:A:284:ASN:HB2	2.08	0.53
1:B:245:LYS:O	1:B:249:ASP:HB2	2.08	0.53
1:B:272:ARG:HH21	1:B:354:THR:HG21	1.72	0.53
1:A:82:MET:O	1:A:232:ILE:HA	2.09	0.53
1:A:320:VAL:HG21	1:A:324:GLN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:TYR:CE1	1:A:341:ILE:HD12	2.43	0.53
1:B:43:THR:HG22	1:B:52:VAL:HA	1.91	0.53
1:B:246:ILE:HB	1:B:257:HIS:HE1	1.74	0.53
1:A:157:LEU:HB2	1:A:160:LEU:HD11	1.91	0.53
1:B:117:GLY:O	1:B:302:ILE:HG13	2.08	0.53
1:A:202:VAL:HA	1:A:206:ILE:HG12	1.90	0.52
1:B:278:ALA:HA	1:B:281:VAL:CG2	2.37	0.52
1:A:308:THR:HG23	1:B:221:LYS:NZ	2.23	0.52
1:A:133:LEU:HD21	1:A:287:ALA:HB2	1.92	0.52
1:B:18:ILE:HG21	1:B:235:PRO:HG3	1.91	0.52
1:B:15:PRO:O	1:B:18:ILE:HG22	2.09	0.52
1:B:41:CYS:HA	1:B:54:GLY:HA3	1.91	0.52
1:A:257:HIS:O	1:B:247:ILE:HG13	2.10	0.52
1:A:324:GLN:HG3	1:A:327:LEU:HD12	1.91	0.52
1:B:30:ILE:HG23	1:B:58:THR:HG21	1.92	0.52
1:B:57:THR:HG22	1:B:98:GLN:HB3	1.92	0.52
1:A:172:TYR:CE1	1:A:177:ILE:HG22	2.44	0.51
1:A:298:VAL:HG21	1:A:335:LEU:HD22	1.92	0.51
1:A:247:ILE:HB	1:B:259:GLY:HA2	1.92	0.51
1:A:121:LEU:HG	1:A:258:GLY:HA3	1.93	0.51
1:A:83:GLY:CA	1:A:236:MET:HB2	2.41	0.51
1:A:300:TYR:CE1	1:A:307:PRO:HB3	2.45	0.51
1:B:44:TYR:HB3	1:B:51:LEU:HD21	1.92	0.51
1:A:3:HIS:HB2	1:A:172:TYR:HB2	1.93	0.50
1:A:242:THR:HG22	1:B:244:ARG:HH21	1.75	0.50
1:B:69:ARG:HG2	1:B:69:ARG:HH11	1.75	0.50
1:A:157:LEU:HD12	1:A:157:LEU:N	2.26	0.50
1:B:170:PHE:CE1	1:B:180:ILE:HD12	2.46	0.50
1:B:189:HIS:O	1:B:231:VAL:HG23	2.11	0.50
1:A:147:ARG:O	1:A:151:VAL:HG22	2.12	0.50
1:A:374:GLN:O	1:A:377:ARG:HG3	2.12	0.50
1:A:174:ASP:C	1:A:176:LYS:H	2.20	0.50
1:B:194:ASP:O	1:B:197:SER:HB3	2.11	0.50
1:B:325:LEU:HA	1:B:328:LEU:HB3	1.93	0.50
1:A:64:ILE:HG22	1:A:68:THR:OG1	2.12	0.50
1:A:133:LEU:HD13	1:A:283:LYS:HE3	1.94	0.50
1:B:202:VAL:HG13	1:B:206:ILE:CG2	2.41	0.50
1:B:8:GLU:HG3	1:B:248:VAL:HG11	1.94	0.50
1:A:245:LYS:HG3	1:A:248:VAL:HG11	1.95	0.49
1:A:276:TYR:HB3	1:A:367:TRP:HB3	1.95	0.49
1:A:324:GLN:O	1:A:327:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:THR:O	1:B:58:THR:HB	2.13	0.49
1:B:161:ARG:HH22	1:B:231:VAL:HG22	1.77	0.49
1:B:144:LEU:HD11	1:B:207:ILE:HA	1.95	0.49
1:B:147:ARG:HB2	1:B:210:ILE:HD11	1.95	0.49
1:A:115:GLY:H	1:A:305:ALA:HB3	1.77	0.49
1:A:116:ALA:N	1:A:305:ALA:HB2	2.28	0.49
1:A:70:ASN:HA	1:A:73:ARG:HD2	1.94	0.49
1:A:188:GLN:HB2	1:A:230:PHE:HD2	1.77	0.49
