



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:21 PM UTC

PDB ID : 3FLM / pdb_00003flm
Title : Crystal structure of menD from E.coli
Authors : Priyadarshi, A.; Hwang, K.Y.
Deposited on : 2008-12-19
Resolution : 2.70 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

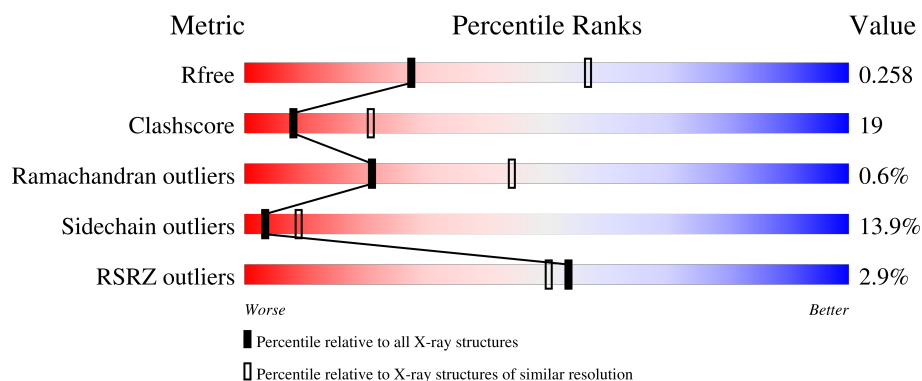
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	556	
1	B	556	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8317 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4158	2636	752	756	14			
1	B	531	Total	C	N	O	S	0	0	0
			4127	2614	747	752	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	LEU	PRO	engineered mutation	UNP P17109
B	36	LEU	PRO	engineered mutation	UNP P17109

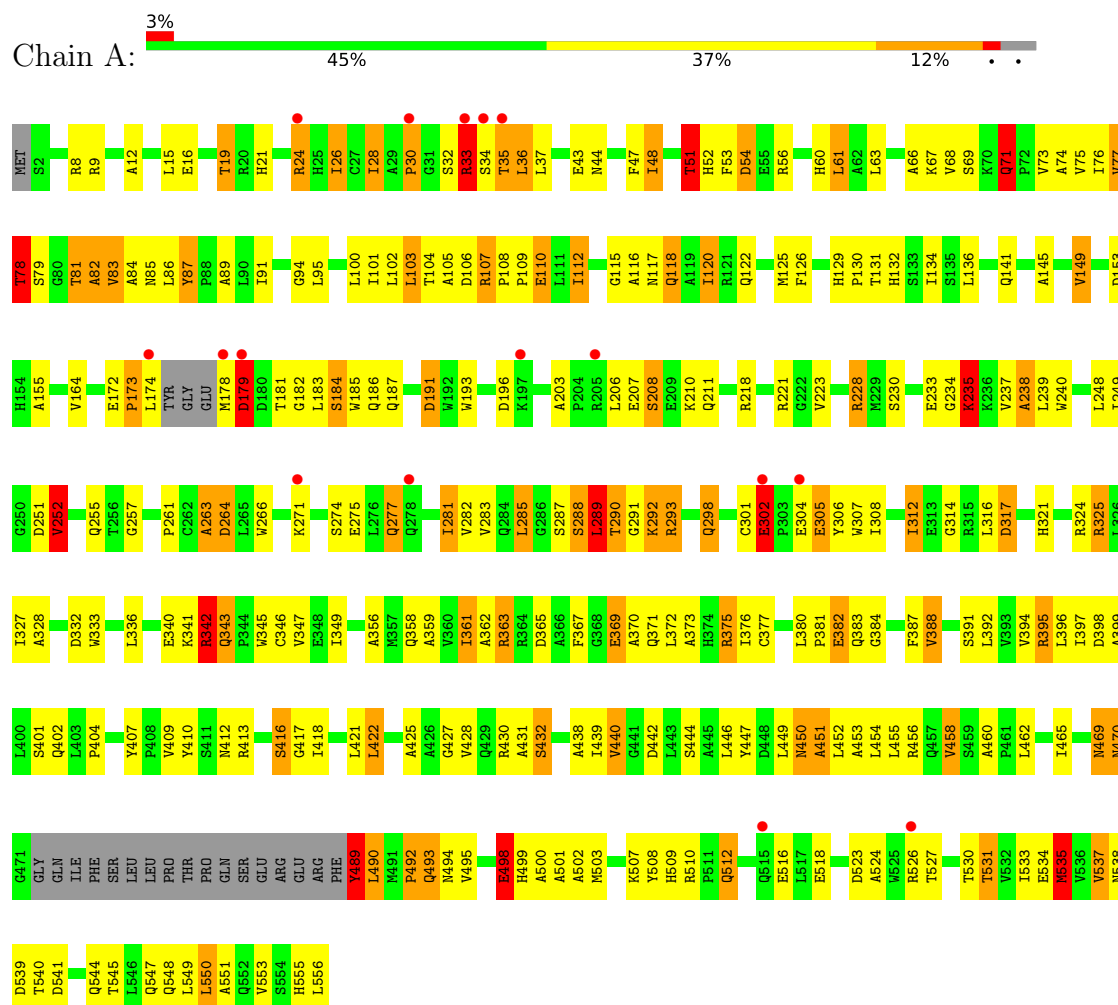
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	18	Total	O	0	0
			18	18		

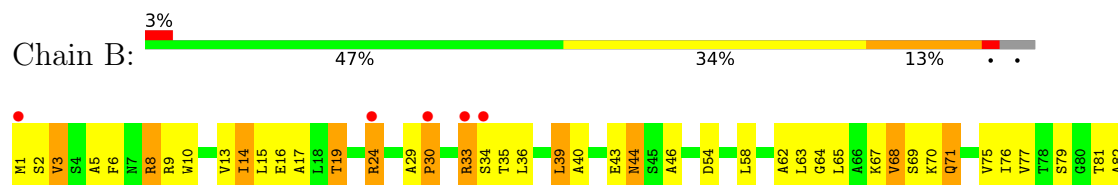
3 Residue-property plots [i](#)

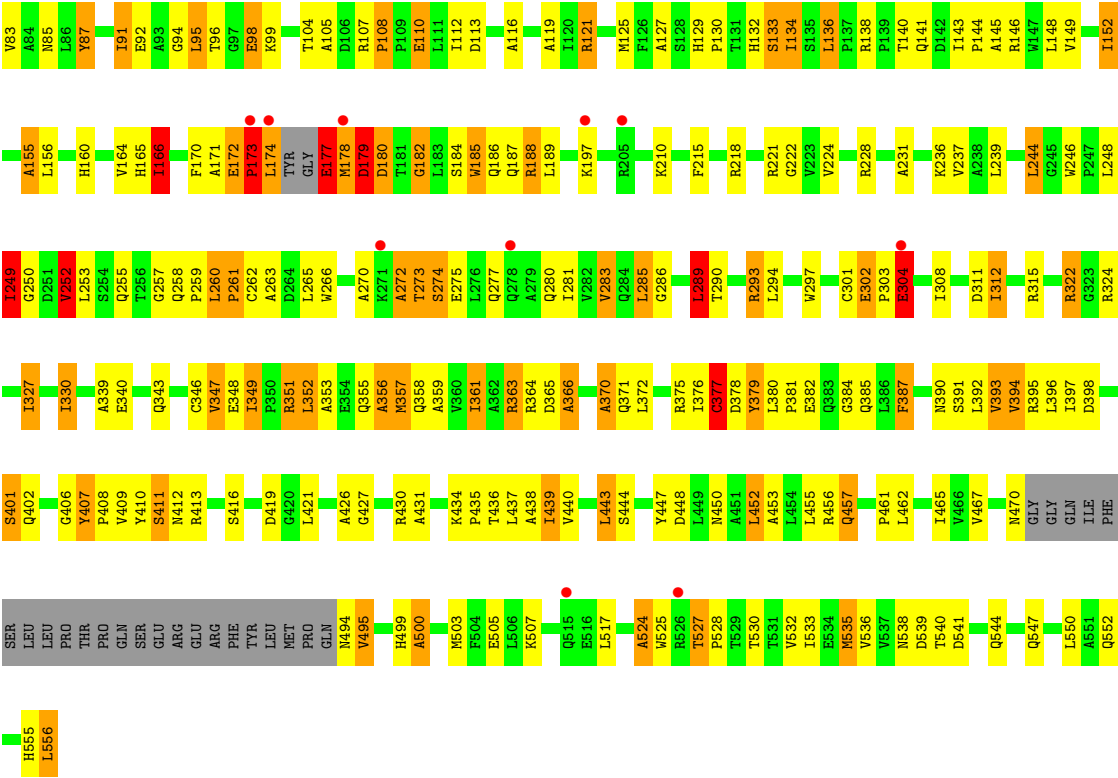
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.07Å 118.07Å 176.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.70) 98.2 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.270 0.178 , 0.258	Depositor DCC
R_{free} test set	1725 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8317	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	1.94	85/4258 (2.0%)	1.79	101/5806 (1.7%)
1	B	1.88	68/4225 (1.6%)	1.82	91/5760 (1.6%)
All	All	1.91	153/8483 (1.8%)	1.80	192/11566 (1.7%)

