



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:10 AM UTC

PDB ID : 1CD1 / pdb_00001cd1
Title : CD1(MOUSE) ANTIGEN PRESENTING MOLECULE
Authors : Zeng, Z.H.; Segelke, B.W.; Wilson, I.A.
Deposited on : 1997-04-02
Resolution : 2.67 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
Xtrriage (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

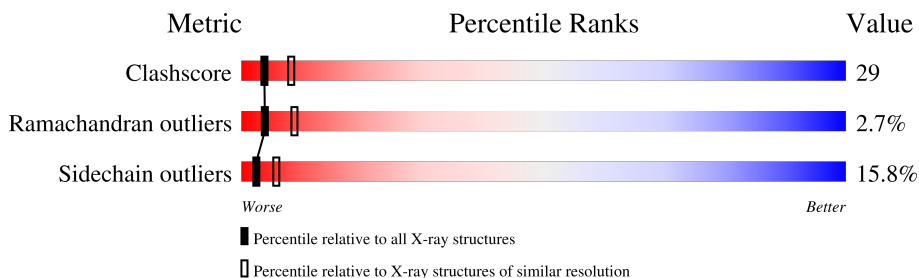
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)

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	315	 24% 37% 23% 13%
1	C	315	 25% 38% 19% 5% 13%
2	B	99	 25% 44% 28% 13%
2	D	99	 31% 44% 22% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6026 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 CD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2192	1396	378	405	13	0	0	0
1	C	273	2192	1396	378	405	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	conflict	UNP P11609
C	201	HIS	ASP	conflict	UNP P11609

- Molecule 2 is a protein called CD1.


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	821	524	138	152	7	0	0	0
2	D	99	821	524	138	152	7	0	0	0

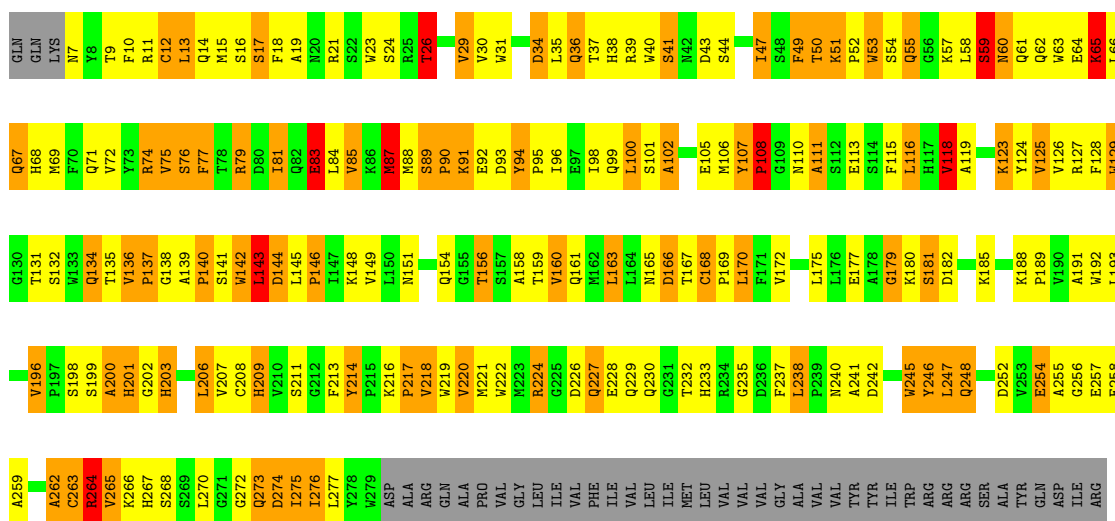
3 Residue-property plots

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. 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.