1:A:224:ILE:HD12	1:A:225:ASN:HB2	1.94	0.48
1:A:61:TRP:CZ3	1:A:97:LYS:HD3	2.48	0.48
1:A:70:ASN:O	1:A:73:ARG:HB2	2.13	0.48
1:B:186:SER:HA	1:B:225:ASN:HB3	1.96	0.48
1:A:34:ASP:HB3	1:A:58:THR:HB	1.94	0.48
1:B:118:ASP:HA	1:B:302:ILE:HB	1.93	0.48
1:B:17:LYS:HD3	1:B:17:LYS:HA	1.77	0.48
1:B:31:LEU:HB3	1:B:349:PRO:HD3	1.95	0.48
1:A:27:LEU:HD13	1:A:39:VAL:CG2	2.43	0.48
1:B:125:TYR:HE2	1:B:135:PRO:HB3	1.79	0.48
1:B:247:ILE:HG23	1:B:252:GLY:O	2.13	0.48
1:B:17:LYS:HD2	1:B:355:ALA:O	2.13	0.48
1:B:26:VAL:HG21	1:B:64:ILE:HG22	1.96	0.48
1:B:124:GLY:HA3	1:B:278:ALA:O	2.14	0.48
1:B:169:THR:HB	1:B:182:ALA:HB3	1.95	0.48
1:A:53:GLY:HA3	1:B:44:TYR:OH	2.14	0.47
1:B:35:PRO:HB2	1:B:347:LEU:HG	1.95	0.47
1:B:37:ALA:HB1	1:B:57:THR:O	2.14	0.47
1:B:185:LEU:HD13	1:B:207:ILE:HD12	1.94	0.47
1:A:15:PRO:HG3	1:A:238:ASP:OD2	2.15	0.47
1:A:66:GLU:O	1:A:70:ASN:HB2	2.15	0.47
1:B:333:PHE:CE1	1:B:372:LYS:HD2	2.49	0.47
1:B:161:ARG:NE	1:B:190:SER:HA	2.29	0.47
1:B:262:PHE:HE1	1:B:275:ALA:HB3	1.80	0.47
1:A:211:LEU:HA	1:A:212:PRO:HD3	1.72	0.47
1:B:138:ILE:HD11	1:B:248:VAL:O	2.15	0.47
1:A:27:LEU:HA	1:A:30:ILE:HG22	1.97	0.47
1:A:77:TYR:HB3	1:A:84:PHE:O	2.13	0.47
1:B:31:LEU:HD12	1:B:35:PRO:HA	1.96	0.47
1:B:239:CYS:SG	1:B:240:GLY:N	2.87	0.47
1:B:23:SER:OG	1:B:43:THR:HG23	2.15	0.47
1:A:7:SER:HB2	1:A:137:PRO:HB2	1.96	0.46
1:B:8:GLU:HA	1:B:166:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ALA:HA	1:B:344:LEU:HD21	1.96	0.46
1:A:245:LYS:HA	1:A:245:LYS:CE	2.45	0.46
1:B:276:TYR:CE1	1:B:359:HIS:HB3	2.37	0.46
1:A:4:LEU:O	1:B:309:SER:HB3	2.15	0.46
1:B:132:VAL:HG13	1:B:134:MET:H	1.80	0.46
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.80	0.46
1:B:262:PHE:CE1	1:B:275:ALA:HB3	2.50	0.46
1:B:33:GLN:OE1	1:B:60:ALA:HA	2.15	0.46
1:B:44:TYR:HB3	1:B:51:LEU:CD2	2.45	0.46
1:B:161:ARG:NH2	1:B:231:VAL:HG22	2.31	0.46
1:B:295:GLU:HG2	1:B:315:PHE:CE1	2.48	0.46
1:A:9:SER:HB2	1:A:141:ALA:CB	2.46	0.45
1:B:5:PHE:CZ	1:B:254:MET:SD	3.09	0.45
1:B:182:ALA:HB2	1:B:221:LYS:HD3	1.98	0.45
1:B:27:LEU:O	1:B:31:LEU:HD22	2.16	0.45
1:B:277:ALA:O	1:B:280:TYR:N	2.50	0.45
1:A:305:ALA:HB1	1:A:336:ARG:HB2	1.97	0.45
1:B:31:LEU:CB	1:B:349:PRO:HD3	2.46	0.45
1:A:152:ARG:HD2	1:A:162:PRO:HG3	1.97	0.45
1:A:337:PRO:O	1:A:340:LEU:HD22	2.17	0.45
1:B:22:ILE:HG21	1:B:68:THR:HG23	1.98	0.45
1:B:77:TYR:OH	1:B:234:GLY:HA2	2.16	0.45
1:B:152:ARG:NH2	1:B:162:PRO:HG3	2.30	0.45