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	3	5
1	B	0	6
All	All	3	11

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	ALA	CA-CB	-12.69	1.32	1.53
1	A	105	ALA	CA-CB	-10.81	1.35	1.53
1	B	224	VAL	CA-CB	-10.46	1.42	1.54
1	B	155	ALA	CA-CB	-10.30	1.37	1.53
1	A	83	VAL	CA-CB	-9.83	1.43	1.54
1	B	83	VAL	CA-CB	-9.50	1.43	1.54
1	B	62	ALA	CA-CB	-9.43	1.38	1.53
1	B	3	VAL	CA-CB	9.30	1.67	1.54
1	B	30	PRO	CA-C	9.17	1.65	1.52
1	A	249	ILE	CA-CB	-8.97	1.43	1.54
1	A	527	THR	N-CA	8.74	1.53	1.45
1	B	444	SER	N-CA	-8.48	1.36	1.46
1	A	545	THR	CA-CB	-8.39	1.39	1.53
1	B	30	PRO	N-CA	8.15	1.57	1.47
1	A	85	ASN	C-O	-8.05	1.13	1.24
1	A	367	PHE	CA-C	-7.79	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	GLY	C-O	-7.74	1.14	1.24
1	B	536	VAL	CA-C	7.69	1.61	1.52
1	A	66	ALA	CA-CB	-7.68	1.41	1.53
1	B	143	ILE	CA-CB	-7.61	1.45	1.54
1	A	356	ALA	CA-CB	-7.59	1.40	1.53
1	B	68	VAL	CA-CB	-7.34	1.46	1.54
1	B	327	ILE	CA-CB	-7.32	1.45	1.53
1	A	425	ALA	CA-CB	-7.12	1.41	1.53
1	B	104	THR	N-CA	7.09	1.54	1.46
1	B	95	LEU	N-CA	-7.04	1.37	1.46
1	A	155	ALA	CA-CB	-7.01	1.42	1.53
1	B	231	ALA	CA-CB	-6.77	1.42	1.53
1	B	136	LEU	CA-C	-6.73	1.46	1.53
1	A	116	ALA	CA-CB	-6.61	1.42	1.53
1	A	110	GLU	CB-CG	-6.57	1.32	1.52
1	A	131	THR	N-CA	-6.52	1.38	1.46
1	A	397	ILE	CA-CB	-6.51	1.46	1.54
1	B	361	ILE	CA-C	6.50	1.61	1.52
1	B	370	ALA	CA-CB	-6.50	1.43	1.53
1	A	382	GLU	CG-CD	6.47	1.68	1.52
1	A	551	ALA	N-CA	6.44	1.54	1.46
1	B	133	SER	C-O	-6.40	1.15	1.24
1	A	86	LEU	C-O	6.39	1.32	1.24
1	A	141	GLN	CD-NE2	6.37	1.46	1.33
1	B	356	ALA	CA-CB	-6.36	1.42	1.53
1	A	230	SER	CA-C	6.35	1.61	1.53
1	B	330	ILE	CA-CB	-6.35	1.47	1.54
1	A	317	ASP	C-O	-6.32	1.18	1.24
1	A	115	GLY	C-O	-6.29	1.15	1.24
1	A	238	ALA	CA-CB	-6.29	1.43	1.53
1	A	91	ILE	CA-CB	-6.28	1.47	1.54
1	B	236	LYS	C-O	6.27	1.31	1.24
1	B	524	ALA	CA-CB	-6.26	1.42	1.53
1	A	30	PRO	CA-C	6.26	1.61	1.52
1	A	105	ALA	CA-C	6.25	1.60	1.52
1	A	77	VAL	CA-C	-6.24	1.45	1.52
1	A	498	GLU	C-O	6.20	1.31	1.24
1	A	531	THR	CA-C	-6.18	1.45	1.52
1	A	347	VAL	CA-C	-6.17	1.45	1.52
1	A	537	VAL	CA-C	6.13	1.59	1.52
1	A	533	ILE	CA-CB	6.10	1.61	1.54
1	A	465	ILE	CA-CB	-6.10	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	ALA	CA-CB	-6.09	1.43	1.53
1	A	305	GLU	CA-C	6.09	1.59	1.52
1	B	505	GLU	CA-C	-6.08	1.45	1.53
1	B	91	ILE	CA-CB	-6.08	1.46	1.54
1	B	179	ASP	CA-C	-6.06	1.46	1.53
1	B	237	VAL	CA-CB	6.04	1.61	1.54
1	A	458	VAL	CA-C	-6.04	1.45	1.52
1	B	75	VAL	CA-C	-5.99	1.45	1.52
1	B	77	VAL	C-O	-5.98	1.17	1.23
1	A	102	LEU	CA-C	-5.97	1.45	1.52
1	B	411	SER	C-O	-5.95	1.16	1.23
1	B	171	ALA	CA-CB	-5.94	1.43	1.53
1	A	502	ALA	CA-CB	-5.93	1.43	1.53
1	B	503	MET	CA-C	5.93	1.61	1.52
1	A	73	VAL	CA-CB	-5.91	1.46	1.54
1	A	288	SER	C-O	5.87	1.31	1.23
1	B	324	ARG	CA-C	-5.87	1.45	1.52
1	A	440	VAL	CA-CB	-5.83	1.46	1.55
1	A	75	VAL	N-CA	-5.82	1.39	1.46
1	A	52	HIS	CA-C	-5.81	1.44	1.52
1	A	333	TRP	CA-C	-5.79	1.45	1.52
1	B	160	HIS	N-CA	5.77	1.53	1.46
1	A	361	ILE	CG1-CD1	5.76	1.74	1.51
1	B	134	ILE	C-O	-5.75	1.18	1.24
1	A	112	ILE	CG1-CD1	-5.74	1.29	1.51
1	A	271	LYS	CA-CB	5.74	1.62	1.53
1	A	287	SER	CA-CB	-5.73	1.46	1.54
1	A	193	TRP	C-O	-5.71	1.16	1.24
1	A	399	ALA	CA-CB	-5.69	1.44	1.53
1	B	447	TYR	N-CA	-5.68	1.39	1.46
1	A	203	ALA	CA-CB	5.65	1.59	1.53
1	A	289	LEU	CA-CB	-5.60	1.44	1.53
1	A	54	ASP	CA-C	5.59	1.59	1.52
1	B	495	VAL	CA-CB	5.55	1.62	1.54
1	A	120	ILE	CA-C	5.55	1.58	1.52
1	B	416	SER	CA-C	-5.55	1.46	1.53
1	B	134	ILE	CA-CB	-5.53	1.47	1.54
1	A	332	ASP	CA-C	-5.51	1.45	1.52
1	B	308	ILE	C-O	5.51	1.30	1.24
1	B	119	ALA	CA-CB	5.51	1.63	1.53
1	B	261	PRO	N-CA	-5.50	1.40	1.47
1	A	328	ALA	CA-CB	-5.50	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	VAL	C-O	-5.47	1.18	1.24
1	B	127	ALA	CA-CB	5.45	1.62	1.53
1	B	412	ASN	N-CA	-5.44	1.38	1.46
1	A	206	LEU	CA-C	-5.44	1.46	1.52
1	A	361	ILE	CA-CB	5.42	1.61	1.54
1	A	81	THR	N-CA	5.42	1.53	1.46
1	B	244	LEU	CA-C	5.42	1.60	1.52
1	A	553	VAL	N-CA	-5.42	1.39	1.46
1	B	44	ASN	CA-C	-5.41	1.46	1.52
1	A	126	PHE	N-CA	-5.39	1.39	1.46
1	B	500	ALA	CA-C	-5.37	1.46	1.52
1	A	173	PRO	CB-CG	5.36	1.72	1.51
1	B	461	PRO	N-CA	5.36	1.53	1.47
1	A	547	GLN	CG-CD	5.36	1.65	1.52
1	B	541	ASP	CA-C	-5.35	1.46	1.52
1	A	510	ARG	CA-C	-5.34	1.46	1.52
1	A	292	LYS	CG-CD	5.32	1.68	1.52
1	B	98	GLU	C-O	-5.30	1.17	1.23
1	A	263	ALA	CA-CB	-5.30	1.44	1.53
1	B	116	ALA	CA-CB	-5.29	1.45	1.53
1	B	435	PRO	C-O	-5.29	1.17	1.23
1	B	83	VAL	N-CA	-5.28	1.40	1.46
1	B	351	ARG	CG-CD	5.27	1.68	1.52
1	A	460	ALA	CA-CB	-5.26	1.46	1.54
1	B	289	LEU	CA-C	5.26	1.59	1.52
1	A	210	LYS	N-CA	-5.26	1.39	1.46
1	B	434	LYS	C-O	-5.25	1.16	1.24
1	A	78	THR	CA-CB	-5.23	1.44	1.53
1	B	286	GLY	N-CA	5.22	1.52	1.45
1	B	185	TRP	N-CA	5.22	1.52	1.46
1	A	373	ALA	CA-CB	-5.20	1.45	1.53
1	A	450	ASN	C-O	-5.18	1.17	1.24
1	A	373	ALA	N-CA	-5.17	1.39	1.46
1	A	89	ALA	CA-CB	-5.16	1.44	1.53
1	A	21	HIS	CA-C	-5.15	1.46	1.52
1	B	143	ILE	CA-C	-5.15	1.48	1.53
1	A	365	ASP	CB-CG	5.14	1.65	1.52
1	A	308	ILE	CA-C	5.14	1.58	1.52
1	A	518	GLU	CG-CD	5.13	1.64	1.52
1	A	134	ILE	CA-CB	-5.13	1.47	1.54
1	A	82	ALA	N-CA	5.12	1.52	1.46
1	B	170	PHE	C-O	-5.11	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	ASP	C-O	5.11	1.30	1.24
1	A	530	THR	CA-C	-5.10	1.46	1.52
1	A	535	MET	CA-C	-5.08	1.46	1.52
1	B	94	GLY	C-O	-5.08	1.17	1.23
1	A	239	LEU	CG-CD2	5.08	1.69	1.52
1	B	221	ARG	N-CA	-5.06	1.40	1.46
1	B	272	ALA	CA-CB	-5.05	1.45	1.53
1	B	145	ALA	CA-CB	-5.04	1.45	1.53
1	B	401	SER	C-O	-5.03	1.17	1.23
1	B	144	PRO	C-O	5.02	1.29	1.23
1	A	507	LYS	CA-C	5.01	1.59	1.52