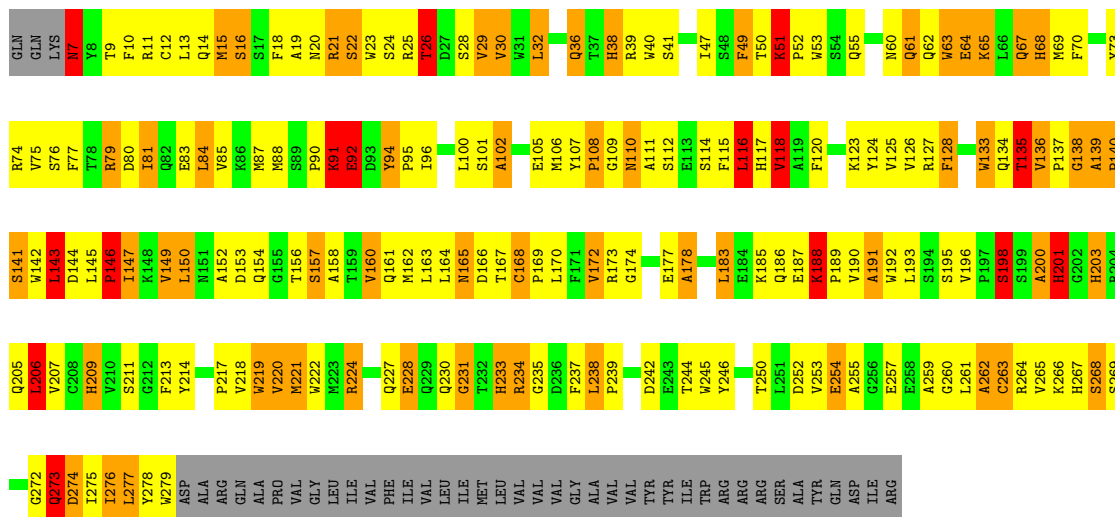
- Molecule 1: CD1

Chain A: 



- Molecule 1: CD1

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.34Å 76.20Å 103.40Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	10.00 – 2.67	Depositor
% Data completeness (in resolution range)	83.7 (10.00-2.67)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.192 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6026	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	2.29	81/2257 (3.6%)	1.94	64/3069 (2.1%)
1	C	2.30	93/2257 (4.1%)	1.92	53/3069 (1.7%)
2	B	2.29	33/847 (3.9%)	1.93	25/1148 (2.2%)
2	D	2.29	28/847 (3.3%)	1.95	19/1148 (1.7%)
All	All	2.29	235/6208 (3.8%)	1.93	161/8434 (1.9%)