1:B:357:TYR:N	1:B:362:ARG:NH2	2.63	0.45
1:A:79:HIS:H	1:A:82:MET:HE3	1.81	0.45
1:A:320:VAL:HG22	1:A:325:LEU:HD12	1.98	0.45
1:B:202:VAL:HA	1:B:206:ILE:HG22	1.99	0.45
1:B:127:THR:O	1:B:133:LEU:HA	2.16	0.45
1:B:131:ASP:OD1	1:B:132:VAL:HG12	2.17	0.45
1:B:328:LEU:HD13	1:B:380:ALA:HB2	1.99	0.45
1:A:24:ASP:OD1	1:A:264:GLY:N	2.50	0.45
1:B:91:VAL:O	1:B:92:LEU:HD23	2.17	0.45
1:A:333:PHE:CD1	1:A:333:PHE:N	2.85	0.45
1:A:338:TYR:CD1	1:A:341:ILE:HD12	2.52	0.45
1:B:325:LEU:HB2	1:B:328:LEU:HD22	1.99	0.45
1:A:167:GLN:HB3	1:A:184:VAL:CG2	2.47	0.44
1:A:20:ASP:HB3	1:A:355:ALA:HB1	1.99	0.44
1:A:276:TYR:CE1	1:A:359:HIS:CD2	3.05	0.44
1:B:296:ILE:HD11	1:B:298:VAL:HG22	1.98	0.44
1:B:246:ILE:HD12	1:B:257:HIS:ND1	2.33	0.44
1:A:306:GLU:HA	1:A:307:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:HB3	1:B:239:CYS:SG	2.57	0.44
1:B:300:TYR:CD2	1:B:337:PRO:HG3	2.53	0.44
1:A:222:PHE:CD1	1:A:222:PHE:N	2.85	0.44
1:A:236:MET:O	1:A:236:MET:SD	2.76	0.44
1:B:70:ASN:O	1:B:73:ARG:HB3	2.18	0.44
1:B:280:TYR:CE2	1:B:343:MET:SD	3.11	0.44
1:A:74:GLU:OE2	1:A:352:LYS:HD2	2.18	0.44
1:B:144:LEU:HD11	1:B:207:ILE:HG13	2.00	0.44
1:B:163:ASP:O	1:B:187:THR:HA	2.18	0.44
1:B:225:ASN:HA	1:B:226:PRO:HD2	1.82	0.44
1:B:280:TYR:HE2	1:B:343:MET:SD	2.41	0.44
1:A:267:PRO:O	1:A:341:ILE:HD11	2.17	0.44
1:B:246:ILE:HB	1:B:257:HIS:CE1	2.53	0.43
1:B:247:ILE:O	1:B:250:THR:N	2.51	0.43
1:A:49:MET:HE3	1:A:49:MET:HB2	1.71	0.43
1:A:210:ILE:HD13	1:A:210:ILE:HA	1.95	0.43
1:A:213:ALA:HA	1:A:216:LEU:HD12	2.00	0.43
1:B:64:ILE:HD11	1:B:93:SER:OG	2.19	0.43
1:B:281:VAL:HG21	1:B:296:ILE:HD12	1.99	0.43
1:B:77:TYR:CZ	1:B:162:PRO:HG2	2.51	0.43
1:B:140:TYR:HD1	1:B:143:ARG:HG3	1.82	0.43
1:B:134:MET:HG3	1:B:135:PRO:CD	2.43	0.43
1:B:140:TYR:CD1	1:B:143:ARG:HG3	2.53	0.43
1:A:1:ALA:N	1:A:173:ASP:O	2.43	0.43
1:A:127:THR:HG23	1:A:129:GLU:H	1.84	0.43
1:A:69:ARG:HD2	1:A:86:ALA:O	2.19	0.43
1:B:14:HIS:O	1:B:15:PRO:C	2.62	0.43
1:B:152:ARG:CB	1:B:160:LEU:HD11	2.43	0.43
1:A:122:MET:HE2	1:A:122:MET:HB2	1.79	0.43
1:B:188:GLN:HA	1:B:230:PHE:HB3	2.00	0.43
1:A:334:ASP:HB3	1:A:336:ARG:NE	2.34	0.43
1:B:27:LEU:HD13	1:B:31:LEU:CD2	2.47	0.43
1:B:49:MET:HE3	1:B:49:MET:HB2	1.73	0.43
1:A:136:ALA:N	1:A:137:PRO:HD2	2.33	0.42
1:A:320:VAL:CG2	1:A:324:GLN:HB3	2.49	0.42
1:B:54:GLY:O	1:B:95:ILE:HA	2.19	0.42
1:B:139:THR:O	1:B:143:ARG:HG2	2.19	0.42
1:B:251:TYR:HE1	1:B:279:ARG:HH21	1.67	0.42