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	ASP	N-CA-C	12.15	126.22	111.40
1	A	33	ARG	CB-CA-C	-11.67	91.25	109.34
1	A	33	ARG	N-CA-C	11.56	128.12	113.55
1	B	304	GLU	N-CA-C	-10.19	100.18	111.28
1	A	196	ASP	CB-CA-C	-9.99	91.50	110.67
1	A	240	TRP	N-CA-C	-9.75	100.73	111.36
1	B	252	VAL	CB-CA-C	-9.60	95.55	111.29
1	A	432	SER	N-CA-C	-9.25	102.13	113.97
1	B	379	TYR	N-CA-C	8.93	123.73	113.01
1	A	257	GLY	N-CA-C	-8.82	104.20	114.69
1	A	371	GLN	N-CA-C	-8.79	101.39	112.90
1	B	536	VAL	N-CA-C	8.42	120.00	108.89
1	B	179	ASP	N-CA-C	-8.25	97.60	109.31
1	B	257	GLY	N-CA-C	-8.21	105.31	115.08
1	A	179	ASP	CB-CA-C	-7.85	95.03	113.02
1	A	343	GLN	CB-CA-C	7.75	120.73	109.11
1	A	71	GLN	CA-C-N	-7.73	112.04	119.85
1	A	71	GLN	C-N-CA	-7.73	112.04	119.85
1	B	500	ALA	N-CA-C	-7.67	102.04	111.40
1	B	71	GLN	CA-C-N	-7.63	112.14	119.85
1	B	71	GLN	C-N-CA	-7.63	112.14	119.85
1	A	94	GLY	N-CA-C	-7.60	104.96	114.16
1	A	179	ASP	CA-C-N	7.47	135.05	122.65
1	A	179	ASP	C-N-CA	7.47	135.05	122.65
1	B	260	LEU	CA-C-N	7.45	129.15	119.84
1	B	260	LEU	C-N-CA	7.45	129.15	119.84
1	B	34	SER	CB-CA-C	-7.27	98.27	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	THR	N-CA-C	-7.20	98.50	109.95
1	B	108	PRO	CA-C-N	-7.20	112.26	120.04
1	B	108	PRO	C-N-CA	-7.20	112.26	120.04
1	B	301	CYS	CA-C-N	-7.02	114.80	122.59
1	B	301	CYS	C-N-CA	-7.02	114.80	122.59
1	A	108	PRO	CA-C-N	-6.99	112.50	120.04
1	A	108	PRO	C-N-CA	-6.99	112.50	120.04
1	A	540	THR	N-CA-C	6.93	121.86	113.41
1	B	533	ILE	CB-CA-C	-6.84	103.50	111.09
1	B	457	GLN	N-CA-C	6.83	121.43	107.69
1	B	532	VAL	CB-CA-C	-6.76	101.95	111.21
1	A	404	PRO	CB-CA-C	6.74	120.12	111.56
1	B	366	ALA	CA-C-N	-6.73	112.07	122.16
1	B	366	ALA	C-N-CA	-6.73	112.07	122.16
1	A	107	ARG	NE-CZ-NH1	-6.71	114.79	121.50
1	A	24	ARG	N-CA-C	-6.71	104.14	112.72
1	A	418	ILE	N-CA-C	-6.69	104.79	111.88
1	A	308	ILE	N-CA-C	6.68	116.34	106.85
1	A	451	ALA	N-CA-C	-6.62	105.19	113.20
1	A	535	MET	CB-CA-C	-6.61	100.02	110.79
1	B	249	ILE	CB-CA-C	-6.60	102.98	110.96
1	B	132	HIS	CA-C-N	-6.54	113.13	122.94
1	B	132	HIS	C-N-CA	-6.54	113.13	122.94
1	A	388	VAL	CB-CA-C	6.53	118.99	110.12
1	A	252	VAL	CB-CA-C	-6.52	103.50	112.04
1	A	394	VAL	N-CA-C	6.52	117.31	110.72
1	A	342	ARG	CB-CG-CD	6.51	126.27	111.30
1	A	417	GLY	N-CA-C	-6.47	104.25	112.54
1	A	223	VAL	CB-CA-C	-6.45	100.57	110.50
1	B	152	ILE	N-CA-C	-6.42	104.60	110.82
1	B	377	CYS	N-CA-CB	6.41	120.85	110.40
1	A	442	ASP	CA-C-N	-6.38	111.22	120.29
1	A	442	ASP	C-N-CA	-6.38	111.22	120.29
1	B	44	ASN	CA-C-N	-6.35	112.48	122.65
1	B	44	ASN	C-N-CA	-6.35	112.48	122.65
1	B	143	ILE	CA-C-N	-6.32	113.77	120.03
1	B	143	ILE	C-N-CA	-6.32	113.77	120.03
1	A	264	ASP	N-CA-C	-6.31	105.07	112.89
1	B	302	GLU	CA-C-N	6.30	127.17	120.11
1	B	302	GLU	C-N-CA	6.30	127.17	120.11
1	B	129	HIS	CA-C-N	-6.30	113.79	120.03
1	B	129	HIS	C-N-CA	-6.30	113.79	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	GLU	CB-CA-C	-6.29	98.27	110.46
1	A	399	ALA	N-CA-C	-6.28	105.45	113.23
1	B	439	ILE	CB-CA-C	-6.28	101.16	110.82
1	B	14	ILE	N-CA-C	-6.26	103.79	110.36
1	A	60	HIS	N-CA-C	6.25	118.89	111.33
1	B	125	MET	CB-CA-C	-6.25	98.35	110.46
1	B	408	PRO	CA-C-N	-6.22	113.49	122.45
1	B	408	PRO	C-N-CA	-6.22	113.49	122.45
1	A	191	ASP	N-CA-C	-6.21	105.57	113.02
1	A	251	ASP	N-CA-C	-6.20	100.53	110.14
1	A	179	ASP	N-CA-C	-6.18	100.67	108.45
1	A	277	GLN	N-CA-C	-6.16	105.02	112.54
1	A	132	HIS	CA-C-N	-6.16	114.12	122.86
1	A	132	HIS	C-N-CA	-6.16	114.12	122.86
1	A	380	LEU	N-CA-C	6.14	117.12	109.57
1	B	358	GLN	N-CA-C	-6.13	104.67	111.36
1	B	94	GLY	N-CA-C	-6.12	105.17	113.37
1	B	166	ILE	N-CA-CB	6.12	119.05	111.41
1	B	197	LYS	CA-C-N	-6.11	112.20	119.84
1	B	197	LYS	C-N-CA	-6.11	112.20	119.84
1	B	98	GLU	CA-C-O	-6.09	114.45	121.15
1	B	555	HIS	CA-C-N	-6.09	110.73	121.70
1	B	555	HIS	C-N-CA	-6.09	110.73	121.70
1	B	538	ASN	CB-CA-C	-6.09	97.20	109.68
1	A	234	GLY	N-CA-C	-6.08	105.43	112.73
1	A	550	LEU	N-CA-C	-6.06	104.59	111.07
1	A	207	GLU	N-CA-C	6.05	117.92	107.93