All (235) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	VAL	CA-CB	-10.82	1.42	1.54
2	D	8	GLN	N-CA	9.99	1.58	1.46
1	C	237	PHE	CA-C	-9.35	1.40	1.52
2	D	67	HIS	ND1-CE1	9.15	1.41	1.32
1	C	190	VAL	CA-C	8.85	1.64	1.52
1	C	152	ALA	CA-CB	8.32	1.63	1.52
1	C	185	LYS	CA-C	-8.16	1.42	1.52
2	B	31	HIS	CG-CD2	8.09	1.44	1.35
1	A	252	ASP	CA-C	-8.03	1.42	1.52
1	A	263	CYS	CA-C	-7.94	1.43	1.52
2	D	81	ARG	N-CA	-7.82	1.36	1.46
1	C	178	ALA	C-O	-7.69	1.15	1.24
2	B	30	PHE	N-CA	7.64	1.55	1.45
1	C	29	VAL	CA-CB	7.58	1.64	1.54
1	C	64	GLU	N-CA	7.57	1.56	1.46
2	B	83	LYS	N-CA	7.38	1.55	1.46
1	A	23	TRP	NE1-CE2	-7.33	1.29	1.37
2	B	66	ALA	C-N	-7.31	1.24	1.33
1	A	119	ALA	C-O	-7.24	1.15	1.24
2	D	85	ASP	C-N	-7.23	1.24	1.33
2	B	21	ASN	C-O	-7.22	1.17	1.24
1	A	11	ARG	CZ-NH1	7.21	1.42	1.32
2	D	17	ASN	C-O	7.17	1.32	1.23
2	B	84	HIS	CA-C	7.16	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	CYS	CA-C	7.16	1.61	1.52
1	A	264	ARG	CZ-NH2	7.15	1.42	1.33
1	C	95	PRO	N-CA	7.14	1.56	1.47
1	A	38	HIS	ND1-CE1	7.04	1.39	1.32
1	A	245	TRP	NE1-CE2	-6.97	1.29	1.37
2	D	68	THR	CA-CB	-6.97	1.43	1.53
2	D	2	GLN	C-O	-6.93	1.16	1.24
1	A	108	PRO	N-CA	6.90	1.56	1.47
1	A	196	VAL	C-N	6.88	1.41	1.33
1	A	268	SER	N-CA	6.83	1.54	1.46
1	A	51	LYS	N-CA	6.81	1.53	1.46
2	D	46	ILE	N-CA	6.80	1.54	1.46
2	D	83	LYS	N-CA	6.78	1.54	1.46
1	A	168	CYS	CA-C	-6.78	1.44	1.52
1	C	253	VAL	C-O	-6.76	1.16	1.24
1	C	7	ASN	N-CA	6.75	1.59	1.46
1	C	238	LEU	C-O	6.74	1.32	1.24
1	C	220	VAL	C-O	-6.73	1.16	1.24
1	A	38	HIS	CG-ND1	-6.71	1.30	1.38
1	C	63	TRP	C-O	-6.70	1.16	1.24
1	C	165	ASN	N-CA	6.70	1.54	1.46
1	C	41	SER	N-CA	-6.68	1.37	1.46
1	C	40	TRP	N-CA	-6.67	1.37	1.46
1	C	136	VAL	CA-C	6.67	1.59	1.52
1	C	231	GLY	N-CA	6.66	1.54	1.45
1	C	209	HIS	CD2-NE2	-6.62	1.30	1.37
2	D	14	PRO	CA-C	6.61	1.58	1.52
2	B	96	ASP	C-O	6.61	1.31	1.23
1	A	201	HIS	CG-CD2	6.58	1.43	1.35
1	C	116	LEU	N-CA	6.56	1.54	1.46
1	A	140	PRO	N-CA	6.54	1.55	1.47
1	C	52	PRO	CA-CB	-6.54	1.44	1.53
2	D	80	CYS	CA-C	6.53	1.60	1.52
1	A	38	HIS	CE1-NE2	6.53	1.39	1.32
1	A	158	ALA	N-CA	6.50	1.54	1.46
2	B	20	PRO	C-O	-6.47	1.15	1.23
2	D	33	PRO	N-CA	-6.47	1.39	1.47
1	C	183	LEU	C-N	-6.45	1.25	1.33
1	C	10	PHE	CA-CB	-6.45	1.44	1.53
1	A	151	ASN	N-CA	-6.41	1.38	1.46
2	D	17	ASN	C-N	-6.41	1.24	1.33
1	C	235	GLY	C-O	6.38	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	GLN	C-O	-6.37	1.16	1.24
1	C	51	LYS	N-CA	6.37	1.55	1.46
1	A	203	HIS	N-CA	6.34	1.54	1.46
2	D	9	VAL	CA-CB	-6.32	1.46	1.54
2	D	93	VAL	N-CA	-6.32	1.38	1.46
2	D	34	HIS	C-O	-6.32	1.16	1.24
1	C	193	LEU	CA-C	-6.31	1.45	1.52
2	D	59	ASP	N-CA	6.31	1.54	1.46
1	A	218	VAL	C-O	-6.31	1.17	1.23
1	C	164	LEU	CA-C	-6.26	1.45	1.52
1	C	196	VAL	N-CA	6.24	1.54	1.46