1:A:64:ILE:HG22	1:A:64:ILE:O	2.19	0.42
1:B:288:ALA:HB2	1:B:373:ALA:HB1	2.01	0.42
1:A:64:ILE:HG21	1:A:64:ILE:HD13	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:SER:HB2	1:A:338:TYR:OH	2.20	0.42
1:B:84:PHE:CD2	1:B:235:PRO:HB2	2.54	0.42
1:A:26:VAL:CG2	1:A:64:ILE:HG23	2.50	0.42
1:A:266:ASP:HB2	1:A:267:PRO:CD	2.45	0.42
1:B:134:MET:SD	1:B:279:ARG:NH1	2.93	0.42
1:B:338:TYR:O	1:B:341:ILE:HB	2.19	0.42
1:A:61:TRP:HZ3	1:A:97:LYS:HD3	1.82	0.42
1:B:211:LEU:HA	1:B:212:PRO:HD3	1.71	0.42
1:A:115:GLY:N	1:A:305:ALA:HB3	2.34	0.42
1:A:217:THR:HB	1:A:218:SER:H	1.73	0.42
1:A:365:PHE:HB2	1:A:368:GLU:HB2	2.02	0.42
1:B:40:ALA:HA	1:B:264:GLY:O	2.20	0.42
1:B:294:CYS:SG	1:B:295:GLU:N	2.93	0.42
1:A:68:THR:HG21	1:A:91:VAL:CG2	2.50	0.42
1:A:133:LEU:HD12	1:A:133:LEU:N	2.35	0.42
1:A:18:ILE:HD11	1:A:75:ILE:HD11	2.02	0.41
1:A:183:VAL:HG11	1:A:211:LEU:HD22	2.02	0.41
1:A:351:TYR:O	1:A:352:LYS:C	2.63	0.41
1:A:250:THR:HG22	1:A:360:PHE:CZ	2.55	0.41
1:B:46:LYS:HB3	1:B:239:CYS:HG	1.85	0.41
1:B:15:PRO:O	1:B:18:ILE:N	2.54	0.41
1:A:123:PHE:CD2	1:A:297:GLN:HB2	2.55	0.41
1:A:217:THR:CB	1:A:219:ALA:H	2.34	0.41
1:A:9:SER:OG	1:A:142:HIS:HA	2.21	0.41
1:A:213:ALA:HA	1:A:216:LEU:HB2	2.03	0.41
1:A:87:ASN:OD1	1:A:87:ASN:N	2.54	0.41
1:A:170:PHE:CZ	1:A:180:ILE:HD12	2.55	0.41
1:A:311:MET:HG2	1:B:3:HIS:CG	2.56	0.41
1:A:358:GLY:N	1:A:362:ARG:HH22	2.18	0.41
1:B:10:VAL:HB	1:B:14:HIS:HB3	2.01	0.41
1:A:3:HIS:O	1:A:172:TYR:N	2.53	0.41
1:A:6:THR:HG23	1:A:169:THR:HG22	2.02	0.41
1:A:154:ASN:N	1:A:154:ASN:HD22	2.18	0.41
1:A:350:ILE:HD12	1:A:350:ILE:HA	1.92	0.41
1:A:377:ARG:HB2	1:A:383:LYS:HA	2.03	0.41
1:B:12:GLU:O	1:B:75:ILE:HG21	2.20	0.41
1:B:15:PRO:HG3	1:B:235:PRO:HA	2.03	0.41
1:B:98:GLN:HE21	1:B:98:GLN:HB2	1.80	0.41
1:B:161:ARG:HG3	1:B:161:ARG:NH1	2.36	0.41
1:A:191:GLU:H	1:A:191:GLU:CD	2.29	0.41
1:A:362:ARG:HD2	1:A:364:HIS:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLN:O	1:B:202:VAL:HB	2.21	0.41
1:A:1:ALA:O	1:A:3:HIS:ND1	2.54	0.40
1:B:193:ILE:HD11	1:B:197:SER:OG	2.22	0.40
1:A:82:MET:SD	1:A:161:ARG:HD2	2.60	0.40
1:B:381:GLY:C	1:B:382:LEU:HG	2.46	0.40
1:A:83:GLY:HA2	1:A:236:MET:HG2	2.02	0.40
1:B:288:ALA:HB3	1:B:290:LEU:HD11	2.02	0.40
1:A:304:VAL:HG12	1:A:306:GLU:O	2.22	0.40
1:B:143:ARG:C	1:B:210:ILE:HG21	2.47	0.40
1:B:161:ARG:HB2	1:B:188:GLN:CD	2.45	0.40
1:B:279:ARG:NH1	1:B:283:LYS:NZ	2.69	0.40