1	B	83	VAL	N-CA-C	6.05	116.22	110.42
1	B	387	PHE	CA-C-N	-6.04	115.31	123.10
1	B	387	PHE	C-N-CA	-6.04	115.31	123.10
1	B	452	LEU	N-CA-C	-6.04	104.03	111.33
1	A	425	ALA	N-CA-C	-6.04	104.63	112.23
1	A	235	LYS	N-CA-C	-6.01	104.65	111.14
1	B	249	ILE	N-CA-CB	5.92	117.74	111.00
1	A	112	ILE	CB-CA-C	5.89	119.40	110.62
1	A	341	LYS	N-CA-C	5.89	119.36	110.64
1	A	304	GLU	N-CA-C	-5.88	104.22	111.33
1	A	510	ARG	N-CA-C	-5.85	96.11	108.39
1	B	427	GLY	N-CA-C	-5.85	99.32	113.18
1	A	181	THR	CA-C-N	-5.82	107.60	122.78
1	A	181	THR	C-N-CA	-5.82	107.60	122.78
1	A	271	LYS	N-CA-C	-5.81	104.85	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	ASP	N-CA-C	5.77	120.48	113.38
1	B	143	ILE	N-CA-C	-5.74	101.19	107.73
1	A	136	LEU	CA-C-N	5.72	125.63	119.85
1	A	136	LEU	C-N-CA	5.72	125.63	119.85
1	A	291	GLY	N-CA-C	5.69	119.00	111.03
1	B	315	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	A	95	LEU	CA-C-N	-5.65	113.27	122.26
1	A	95	LEU	C-N-CA	-5.65	113.27	122.26
1	B	138	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	A	343	GLN	CA-C-N	-5.64	113.73	119.83
1	A	343	GLN	C-N-CA	-5.64	113.73	119.83
1	B	8	ARG	N-CA-C	5.61	118.12	111.33
1	A	101	ILE	CA-C-N	-5.60	115.33	122.77
1	A	101	ILE	C-N-CA	-5.60	115.33	122.77
1	B	129	HIS	N-CA-C	5.60	121.11	113.16
1	B	165	HIS	CA-C-N	-5.59	115.60	122.93
1	B	165	HIS	C-N-CA	-5.59	115.60	122.93
1	A	290	THR	N-CA-C	5.58	120.07	112.04
1	B	110	GLU	CB-CA-C	-5.58	98.55	110.32
1	A	548	GLN	N-CA-C	-5.57	105.12	111.14
1	B	107	ARG	N-CA-C	-5.57	102.09	109.84
1	B	352	LEU	N-CA-C	5.52	119.11	112.38
1	B	136	LEU	CA-C-N	-5.50	115.08	120.52
1	B	136	LEU	C-N-CA	-5.50	115.08	120.52
1	A	104	THR	CA-C-N	-5.50	112.91	120.71
1	A	104	THR	C-N-CA	-5.50	112.91	120.71
1	A	526	ARG	N-CA-C	5.49	117.35	111.36
1	B	3	VAL	N-CA-C	-5.46	105.05	111.00
1	A	382	GLU	N-CA-C	-5.46	101.77	109.96
1	A	118	GLN	N-CA-C	-5.44	104.14	111.54
1	A	61	LEU	CB-CG-CD1	-5.44	94.39	110.70
1	B	324	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	B	79	SER	CA-C-O	-5.42	115.41	121.81
1	A	37	LEU	N-CA-C	-5.38	105.85	112.90
1	B	378	ASP	N-CA-CB	5.37	117.94	109.94
1	A	51	THR	CB-CA-C	-5.36	98.29	110.07
1	B	421	LEU	CA-C-N	-5.34	112.70	120.29
1	B	421	LEU	C-N-CA	-5.34	112.70	120.29
1	B	283	VAL	CA-C-N	-5.34	115.63	123.00
1	B	283	VAL	C-N-CA	-5.34	115.63	123.00
1	A	196	ASP	N-CA-C	5.34	118.01	111.82
1	B	311	ASP	CB-CA-C	-5.34	104.60	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	LEU	N-CA-C	5.33	116.95	111.03
1	B	224	VAL	N-CA-C	5.32	115.76	107.99
1	B	412	ASN	CB-CA-C	-5.31	104.21	112.07
1	A	531	THR	CA-C-N	-5.28	115.56	122.37
1	A	531	THR	C-N-CA	-5.28	115.56	122.37
1	A	12	ALA	N-CA-C	-5.26	105.71	111.82
1	A	509	HIS	CA-C-N	-5.24	116.71	123.16
1	A	509	HIS	C-N-CA	-5.24	116.71	123.16
1	A	388	VAL	N-CA-CB	-5.23	104.25	111.99
1	A	555	HIS	CB-CA-C	-5.23	99.38	110.31
1	A	228	ARG	N-CA-C	-5.22	102.13	109.96
1	B	527	THR	CA-C-N	5.22	126.36	119.84
1	B	527	THR	C-N-CA	5.22	126.36	119.84
1	A	325	ARG	CA-CB-CG	5.20	124.49	114.10
1	A	416	SER	CB-CA-C	-5.20	104.51	111.89
1	A	100	LEU	CA-C-N	-5.16	115.93	122.43
1	A	100	LEU	C-N-CA	-5.16	115.93	122.43
1	A	153	ASP	N-CA-C	5.16	116.90	111.28
1	A	361	ILE	CB-CG1-CD1	5.15	124.61	113.80
1	A	126	PHE	N-CA-C	-5.13	105.70	112.94
1	B	39	LEU	CA-C-N	-5.13	113.01	120.29
1	B	39	LEU	C-N-CA	-5.13	113.01	120.29
1	A	431	ALA	N-CA-C	5.12	116.86	111.28
1	A	527	THR	N-CA-C	5.12	118.00	109.09
1	B	297	TRP	CA-CB-CG	-5.12	103.88	113.60
1	A	523	ASP	N-CA-C	-5.11	104.78	111.02
1	B	448	ASP	N-CA-C	-5.11	105.52	112.26
1	B	407	TYR	CA-C-N	5.11	126.22	119.84
1	B	407	TYR	C-N-CA	5.11	126.22	119.84
1	A	498	GLU	N-CA-C	5.10	116.53	110.97
1	A	430	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	B	99	LYS	N-CA-C	5.06	117.36	108.56
1	B	406	GLY	CA-C-N	-5.03	114.61	121.61
1	B	406	GLY	C-N-CA	-5.03	114.61	121.61
1	A	409	VAL	N-CA-C	5.02	115.72	108.48
1	B	224	VAL	N-CA-CB	-5.02	105.34	111.21
1	A	391	SER	N-CA-CB	-5.01	102.63	111.39
1	A	183	LEU	CA-C-N	-5.01	112.36	120.72
1	A	183	LEU	C-N-CA	-5.01	112.36	120.72