2	B	26	TYR	CA-C	-6.23	1.45	1.53
1	A	10	PHE	CA-C	-6.22	1.45	1.52
1	C	253	VAL	N-CA	-6.21	1.39	1.46
2	B	89	GLU	N-CA	6.18	1.51	1.45
1	A	118	VAL	N-CA	6.18	1.54	1.46
2	B	58	LYS	C-O	-6.17	1.16	1.24
1	A	47	ILE	C-O	-6.16	1.17	1.24
2	B	33	PRO	CA-CB	-6.15	1.45	1.53
1	A	209	HIS	ND1-CE1	-6.14	1.26	1.32
1	C	68	HIS	ND1-CE1	6.14	1.38	1.32
2	B	67	HIS	CG-ND1	6.12	1.45	1.38
1	C	203	HIS	ND1-CE1	6.08	1.38	1.32
1	A	129	TRP	NE1-CE2	6.08	1.44	1.37
2	D	8	GLN	CA-CB	-6.08	1.43	1.53
1	C	133	TRP	C-O	-6.08	1.16	1.24
1	A	52	PRO	C-N	6.07	1.40	1.33
2	B	92	THR	C-N	-6.07	1.24	1.33
1	C	262	ALA	CA-CB	-6.06	1.43	1.53
1	C	195	SER	CA-C	-6.04	1.45	1.52
2	D	44	LYS	C-O	6.04	1.31	1.23
2	B	29	GLN	C-O	-6.04	1.16	1.24
1	A	229	GLN	CA-C	-6.04	1.45	1.52
2	B	82	VAL	C-O	-6.03	1.18	1.24
1	C	25	ARG	CZ-NH2	6.03	1.41	1.33
1	C	260	GLY	CA-C	6.02	1.57	1.52
1	A	110	ASN	CA-C	6.02	1.60	1.52
1	C	84	LEU	N-CA	-6.02	1.38	1.46
1	A	259	ALA	C-O	-6.01	1.17	1.24
1	C	38	HIS	CD2-NE2	-6.01	1.31	1.37
1	C	273	GLN	C-N	-6.01	1.25	1.33
2	B	28	THR	C-O	6.00	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	239	PRO	C-N	5.99	1.41	1.33
2	B	51	MET	CA-C	-5.96	1.45	1.52
1	C	55	GLN	CA-C	-5.95	1.45	1.52
1	C	146	PRO	CA-C	5.93	1.60	1.52
1	A	156	THR	CA-C	5.90	1.60	1.52
1	A	140	PRO	CA-C	-5.90	1.45	1.52
1	A	59	SER	C-O	-5.90	1.16	1.23
1	C	147	ILE	C-O	-5.86	1.16	1.24
1	A	224	ARG	NE-CZ	5.86	1.39	1.33
1	A	140	PRO	C-N	5.84	1.41	1.33
1	C	14	GLN	C-N	-5.83	1.25	1.33
1	A	256	GLY	N-CA	-5.83	1.36	1.45
1	A	132	SER	C-O	-5.82	1.16	1.23
2	B	65	LEU	C-O	-5.80	1.17	1.23
1	A	19	ALA	C-O	-5.79	1.16	1.24
2	D	34	HIS	CA-CB	-5.79	1.44	1.53
1	C	84	LEU	CA-C	5.79	1.60	1.52
1	C	205	GLN	C-O	5.78	1.30	1.24
1	A	148	LYS	N-CA	5.77	1.53	1.46
1	A	233	HIS	CG-ND1	-5.76	1.31	1.38
2	D	45	LYS	CA-C	-5.76	1.45	1.52
1	C	198	SER	C-O	5.74	1.31	1.24
1	C	24	SER	N-CA	-5.74	1.38	1.45
1	C	203	HIS	CE1-NE2	-5.72	1.26	1.32
1	A	214	TYR	CA-CB	5.71	1.62	1.53
1	A	247	LEU	C-O	-5.71	1.16	1.23
2	D	22	ILE	C-O	-5.71	1.18	1.24
1	C	245	TRP	CA-CB	-5.70	1.45	1.53
1	A	74	ARG	CZ-NH2	-5.68	1.26	1.33
1	A	248	GLN	CA-C	-5.68	1.45	1.52
2	B	13	HIS	C-O	5.68	1.29	1.24
1	C	11	ARG	N-CA	5.68	1.52	1.45
1	A	29	VAL	C-O	5.67	1.30	1.24
1	C	162	MET	N-CA	-5.67	1.39	1.46
1	C	94	TYR	N-CA	5.66	1.54	1.46
1	A	211	SER	C-O	-5.66	1.17	1.23
2	B	54	MET	CA-CB	-5.64	1.44	1.53
1	C	245	TRP	NE1-CE2	-5.63	1.31	1.37
1	C	191	ALA	C-N	5.62	1.40	1.33
1	A	201	HIS	N-CA	5.61	1.53	1.46
1	A	255	ALA	CA-C	5.59	1.60	1.52
2	B	48	LYS	CA-CB	5.58	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	TYR	CA-C	-5.58	1.45	1.52
1	C	117	HIS	CE1-NE2	-5.57	1.26	1.32
2	B	12	ARG	C-O	5.56	1.31	1.23
1	A	26	THR	CA-CB	5.55	1.62	1.53
1	C	153	ASP	C-O	-5.54	1.17	1.24
2	B	54	MET	C-N	-5.54	1.26	1.33