There are no symmetry-related clashes.

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	381/383 (100%)	303 (80%)	69 (18%)	9 (2%)	4	28
1	B	381/383 (100%)	295 (77%)	71 (19%)	15 (4%)	2	18
All	All	762/766 (100%)	598 (78%)	140 (18%)	24 (3%)	3	22

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	THR
1	B	136	ALA
1	A	228	GLY
1	B	47	THR
1	B	227	THR
1	B	231	VAL
1	B	241	LEU

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Mol	Chain	Res	Type
1	B	350	ILE
1	A	60	ALA
1	A	110	ASP
1	A	115	GLY
1	A	252	GLY
1	B	100	PRO
1	B	110	ASP
1	B	218	SER
1	B	254	MET
1	B	322	SER
1	B	334	ASP
1	B	158	PRO
1	B	267	PRO
1	A	259	GLY
1	B	321	PRO
1	A	137	PRO
1	A	349	PRO

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	311/311 (100%)	223 (72%)	88 (28%)	0	2
1	B	311/311 (100%)	221 (71%)	90 (29%)	0	1
All	All	622/622 (100%)	444 (71%)	178 (29%)	0	2

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	7	SER
1	A	10	VAL
1	A	17	LYS
1	A	18	ILE
1	A	38	ARG

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Mol	Chain	Res	Type
1	A	41	CYS
1	A	43	THR
1	A	45	VAL
1	A	46	LYS
1	A	52	VAL
1	A	61	TRP
1	A	67	ILE
1	A	69	ARG
1	A	75	ILE
1	A	78	VAL
1	A	80	SER
1	A	84	PHE
1	A	87	ASN
1	A	88	SER
1	A	99	SER
1	A	104	GLN
1	A	107	ASP
1	A	108	ARG
1	A	118	ASP
1	A	121	LEU
1	A	127	THR
1	A	130	THR
1	A	132	VAL
1	A	139	THR
1	A	145	VAL
1	A	152	ARG
1	A	154	ASN
1	A	156	THR
1	A	157	LEU
1	A	160	LEU
1	A	163	ASP
1	A	177	ILE
1	A	184	VAL
1	A	194	ASP
1	A	195	GLN
1	A	196	LYS
1	A	198	LEU
1	A	199	GLN
1	A	206	ILE
1	A	207	ILE
1	A	210	ILE
1	A	214	GLU