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	35	THR	CB
1	A	302	GLU	CA
1	A	493	GLN	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	ASP	Peptide
1	A	302	GLU	Peptide
1	A	469	ASN	Peptide
1	A	489	TYR	Peptide
1	A	492	PRO	Peptide
1	B	172	GLU	Peptide
1	B	173	PRO	Peptide
1	B	177	GLU	Peptide
1	B	179	ASP	Peptide
1	B	182	GLY	Peptide
1	B	390	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4158	0	4131	161	0
1	B	4127	0	4102	167	0
2	A	14	0	0	0	0
2	B	18	0	0	0	0
All	All	8317	0	8233	319	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 19.

All (319) 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:33:ARG:NH2	1:B:174:LEU:HD21	1.51	1.25
1:A:493:GLN:HG2	1:A:494:ASN:N	1.60	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HH22	1:B:174:LEU:HD21	1.00	1.14
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.03	1.13
1:B:363:ARG:HB3	1:B:363:ARG:HH11	1.16	1.10
1:B:252:VAL:HG22	1:B:398:ASP:HB2	1.44	0.97
1:A:179:ASP:OD2	1:A:179:ASP:C	2.10	0.94
1:B:293:ARG:HH11	1:B:293:ARG:HG2	1.29	0.93
1:A:281:ILE:HD12	1:A:282:VAL:N	1.84	0.91
1:A:489:TYR:O	1:A:489:TYR:CD1	2.23	0.90
1:A:493:GLN:CG	1:A:494:ASN:N	2.30	0.90
1:A:372:LEU:HD22	1:A:535:MET:CE	2.02	0.90
1:A:16:GLU:O	1:A:19:THR:HB	1.72	0.89
1:A:358:GLN:O	1:A:361:ILE:HG12	1.74	0.88
1:B:179:ASP:C	1:B:179:ASP:OD1	2.13	0.88
1:A:33:ARG:O	1:A:33:ARG:HG3	1.66	0.87
1:B:174:LEU:N	1:B:174:LEU:HD23	1.88	0.87
1:A:538:ASN:HB2	1:A:541:ASP:OD2	1.74	0.86
1:B:33:ARG:HH22	1:B:174:LEU:CD2	1.87	0.86
1:B:372:LEU:HD22	1:B:535:MET:CE	2.05	0.86
1:A:493:GLN:CG	1:A:494:ASN:H	1.88	0.86
1:B:363:ARG:HB3	1:B:363:ARG:NH1	1.92	0.85
1:A:489:TYR:O	1:A:489:TYR:CG	2.29	0.83
1:A:381:PRO:HG2	1:A:384:GLY:HA3	1.61	0.82
1:A:122:GLN:O	1:A:125:MET:HB2	1.81	0.81
1:A:293:ARG:HH11	1:A:293:ARG:CG	1.89	0.81
1:A:264:ASP:O	1:A:293:ARG:HG3	1.80	0.81
1:A:301:CYS:O	1:A:302:GLU:HB3	1.81	0.81
1:B:33:ARG:O	1:B:33:ARG:CD	2.30	0.80
1:B:177:GLU:CA	1:B:177:GLU:OE2	2.30	0.79
1:A:375:ARG:HG2	1:A:375:ARG:HH11	1.47	0.79
1:A:361:ILE:HG13	1:A:362:ALA:N	1.99	0.78
1:B:293:ARG:HG2	1:B:293:ARG:NH1	1.87	0.78
1:B:381:PRO:HG2	1:B:384:GLY:HA3	1.66	0.77
1:A:372:LEU:HD22	1:A:535:MET:HE3	1.65	0.77
1:A:9:ARG:HG3	1:A:182:GLY:HA3	1.67	0.77
1:A:281:ILE:HD12	1:A:282:VAL:H	1.49	0.77
1:A:422:LEU:N	1:A:422:LEU:HD23	2.00	0.77
1:B:177:GLU:OE2	1:B:177:GLU:HA	1.86	0.76
1:A:293:ARG:HG2	1:A:293:ARG:NH1	1.77	0.76
1:A:498:GLU:HG3	1:A:508:TYR:CE2	2.21	0.74
1:B:363:ARG:HH11	1:B:363:ARG:CB	1.98	0.74
1:A:372:LEU:HD22	1:A:535:MET:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:HD3	1:B:46:ALA:O	1.87	0.74
1:B:372:LEU:HD22	1:B:535:MET:HE3	1.68	0.74
1:B:357:MET:O	1:B:361:ILE:HG13	1.88	0.74
1:B:372:LEU:HD22	1:B:535:MET:HE2	1.70	0.74
1:B:173:PRO:C	1:B:174:LEU:HD23	2.14	0.73
1:B:24:ARG:CD	1:B:46:ALA:O	2.37	0.73
1:A:178:MET:O	1:A:178:MET:HG3	1.87	0.72
1:B:174:LEU:N	1:B:174:LEU:CD2	2.49	0.72
1:A:28:ILE:O	1:A:51:THR:HA	1.89	0.72
1:A:173:PRO:HD2	1:A:173:PRO:O	1.91	0.71
1:A:68:VAL:HG22	1:A:410:TYR:CZ	2.26	0.70
1:A:84:ALA:HB1	1:B:87:TYR:HB3	1.74	0.70
1:A:252:VAL:HG22	1:A:398:ASP:HB2	1.73	0.70
1:A:34:SER:OG	1:A:78:THR:CA	2.40	0.70
1:B:33:ARG:O	1:B:33:ARG:CG	2.40	0.69
1:B:409:VAL:HG12	1:B:410:TYR:N	2.07	0.68
1:B:33:ARG:O	1:B:33:ARG:HD3	1.93	0.68
1:A:395:ARG:HG3	1:A:395:ARG:HH11	1.59	0.68
1:B:121:ARG:NH2	1:B:121:ARG:HG3	2.09	0.68
1:A:261:PRO:HG3	1:A:402:GLN:NE2	2.08	0.68
1:B:164:VAL:HG12	1:B:166:ILE:HD12	1.76	0.68
1:A:129:HIS:N	1:A:130:PRO:CD	2.57	0.67
1:A:305:GLU:HG2	1:A:307:TRP:HE1	1.60	0.67
1:A:489:TYR:N	1:A:490:LEU:HA	2.09	0.67
1:A:470:ASN:OD1	1:A:470:ASN:N	2.28	0.67
1:A:275:GLU:OE1	1:A:349:ILE:HG12	1.96	0.66
1:A:421:LEU:HD12	1:A:444:SER:HB3	1.77	0.66
1:B:69:SER:OG	1:B:71:GLN:HG2	1.95	0.66
1:B:177:GLU:OE2	1:B:177:GLU:N	2.29	0.66
1:B:179:ASP:OD1	1:B:180:ASP:N	2.30	0.64
1:A:179:ASP:OD2	1:A:179:ASP:O	2.16	0.64
1:A:342:ARG:HB3	1:A:342:ARG:NH1	2.13	0.64
1:B:259:PRO:C	1:B:261:PRO:HD3	2.22	0.64
1:B:293:ARG:HH11	1:B:293:ARG:CG	2.07	0.64
1:A:76:ILE:HG12	1:A:103:LEU:HD12	1.78	0.64
1:A:512:GLN:HB2	1:A:516:GLU:OE1	1.97	0.64
1:A:34:SER:O	1:A:36:LEU:N	2.32	0.63
1:A:34:SER:OG	1:A:78:THR:N	2.32	0.61
1:A:342:ARG:CB	1:A:342:ARG:HH11	2.14	0.61
1:A:173:PRO:O	1:A:173:PRO:CD	2.48	0.61
1:A:191:ASP:OD1	1:A:191:ASP:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:VAL:HG12	1:B:166:ILE:CD1	2.32	0.60
1:B:263:ALA:HA	1:B:266:TRP:CE2	2.37	0.60
1:B:393:VAL:HG21	1:B:467:VAL:HG21	1.84	0.59
1:B:355:GLN:NE2	1:B:556:LEU:HG	2.18	0.59
1:B:33:ARG:HE	1:B:33:ARG:HA	1.67	0.59
1:B:381:PRO:HD2	1:B:407:TYR:OH	2.02	0.59
1:A:342:ARG:NH1	1:A:342:ARG:CB	2.65	0.59
1:B:121:ARG:CG	1:B:121:ARG:HH21	2.16	0.59
1:B:252:VAL:CG2	1:B:398:ASP:HB2	2.25	0.59
1:A:538:ASN:CB	1:A:541:ASP:OD2	2.50	0.58
1:B:327:ILE:HD12	1:B:327:ILE:N	2.18	0.58
1:A:499:HIS:HB3	1:B:499:HIS:HB3	1.85	0.58
1:B:6:PHE:CE1	1:B:141:GLN:HG2	2.38	0.58
1:B:263:ALA:HA	1:B:266:TRP:NE1	2.19	0.58
1:A:26:ILE:HG12	1:A:74:ALA:HB3	1.86	0.57