1	A	170	LEU	C-O	5.54	1.30	1.24
1	A	62	GLN	CA-C	-5.54	1.45	1.52
1	C	149	VAL	CA-CB	5.51	1.62	1.54
1	C	221	MET	N-CA	-5.51	1.39	1.46
1	C	173	ARG	CD-NE	5.50	1.53	1.46
1	C	201	HIS	C-N	-5.50	1.25	1.33
1	C	120	PHE	C-N	5.50	1.41	1.33
1	A	111	ALA	CA-C	-5.50	1.45	1.52
2	D	34	HIS	CG-ND1	5.48	1.44	1.38
1	A	90	PRO	C-N	-5.47	1.26	1.33
1	A	160	VAL	C-N	5.46	1.41	1.33
1	A	168	CYS	CA-CB	5.44	1.60	1.53
1	C	65	LYS	CA-C	-5.43	1.45	1.52
1	C	195	SER	N-CA	5.42	1.52	1.46
2	B	13	HIS	C-N	-5.41	1.26	1.33
1	C	22	SER	CA-CB	5.40	1.62	1.54
1	C	228	GLU	N-CA	-5.40	1.38	1.45
1	C	233	HIS	CG-CD2	-5.40	1.29	1.35
1	A	49	PHE	C-O	-5.40	1.17	1.23
2	B	33	PRO	CA-C	5.40	1.60	1.52
2	D	82	VAL	N-CA	-5.35	1.40	1.46
2	B	47	PRO	C-N	-5.34	1.24	1.33
1	A	276	ILE	CA-C	-5.33	1.47	1.53
2	D	49	VAL	C-O	5.33	1.29	1.24
1	C	206	LEU	CA-CB	-5.33	1.45	1.53
2	B	66	ALA	C-O	5.33	1.30	1.23
1	A	53	TRP	CA-CB	5.32	1.60	1.53
1	C	172	VAL	C-O	-5.32	1.18	1.24
1	A	168	CYS	N-CA	5.31	1.51	1.46
2	D	55	SER	C-O	5.31	1.30	1.23
1	A	57	LYS	C-N	-5.30	1.26	1.33
1	C	60	ASN	N-CA	-5.30	1.40	1.46
1	C	238	LEU	CA-CB	5.30	1.62	1.53
1	A	65	LYS	N-CA	-5.30	1.39	1.46
1	C	67	GLN	C-O	-5.30	1.17	1.24
1	C	102	ALA	CA-C	-5.29	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	SER	C-N	5.29	1.40	1.33
1	A	34	ASP	N-CA	-5.28	1.40	1.46
1	C	81	ILE	CA-C	-5.26	1.46	1.52
1	A	179	GLY	C-O	-5.26	1.17	1.24
2	B	98	ASP	CG-OD2	-5.26	1.15	1.25
1	A	207	VAL	CA-C	-5.25	1.46	1.52
1	A	273	GLN	N-CA	5.25	1.52	1.45
2	B	14	PRO	CA-CB	5.23	1.61	1.54
1	C	52	PRO	C-N	-5.22	1.26	1.33
1	C	118	VAL	C-O	5.21	1.29	1.24
1	C	166	ASP	C-N	-5.20	1.26	1.34
1	C	75	VAL	CA-C	5.19	1.59	1.52
1	A	119	ALA	CA-CB	-5.18	1.46	1.53
1	C	26	THR	CB-OG1	5.18	1.52	1.43
2	B	45	LYS	C-N	5.17	1.39	1.33
1	C	91	LYS	C-O	5.17	1.30	1.24
1	A	14	GLN	N-CA	-5.17	1.39	1.46
1	A	98	ILE	N-CA	-5.16	1.40	1.46
1	A	12	CYS	CA-C	5.16	1.59	1.53
1	A	67	GLN	CA-C	-5.13	1.45	1.52
1	A	101	SER	N-CA	5.13	1.52	1.46
1	A	182	ASP	N-CA	-5.13	1.39	1.46
1	C	115	PHE	N-CA	-5.13	1.39	1.45
2	D	22	ILE	CA-CB	5.12	1.62	1.54
1	A	191	ALA	CA-C	-5.12	1.46	1.52
1	A	123	LYS	N-CA	5.12	1.52	1.46
1	C	191	ALA	CA-C	-5.12	1.46	1.52
1	C	36	GLN	CA-C	-5.10	1.46	1.52
1	C	111	ALA	CA-C	5.10	1.59	1.52
1	C	16	SER	CA-C	5.10	1.59	1.52
1	C	138	GLY	N-CA	5.09	1.52	1.44
1	C	168	CYS	N-CA	5.08	1.50	1.46
2	B	30	PHE	C-O	5.08	1.30	1.23
1	A	79	ARG	C-O	-5.07	1.18	1.24
1	A	64	GLU	N-CA	-5.06	1.39	1.46
2	D	61	SER	N-CA	5.06	1.52	1.45
1	C	101	SER	CA-CB	5.05	1.60	1.53
2	B	27	VAL	CA-CB	5.05	1.61	1.54
1	A	102	ALA	N-CA	5.03	1.52	1.45
1	C	230	GLN	C-N	-5.03	1.27	1.33
1	A	37	THR	CA-CB	5.03	1.61	1.54
1	A	41	SER	C-N	-5.03	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	PRO	CA-C	5.03	1.58	1.52