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Mol	Chain	Res	Type
1	A	218	SER
1	A	224	ILE
1	A	232	ILE
1	A	236	MET
1	A	241	LEU
1	A	244	ARG
1	A	245	LYS
1	A	246	ILE
1	A	247	ILE
1	A	248	VAL
1	A	249	ASP
1	A	251	TYR
1	A	262	PHE
1	A	267	PRO
1	A	270	VAL
1	A	273	SER
1	A	285	ILE
1	A	296	ILE
1	A	309	SER
1	A	311	MET
1	A	314	THR
1	A	315	PHE
1	A	317	THR
1	A	318	GLU
1	A	330	ARG
1	A	333	PHE
1	A	335	LEU
1	A	336	ARG
1	A	340	LEU
1	A	341	ILE
1	A	342	GLN
1	A	344	LEU
1	A	346	LEU
1	A	347	LEU
1	A	349	PRO
1	A	352	LYS
1	A	360	PHE
1	A	363	GLU
1	A	376	LEU
1	A	377	ARG
1	B	5	PHE
1	B	7	SER

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Mol	Chain	Res	Type
1	B	9	SER
1	B	15	PRO
1	B	18	ILE
1	B	26	VAL
1	B	28	ASP
1	B	31	LEU
1	B	38	ARG
1	B	39	VAL
1	B	55	GLU
1	B	63	ASP
1	B	64	ILE
1	B	67	ILE
1	B	68	THR
1	B	70	ASN
1	B	74	GLU
1	B	75	ILE
1	B	84	PHE
1	B	93	SER
1	B	98	GLN
1	B	101	ASP
1	B	106	VAL
1	B	107	ASP
1	B	110	ASP
1	B	113	GLU
1	B	118	ASP
1	B	119	GLN
1	B	121	LEU
1	B	127	THR
1	B	130	THR
1	B	131	ASP
1	B	134	MET
1	B	139	THR
1	B	142	HIS
1	B	146	GLN
1	B	158	PRO
1	B	159	TRP
1	B	161	ARG
1	B	174	ASP
1	B	177	ILE
1	B	184	VAL
1	B	185	LEU
1	B	188	GLN

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Mol	Chain	Res	Type
1	B	189	HIS
1	B	192	GLU
1	B	194	ASP
1	B	198	LEU
1	B	204	GLU
1	B	205	GLU
1	B	207	ILE
1	B	211	LEU
1	B	216	LEU
1	B	218	SER
1	B	222	PHE
1	B	225	ASN
1	B	227	THR
1	B	242	THR
1	B	247	ILE
1	B	254	MET
1	B	262	PHE
1	B	263	SER
1	B	268	SER
1	B	281	VAL
1	B	283	LYS
1	B	284	ASN
1	B	285	ILE
1	B	290	LEU
1	B	296	ILE
1	B	298	VAL
1	B	308	THR
1	B	310	ILE
1	B	311	MET
1	B	312	VAL
1	B	314	THR
1	B	315	PHE
1	B	317	THR
1	B	318	GLU
1	B	320	VAL
1	B	325	LEU
1	B	328	LEU
1	B	331	GLU
1	B	332	PHE
1	B	336	ARG
1	B	347	LEU
1	B	352	LYS

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Mol	Chain	Res	Type
1	B	360	PHE
1	B	362	ARG
1	B	364	HIS
1	B	383	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	79	HIS
1	A	104	GLN
1	A	142	HIS
1	A	146	GLN
1	A	154	ASN
1	A	297	GLN
1	A	364	HIS
1	B	70	ASN
1	B	98	GLN
1	B	119	GLN
1	B	128	ASN
1	B	257	HIS
1	B	348	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.