1:A:375:ARG:HG2	1:A:375:ARG:NH1	2.11	0.57
1:B:262:CYS:O	1:B:263:ALA:C	2.48	0.57
1:A:469:ASN:C	1:A:469:ASN:OD1	2.43	0.57
1:A:290:THR:OG1	1:A:413:ARG:NH1	2.35	0.57
1:B:15:LEU:HD12	1:B:40:ALA:HB3	1.85	0.57
1:B:8:ARG:HD3	1:B:36:LEU:CD2	2.35	0.57
1:B:121:ARG:HG3	1:B:121:ARG:HH21	1.69	0.57
1:A:301:CYS:O	1:A:302:GLU:CB	2.52	0.57
1:A:33:ARG:NH1	1:A:106:ASP:O	2.38	0.56
1:A:228:ARG:NH2	1:A:288:SER:OG	2.38	0.56
1:B:283:VAL:HG12	1:B:285:LEU:HD22	1.87	0.56
1:B:290:THR:HA	1:B:413:ARG:NH1	2.21	0.56
1:A:361:ILE:C	1:A:363:ARG:H	2.11	0.56
1:A:490:LEU:H	1:B:457:GLN:NE2	2.02	0.56
1:B:394:VAL:HA	1:B:397:ILE:HD12	1.86	0.56
1:A:34:SER:OG	1:A:78:THR:HA	2.05	0.56
1:A:489:TYR:CD1	1:A:489:TYR:C	2.84	0.56
1:B:244:LEU:HG	1:B:339:ALA:HB1	1.88	0.56
1:B:272:ALA:HB1	1:B:349:ILE:HD13	1.87	0.56
1:B:9:ARG:HB3	1:B:186:GLN:NE2	2.21	0.56
1:A:489:TYR:HA	1:A:490:LEU:HD13	1.87	0.55
1:B:430:ARG:NH2	1:B:457:GLN:HB2	2.22	0.55
1:A:422:LEU:HB2	1:A:451:ALA:HB3	1.89	0.55
1:B:24:ARG:HD2	1:B:46:ALA:O	2.05	0.55
1:A:84:ALA:O	1:A:87:TYR:HB2	2.07	0.54
1:B:182:GLY:O	1:B:185:TRP:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLN:C	1:B:189:LEU:N	2.64	0.54
1:B:259:PRO:C	1:B:261:PRO:CD	2.80	0.54
1:B:108:PRO:HB2	1:B:110:GLU:OE1	2.08	0.54
1:B:259:PRO:O	1:B:261:PRO:CD	2.56	0.54
1:B:33:ARG:O	1:B:33:ARG:HG3	2.07	0.53
1:A:372:LEU:CD2	1:A:535:MET:HE3	2.38	0.53
1:B:249:ILE:N	1:B:249:ILE:HD12	2.24	0.53
1:A:34:SER:O	1:A:35:THR:C	2.50	0.53
1:A:129:HIS:H	1:A:130:PRO:CD	2.22	0.53
1:B:259:PRO:O	1:B:261:PRO:HD2	2.09	0.53
1:A:469:ASN:CG	1:A:469:ASN:O	2.50	0.52
1:A:490:LEU:H	1:B:457:GLN:HE22	1.57	0.52
1:B:409:VAL:CG1	1:B:410:TYR:N	2.72	0.52
1:B:16:GLU:O	1:B:19:THR:HB	2.10	0.52
1:B:15:LEU:CD1	1:B:40:ALA:HB3	2.40	0.52
1:B:112:ILE:O	1:B:113:ASP:HB2	2.09	0.51
1:A:208:SER:HB2	1:A:327:ILE:H	1.75	0.51
1:B:17:ALA:HB2	1:B:149:VAL:HG23	1.91	0.51
1:B:372:LEU:CD2	1:B:535:MET:HE3	2.39	0.51
1:A:382:GLU:O	1:A:383:GLN:HB2	2.10	0.51
1:B:262:CYS:O	1:B:265:LEU:N	2.33	0.51
1:B:285:LEU:HD12	1:B:330:ILE:HG23	1.91	0.51
1:B:455:LEU:HD22	1:B:462:LEU:HD13	1.93	0.51
1:B:81:THR:O	1:B:82:ALA:C	2.53	0.51
1:A:145:ALA:O	1:A:149:VAL:HG12	2.11	0.50
1:A:107:ARG:NH1	1:A:117:ASN:O	2.44	0.50
1:B:426:ALA:O	1:B:430:ARG:HG3	2.10	0.50
1:B:437:LEU:HD11	1:B:465:ILE:HG13	1.92	0.50
1:B:8:ARG:HD3	1:B:36:LEU:HD21	1.93	0.50
1:B:215:PHE:HA	1:B:218:ARG:HE	1.77	0.50
1:B:409:VAL:HG12	1:B:410:TYR:H	1.75	0.50
1:B:452:LEU:O	1:B:453:ALA:C	2.53	0.50
1:A:469:ASN:OD1	1:A:469:ASN:O	2.30	0.50
1:B:258:GLN:O	1:B:261:PRO:HD3	2.12	0.50
1:A:361:ILE:O	1:A:363:ARG:N	2.46	0.49
1:A:358:GLN:O	1:A:361:ILE:CG1	2.56	0.49
1:B:379:TYR:CZ	1:B:517:LEU:HD23	2.47	0.49
1:B:33:ARG:HE	1:B:33:ARG:CA	2.23	0.49
1:B:187:GLN:O	1:B:188:ARG:C	2.53	0.49
1:B:363:ARG:NH1	1:B:363:ARG:CB	2.67	0.49
1:B:387:PHE:O	1:B:438:ALA:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:SER:HA	1:B:277:GLN:HE21	1.76	0.49
1:B:430:ARG:HH21	1:B:457:GLN:HB2	1.77	0.49
1:A:33:ARG:NH2	1:A:172:GLU:OE2	2.46	0.49
1:A:221:ARG:HD2	1:A:345:TRP:CE3	2.48	0.49
1:A:452:LEU:HD23	1:A:455:LEU:HD12	1.95	0.49
1:B:218:ARG:NH2	1:B:340:GLU:HB2	2.27	0.49
1:A:462:LEU:C	1:A:462:LEU:HD23	2.38	0.49
1:A:34:SER:HG	1:A:78:THR:N	2.10	0.48
1:A:500:ALA:O	1:A:501:ALA:C	2.54	0.48
1:B:462:LEU:HD23	1:B:462:LEU:C	2.38	0.48
1:A:524:ALA:HB2	1:A:531:THR:HG21	1.96	0.48
1:B:372:LEU:CD2	1:B:535:MET:CE	2.85	0.48
1:A:33:ARG:C	1:A:35:THR:H	2.21	0.48
1:B:17:ALA:CB	1:B:149:VAL:HG23	2.44	0.48
1:A:281:ILE:HD12	1:A:281:ILE:C	2.37	0.48
1:B:1:MET:O	1:B:2:SER:C	2.56	0.48
1:B:249:ILE:N	1:B:249:ILE:CD1	2.77	0.48
1:A:211:GLN:OE1	1:A:324:ARG:NH2	2.44	0.48
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.68	0.47
1:B:9:ARG:O	1:B:13:VAL:HG23	2.14	0.47
1:B:67:LYS:O	1:B:70:LYS:HE2	2.15	0.47
1:B:270:ALA:HA	1:B:273:THR:OG1	2.15	0.47
1:A:361:ILE:C	1:A:363:ARG:N	2.72	0.47
1:A:446:LEU:HD21	1:A:495:VAL:HG11	1.97	0.47
1:A:503:MET:HE3	1:B:500:ALA:HB2	1.97	0.47
1:A:252:VAL:HG13	1:A:398:ASP:HA	1.97	0.47
1:A:375:ARG:HH11	1:A:375:ARG:CG	2.22	0.47
1:B:67:LYS:HE2	1:B:98:GLU:OE2	2.14	0.47
1:A:44:ASN:HB3	1:A:47:PHE:CE2	2.50	0.47
1:A:450:ASN:C	1:A:450:ASN:OD1	2.58	0.47
1:A:538:ASN:ND2	1:A:541:ASP:OD2	2.47	0.47
1:B:280:GLN:O	1:B:304:GLU:N	2.46	0.47
1:A:317:ASP:OD1	1:A:317:ASP:C	2.58	0.47
1:A:412:ASN:O	1:A:416:SER:HA	2.15	0.47
1:A:469:ASN:HA	1:A:537:VAL:O	2.15	0.46
1:B:63:LEU:HD21	1:B:92:GLU:HG2	1.97	0.46
1:A:48:ILE:N	1:A:48:ILE:HD13	2.30	0.46
1:A:387:PHE:O	1:A:438:ALA:HA	2.15	0.46
1:A:83:VAL:O	1:A:84:ALA:C	2.58	0.46
1:B:69:SER:O	1:B:70:LYS:HB2	2.15	0.46
1:B:8:ARG:NH2	1:B:43:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ALA:O	1:B:371:GLN:HG2	2.16	0.46
1:B:456:ARG:C	1:B:457:GLN:HG2	2.41	0.46
1:A:109:PRO:O	1:A:110:GLU:C	2.53	0.46
1:B:275:GLU:OE1	1:B:349:ILE:HG12	2.16	0.46
1:A:508:TYR:OH	1:A:534:GLU:OE1	2.31	0.46
1:A:407:TYR:CD1	1:A:407:TYR:C	2.94	0.46
1:B:391:SER:O	1:B:392:LEU:C	2.58	0.46
1:B:35:THR:O	1:B:39:LEU:HG	2.16	0.46
1:B:130:PRO:HG2	1:B:133:SER:OG	2.16	0.46