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	GLN	N-CA-C	12.45	126.97	110.53
1	A	273	GLN	N-CA-C	10.45	125.98	110.52
2	B	59	ASP	N-CA-C	-10.10	101.20	112.72
1	C	94	TYR	CA-C-N	-9.74	107.66	119.84
1	C	94	TYR	C-N-CA	-9.74	107.66	119.84
2	D	19	LYS	CA-C-N	9.69	129.75	119.76
2	D	19	LYS	C-N-CA	9.69	129.75	119.76
1	C	228	GLU	N-CA-C	-9.64	97.80	110.53
1	C	168	CYS	O-C-N	9.44	126.78	120.27
2	D	59	ASP	N-CA-C	-8.85	102.40	113.02
1	C	231	GLY	N-CA-C	-8.63	104.21	114.48
2	D	66	ALA	N-CA-C	-8.60	97.80	110.52
2	D	76	ASP	N-CA-C	8.46	123.22	109.59
1	C	188	LYS	CA-C-N	8.28	130.94	120.51
1	C	188	LYS	C-N-CA	8.28	130.94	120.51
1	A	141	SER	N-CA-C	8.08	121.11	111.33
2	B	82	VAL	O-C-N	7.99	131.65	123.10
1	C	110	ASN	N-CA-C	-7.93	93.91	110.80
2	D	86	SER	N-CA-C	-7.59	103.01	111.28
1	A	68	HIS	N-CA-C	-7.56	103.04	111.28
1	A	226	ASP	N-CA-C	-7.55	104.21	113.50
1	C	65	LYS	N-CA-C	-7.46	104.31	113.41
1	A	98	ILE	CA-C-O	7.45	128.25	120.36
1	A	140	PRO	CA-C-O	7.38	129.70	121.43
2	B	89	GLU	CA-C-N	7.35	127.80	119.93
2	B	89	GLU	C-N-CA	7.35	127.80	119.93
1	A	254	GLU	N-CA-C	-7.35	96.56	109.06
1	A	59	SER	N-CA-C	-7.28	99.70	110.48
1	A	230	GLN	N-CA-C	-7.25	99.09	109.96
1	A	258	GLU	N-CA-C	-7.19	104.54	113.38
1	C	245	TRP	N-CA-C	7.19	120.70	110.14
1	A	88	MET	N-CA-C	7.09	121.07	108.24
1	A	57	LYS	N-CA-C	-7.05	103.98	112.59
2	B	42	ASN	N-CA-C	7.01	121.07	111.54
1	A	144	ASP	N-CA-C	6.98	119.92	111.82
1	A	163	LEU	CA-C-O	6.97	128.14	120.82
2	D	69	GLU	N-CA-C	-6.96	97.17	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	SER	N-CA-C	6.96	119.75	111.33
1	A	192	TRP	O-C-N	-6.90	115.54	123.33
1	C	165	ASN	N-CA-C	6.88	120.90	112.23
2	B	12	ARG	N-CA-C	-6.73	105.60	113.88
1	C	230	GLN	CA-C-N	-6.71	115.56	123.08
1	C	230	GLN	C-N-CA	-6.71	115.56	123.08
1	A	134	GLN	N-CA-C	6.64	120.45	108.69
1	A	94	TYR	N-CA-C	6.62	124.45	109.81
1	A	87	MET	N-CA-C	-6.57	105.14	112.57
1	C	200	ALA	N-CA-C	6.57	120.43	111.17
1	A	166	ASP	N-CA-C	6.56	121.49	112.04
2	B	19	LYS	CA-C-N	6.56	126.58	119.89
2	B	19	LYS	C-N-CA	6.56	126.58	119.89
1	A	89	SER	N-CA-C	-6.55	100.54	110.50
1	C	125	VAL	N-CA-C	6.47	122.79	109.34
1	A	196	VAL	CB-CA-C	6.38	116.32	110.13
2	D	5	PRO	N-CA-C	6.38	120.85	111.03
1	C	244	THR	N-CA-C	-6.37	100.77	109.95
1	A	128	PHE	N-CA-C	-6.36	98.87	109.24
2	B	93	VAL	N-CA-C	-6.35	99.33	108.53
2	B	40	LEU	N-CA-C	6.18	119.02	109.07
2	B	76	ASP	N-CA-C	6.16	118.94	108.90
1	A	238	LEU	CA-C-N	6.14	126.60	120.52
1	A	238	LEU	C-N-CA	6.14	126.60	120.52
1	C	230	GLN	N-CA-C	-6.14	101.84	110.50
1	C	238	LEU	CA-C-N	6.13	126.10	120.03
1	C	238	LEU	C-N-CA	6.13	126.10	120.03
1	C	128	PHE	N-CA-C	-6.12	99.22	109.07
1	C	221	MET	CA-C-N	6.08	129.47	120.95
1	C	221	MET	C-N-CA	6.08	129.47	120.95
1	C	49	PHE	N-CA-C	-6.08	100.60	110.20
1	A	107	TYR	CA-C-N	6.04	127.39	119.84
1	A	107	TYR	C-N-CA	6.04	127.39	119.84
1	A	158	ALA	N-CA-C	-6.04	103.45	111.24
2	B	60	TRP	N-CA-C	6.03	123.65	110.80
1	C	135	THR	N-CA-C	-6.00	100.71	110.20
1	C	273	GLN	O-C-N	5.99	129.62	122.79
1	A	55	GLN	N-CA-C	-5.95	105.67	113.17
2	D	88	ALA	N-CA-C	-5.94	104.74	112.23
1	A	72	VAL	CA-C-O	5.92	127.05	120.71
1	C	209	HIS	ND1-CG-CD2	-5.91	100.19	106.10
1	C	157	SER	CA-C-O	-5.90	114.30	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	LEU	N-CA-C	5.88	119.26	110.14