1:B:244:LEU:HG	1:B:339:ALA:CB	2.45	0.46
1:B:91:ILE:O	1:B:92:GLU:C	2.59	0.45
1:B:353:ALA:O	1:B:356:ALA:HB3	2.15	0.45
1:B:381:PRO:HB3	1:B:525:TRP:CZ2	2.51	0.45
1:A:69:SER:CB	1:A:71:GLN:HG3	2.47	0.45
1:A:283:VAL:HG12	1:A:285:LEU:HD22	1.97	0.45
1:A:395:ARG:HG3	1:A:395:ARG:NH1	2.30	0.45
1:A:499:HIS:HB3	1:B:499:HIS:O	2.17	0.45
1:B:134:ILE:HD11	1:B:155:ALA:HB2	1.98	0.45
1:B:289:LEU:HG	1:B:294:LEU:HD21	1.98	0.45
1:B:392:LEU:HD12	1:B:395:ARG:NH1	2.32	0.45
1:B:401:SER:OG	1:B:402:GLN:N	2.48	0.45
1:A:33:ARG:HB3	1:A:78:THR:OG1	2.17	0.45
1:A:33:ARG:C	1:A:35:THR:N	2.73	0.45
1:A:263:ALA:HA	1:A:266:TRP:CD1	2.52	0.45
1:A:298:GLN:HG3	1:A:306:TYR:OH	2.16	0.45
1:B:527:THR:HB	1:B:528:PRO:CD	2.46	0.45
1:A:117:ASN:O	1:A:118:GLN:C	2.60	0.45
1:A:305:GLU:HG2	1:A:307:TRP:NE1	2.30	0.45
1:B:361:ILE:O	1:B:364:ARG:HB3	2.16	0.45
1:A:34:SER:OG	1:A:77:VAL:C	2.61	0.44
1:B:5:ALA:O	1:B:8:ARG:HB2	2.17	0.44
1:B:260:LEU:HA	1:B:261:PRO:HD2	1.67	0.44
1:A:33:ARG:HD2	1:A:79:SER:HB3	1.99	0.44
1:A:53:PHE:CD1	1:A:54:ASP:N	2.85	0.44
1:A:453:ALA:O	1:A:456:ARG:HG3	2.18	0.44
1:A:493:GLN:HG3	1:A:494:ASN:H	1.78	0.44
1:B:312:ILE:HD13	1:B:312:ILE:HG21	1.64	0.44
1:B:356:ALA:O	1:B:359:ALA:HB3	2.17	0.44
1:B:370:ALA:HA	1:B:396:LEU:HD13	1.99	0.44
1:B:347:VAL:HG12	1:B:348:GLU:HG2	2.00	0.44
1:A:56:ARG:NH1	1:A:447:TYR:HE1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:O	1:A:550:LEU:C	2.61	0.43
1:B:76:ILE:HD13	1:B:76:ILE:HG21	1.82	0.43
1:A:184:SER:HA	1:A:187:GLN:HB2	1.99	0.43
1:A:261:PRO:HG3	1:A:402:GLN:HE21	1.80	0.43
1:A:9:ARG:HD2	1:A:186:GLN:CD	2.43	0.43
1:A:120:ILE:HG22	1:B:95:LEU:HD11	2.00	0.43
1:A:489:TYR:N	1:A:490:LEU:HD12	2.33	0.43
1:B:259:PRO:O	1:B:261:PRO:HD3	2.16	0.43
1:B:452:LEU:HD23	1:B:455:LEU:HD12	2.00	0.43
1:B:156:LEU:HA	1:B:156:LEU:HD13	1.65	0.43
1:A:314:GLY:O	1:A:325:ARG:HD3	2.19	0.43
1:B:397:ILE:O	1:B:401:SER:HB3	2.18	0.43
1:A:456:ARG:HE	1:A:456:ARG:HB3	1.66	0.43
1:B:96:THR:HG22	1:B:228:ARG:NH2	2.34	0.43
1:B:13:VAL:O	1:B:14:ILE:C	2.61	0.43
1:B:272:ALA:HB2	1:B:352:LEU:CD1	2.49	0.43
1:B:462:LEU:O	1:B:530:THR:HA	2.18	0.43
1:A:235:LYS:O	1:A:238:ALA:HB3	2.19	0.43
1:B:450:ASN:OD1	1:B:450:ASN:C	2.62	0.43
1:A:69:SER:HB2	1:A:71:GLN:HG3	2.00	0.42
1:B:8:ARG:CD	1:B:36:LEU:CD2	2.96	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.43	0.42
1:B:222:GLY:HA3	1:B:246:TRP:CD2	2.54	0.42
1:A:361:ILE:CG1	1:A:362:ALA:N	2.76	0.42
1:B:377:CYS:HA	1:B:380:LEU:HG	2.02	0.42
1:B:507:LYS:NZ	1:B:524:ALA:HA	2.34	0.42
1:A:452:LEU:O	1:A:453:ALA:C	2.62	0.42
1:B:272:ALA:CB	1:B:349:ILE:HD13	2.49	0.42
1:A:33:ARG:NH1	1:A:107:ARG:HA	2.35	0.42
1:B:187:GLN:C	1:B:189:LEU:H	2.26	0.42
1:B:302:GLU:N	1:B:303:PRO:CD	2.82	0.42
1:A:63:LEU:O	1:A:67:LYS:HB2	2.20	0.42
1:B:385:GLN:HG3	1:B:436:THR:HG23	2.00	0.42
1:B:552:GLN:O	1:B:556:LEU:HD13	2.19	0.42
1:A:252:VAL:CG2	1:A:398:ASP:HB2	2.46	0.42
1:A:317:ASP:OD2	1:A:321:HIS:ND1	2.45	0.42
1:A:107:ARG:HH11	1:A:107:ARG:HD3	1.62	0.42
1:A:182:GLY:O	1:A:185:TRP:HB3	2.20	0.42
1:B:136:LEU:HD22	1:B:148:LEU:CD1	2.50	0.42
1:B:250:GLY:O	1:B:258:GLN:HG2	2.20	0.41
1:B:443:LEU:HD23	1:B:443:LEU:HA	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:SER:OG	1:A:78:THR:CB	2.68	0.41
1:A:68:VAL:HG11	1:A:432:SER:HB3	2.02	0.41
1:A:427:GLY:O	1:A:428:VAL:C	2.64	0.41
1:A:81:THR:O	1:A:82:ALA:C	2.64	0.41
1:A:449:LEU:HD12	1:A:449:LEU:HA	1.79	0.41
1:A:8:ARG:NH1	1:A:43:GLU:OE2	2.53	0.41
1:A:56:ARG:HD3	1:B:85:ASN:OD1	2.20	0.41
1:A:218:ARG:O	1:A:218:ARG:HG3	2.21	0.41
1:A:369:GLU:HG2	1:A:396:LEU:CD1	2.50	0.41
1:A:15:LEU:O	1:A:16:GLU:C	2.64	0.41
1:A:312:ILE:HG13	1:A:316:LEU:HD11	2.02	0.41
1:A:370:ALA:HA	1:A:396:LEU:HD13	2.03	0.41
1:B:44:ASN:OD1	1:B:44:ASN:C	2.64	0.41
1:B:455:LEU:O	1:B:456:ARG:C	2.61	0.41
1:A:61:LEU:HA	1:A:61:LEU:HD12	1.88	0.41
1:A:129:HIS:H	1:A:130:PRO:HD3	1.86	0.41
1:B:178:MET:HE2	1:B:178:MET:HB3	1.66	0.41
1:B:409:VAL:CG1	1:B:410:TYR:H	2.32	0.41
1:A:34:SER:C	1:A:36:LEU:N	2.74	0.41
1:A:233:GLU:O	1:A:237:VAL:HG23	2.21	0.41
1:A:493:GLN:HB3	1:B:456:ARG:CZ	2.52	0.40
1:B:10:TRP:O	1:B:14:ILE:HG13	2.20	0.40
1:B:14:ILE:HG23	1:B:152:ILE:HD11	2.03	0.40
1:B:65:LEU:HA	1:B:431:ALA:HB2	2.02	0.40
1:B:29:ALA:HB2	1:B:58:LEU:HD22	2.03	0.40
1:B:68:VAL:HG22	1:B:410:TYR:CZ	2.56	0.40
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.86	0.40
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.89	0.40
1:B:527:THR:HB	1:B:528:PRO:HD2	2.02	0.40
1:B:9:ARG:HH11	1:B:9:ARG:HD3	1.76	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	529/556 (95%)	489 (92%)	37 (7%)	3 (1%)	21	44
1	B	525/556 (94%)	487 (93%)	35 (7%)	3 (1%)	21	44
All	All	1054/1112 (95%)	976 (93%)	72 (7%)	6 (1%)	21	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173	PRO
1	A	492	PRO
1	A	30	PRO
1	B	64	GLY
1	A	302	GLU
1	B	30	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	433/452 (96%)	372 (86%)	61 (14%)	3	9
1	B	430/452 (95%)	371 (86%)	59 (14%)	3	9
All	All	863/904 (96%)	743 (86%)	120 (14%)	3	9

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	24	ARG
1	A	26	ILE
1	A	28	ILE
1	A	32	SER
1	A	33	ARG
1	A	35	THR

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	48	ILE
1	A	51	THR
1	A	71	GLN
1	A	78	THR
1	A	87	TYR
1	A	103	LEU
1	A	112	ILE
1	A	149	VAL
1	A	174	LEU
1	A	184	SER
1	A	208	SER
1	A	235	LYS
1	A	248	LEU
1	A	252	VAL
1	A	255	GLN
1	A	274	SER
1	A	277	GLN
1	A	281	ILE
1	A	285	LEU
1	A	289	LEU
1	A	292	LYS
1	A	293	ARG
1	A	298	GLN
1	A	302	GLU
1	A	312	ILE
1	A	336	LEU
1	A	340	GLU
1	A	342	ARG
1	A	343	GLN
1	A	346	CYS
1	A	363	ARG
1	A	369	GLU
1	A	375	ARG
1	A	376	ILE
1	A	377	CYS
1	A	388	VAL
1	A	392	LEU
1	A	395	ARG
1	A	401	SER
1	A	422	LEU
1	A	439	ILE

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Mol	Chain	Res	Type
1	A	440	VAL
1	A	458	VAL
1	A	470	ASN
1	A	489	TYR
1	A	490	LEU
1	A	493	GLN
1	A	498	GLU
1	A	512	GLN
1	A	535	MET
1	A	539	ASP
1	A	544	GLN
1	A	556	LEU
1	B	3	VAL
1	B	19	THR
1	B	24	ARG
1	B	33	ARG
1	B	87	TYR
1	B	121	ARG
1	B	140	THR
1	B	146	ARG
1	B	166	ILE
1	B	172	GLU
1	B	174	LEU
1	B	177	GLU
1	B	178	MET
1	B	180	ASP
1	B	184	SER
1	B	188	ARG
1	B	210	LYS
1	B	239	LEU
1	B	248	LEU
1	B	249	ILE
1	B	252	VAL
1	B	253	LEU
1	B	255	GLN
1	B	273	THR
1	B	274	SER
1	B	281	ILE
1	B	285	LEU
1	B	289	LEU
1	B	293	ARG
1	B	304	GLU

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Mol	Chain	Res	Type
1	B	312	ILE
1	B	322	ARG
1	B	343	GLN
1	B	346	CYS
1	B	347	VAL
1	B	349	ILE
1	B	351	ARG
1	B	357	MET
1	B	363	ARG
1	B	375	ARG
1	B	376	ILE
1	B	377	CYS
1	B	382	GLU
1	B	393	VAL
1	B	394	VAL
1	B	411	SER
1	B	439	ILE
1	B	440	VAL
1	B	443	LEU
1	B	470	ASN
1	B	494	ASN
1	B	495	VAL
1	B	535	MET
1	B	539	ASP
1	B	540	THR
1	B	544	GLN
1	B	547	GLN
1	B	550	LEU
1	B	556	LEU

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	7	ASN
1	A	194	GLN
1	A	284	GLN
1	A	343	GLN
1	A	402	GLN
1	B	7	ASN
1	B	71	GLN
1	B	117	ASN
1	B	141	GLN

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Mol	Chain	Res	Type
1	B	277	GLN
1	B	320	HIS
1	B	355	GLN
1	B	457	GLN
1	B	538	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 [i](#)

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	535/556 (96%)	-0.57	16 (2%)	52	49	13, 25, 49, 80	10 (1%)
1	B	531/556 (95%)	-0.53	15 (2%)	55	51	13, 27, 50, 87	11 (2%)
All	All	1066/1112 (95%)	-0.55	31 (2%)	53	50	13, 26, 49, 87	21 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	526	ARG	9.5
1	B	526	ARG	7.3
1	B	271	LYS	6.7
1	B	278	GLN	6.4
1	A	205	ARG	5.4
1	B	205	ARG	5.4
1	B	1	MET	5.3
1	A	515	GLN	5.2
1	A	304	GLU	5.1
1	A	271	LYS	4.7
1	B	515	GLN	4.7
1	A	34	SER	4.5
1	B	174	LEU	4.2
1	A	278	GLN	4.1
1	B	304	GLU	3.8
1	B	33	ARG	3.7
1	B	30	PRO	3.3
1	A	33	ARG	3.2
1	A	174	LEU	3.2
1	B	178	MET	2.9
1	B	197	LYS	2.9
1	B	173	PRO	2.8
1	A	302	GLU	2.8
1	B	34	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	197	LYS	2.6
1	B	24	ARG	2.6
1	A	179	ASP	2.3
1	A	24	ARG	2.3
1	A	178	MET	2.2
1	A	30	PRO	2.2
1	A	35	THR	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.