1	A	100	LEU	CA-C-N	-5.88	114.94	122.77
1	A	100	LEU	C-N-CA	-5.88	114.94	122.77
1	C	29	VAL	CA-C-N	-5.88	112.79	122.67
1	C	29	VAL	C-N-CA	-5.88	112.79	122.67
2	D	86	SER	CA-C-N	5.87	129.90	121.50
2	D	86	SER	C-N-CA	5.87	129.90	121.50
2	D	6	GLN	N-CA-C	-5.84	100.47	109.76
1	A	138	GLY	N-CA-C	-5.84	107.74	114.69
1	A	170	LEU	O-C-N	5.83	128.07	122.07
1	A	245	TRP	CE3-CZ3-CH2	5.81	128.66	121.10
1	A	71	GLN	N-CA-C	-5.79	105.10	111.82
1	C	173	ARG	N-CA-C	-5.71	105.58	112.54
1	C	276	ILE	CB-CA-C	5.68	117.36	111.23
1	A	272	GLY	N-CA-C	-5.66	99.76	113.18
1	A	85	VAL	CB-CA-C	-5.65	103.40	112.16
1	A	83	GLU	N-CA-C	-5.65	105.21	111.36
1	A	76	SER	N-CA-C	5.62	120.17	111.56
1	A	81	ILE	N-CA-C	-5.62	105.05	110.72
2	B	4	THR	CA-C-O	5.58	124.73	119.76
1	A	115	PHE	CA-C-O	5.57	127.19	121.23
2	D	71	THR	CA-C-N	5.56	125.74	119.90
2	D	71	THR	C-N-CA	5.56	125.74	119.90
1	C	149	VAL	CB-CA-C	-5.54	104.66	111.92
1	C	272	GLY	N-CA-C	-5.53	100.07	113.18
1	C	81	ILE	O-C-N	-5.50	116.52	121.91
1	A	209	HIS	ND1-CE1-NE2	5.50	113.90	108.40
1	A	125	VAL	N-CA-C	5.49	118.93	113.71
1	C	81	ILE	CA-C-N	5.49	127.95	120.54
1	C	81	ILE	C-N-CA	5.49	127.95	120.54
2	D	7	ILE	O-C-N	5.48	129.10	123.18
1	A	257	GLU	N-CA-C	5.46	119.03	111.55
2	B	14	PRO	O-C-N	5.45	127.89	121.46
1	C	157	SER	O-C-N	5.45	127.89	122.12
2	B	14	PRO	CA-C-N	-5.43	114.36	119.85
2	B	14	PRO	C-N-CA	-5.43	114.36	119.85
2	D	55	SER	N-CA-C	-5.43	100.87	108.96
1	A	218	VAL	CA-C-O	5.42	127.02	121.28
1	A	220	VAL	N-CA-C	-5.36	100.13	108.81
1	C	254	GLU	N-CA-C	-5.35	102.83	110.59
2	D	61	SER	N-CA-C	-5.34	103.34	110.55
1	A	227	GLN	CB-CG-CD	5.34	121.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	26	TYR	N-CA-C	5.34	117.44	107.99
1	A	245	TRP	N-CA-C	5.33	118.26	109.85
1	C	139	ALA	O-C-N	5.31	125.93	121.31
2	B	66	ALA	N-CA-C	-5.30	101.06	109.96
1	C	32	LEU	N-CA-C	-5.29	96.64	107.70
1	C	209	HIS	CG-CD2-NE2	5.29	112.49	107.20
1	A	74	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	275	ILE	N-CA-C	-5.27	98.34	106.72
1	A	98	ILE	O-C-N	-5.24	117.54	123.20
2	B	43	GLY	O-C-N	5.23	128.09	122.65
1	A	192	TRP	CA-C-O	5.23	126.84	120.99
2	B	17	ASN	OD1-CG-ND2	5.22	127.82	122.60
1	C	234	ARG	N-CA-C	-5.19	101.24	109.96
1	C	63	TRP	CE2-CD2-CE3	-5.18	113.62	118.80
1	A	181	SER	N-CA-C	5.16	116.59	111.07
1	C	74	ARG	O-C-N	5.16	127.60	122.08
2	B	52	SER	N-CA-C	-5.14	103.25	110.35
1	C	111	ALA	N-CA-C	-5.13	99.87	110.80
1	C	102	ALA	O-C-N	-5.12	116.98	123.17
1	A	188	LYS	N-CA-C	5.11	116.27	109.93
1	A	182	ASP	N-CA-C	5.11	119.52	113.28
1	A	31	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	A	224	ARG	N-CA-C	-5.10	95.80	107.48
1	A	262	ALA	N-CA-C	5.09	115.88	108.14
2	B	83	LYS	N-CA-C	-5.09	100.11	108.41
1	A	53	TRP	N-CA-C	5.09	119.17	112.25
1	C	234	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	50	THR	CA-C-O	5.09	126.91	120.65
2	B	53	ASP	CA-C-O	5.08	126.77	120.92
2	B	46	ILE	N-CA-C	-5.08	97.92	108.88
2	D	26	TYR	N-CA-CB	-5.07	102.05	110.47
1	C	74	ARG	CA-C-O	-5.07	115.50	121.07
1	C	158	ALA	CA-C-O	5.07	126.32	121.00
1	C	149	VAL	CA-C-N	5.05	127.36	120.54
1	C	149	VAL	C-N-CA	5.05	127.36	120.54
2	B	2	GLN	O-C-N	-5.05	117.20	123.36
1	A	49	PHE	N-CA-C	-5.05	102.30	110.32
1	A	17	SER	O-C-N	-5.04	117.37	123.27
2	B	26	TYR	N-CA-CB	-5.04	101.94	110.46
1	A	241	ALA	O-C-N	5.01	129.15	122.43

There are no chirality outliers.

There are no planarity outliers.

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	2192	0	2097	126	0
1	C	2192	0	2097	139	0
2	B	821	0	796	43	0
2	D	821	0	796	41	0
All	All	6026	0	5786	339	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 (339) 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:C:198:SER:HB2	1:C:201:HIS:HE1	1.26	1.00
1:C:102:ALA:HB2	1:C:116:LEU:HD23	1.43	0.97
1:C:9:THR:HG23	1:C:105:GLU:HG2	1.47	0.96
1:C:88:MET:HG3	1:C:92:GLU:HA	1.47	0.93
1:C:168:CYS:HB3	1:C:169:PRO:HD3	1.50	0.92
2:B:83:LYS:HG3	2:B:90:PRO:HG3	1.52	0.92
1:A:262:ALA:HB2	1:A:277:LEU:HD13	1.51	0.89
1:A:265:VAL:HG23	1:A:274:ASP:HB2	1.57	0.86
1:C:36:GLN:O	1:C:51:LYS:HE2	1.77	0.84
1:C:69:MET:HE1	1:C:163:LEU:HD11	1.57	0.84
1:C:135:THR:HG23	1:C:139:ALA:HB3	1.60	0.83
1:C:189:PRO:HB3	1:C:213:PHE:HB3	1.59	0.82
1:A:118:VAL:HG22	1:A:126:VAL:HB	1.61	0.80
1:C:198:SER:HB2	1:C:201:HIS:CE1	2.14	0.80
1:A:203:HIS:CE1	1:A:254:GLU:HG3	2.18	0.79
1:C:102:ALA:HB2	1:C:116:LEU:CD2	2.13	0.78
2:D:83:LYS:HG2	2:D:90:PRO:HG3	1.65	0.78
2:B:1:ILE:HB	2:B:2:GLN:OE1	1.84	0.78
1:C:156:THR:O	1:C:160:VAL:HG23	1.83	0.76
1:C:18:PHE:HB2	1:C:96:ILE:HG13	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:MET:HG3	1:C:172:VAL:HG11	1.66	0.76
1:C:263:CYS:O	1:C:275:ILE:HA	1.87	0.75
1:C:186:GLN:HE22	1:C:268:SER:HB2	1.51	0.75
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.67	0.75
1:A:140:PRO:HG2	1:A:143:LEU:HD23	1.69	0.74
1:A:201:HIS:CD2	1:A:203:HIS:HB2	2.22	0.74
2:B:87:MET:HE1	2:B:91:LYS:HD2	1.69	0.74
2:D:30:PHE:HZ	2:D:54:MET:HE2	1.52	0.74
1:C:88:MET:SD	1:C:91:LYS:O	2.46	0.74
1:C:262:ALA:HB2	1:C:277:LEU:HA	1.70	0.74
1:C:18:PHE:HB2	1:C:96:ILE:CG1	2.18	0.73
1:A:16:SER:HB3	1:A:18:PHE:HE1	1.56	0.71
1:C:47:ILE:HD13	1:C:67:GLN:HG3	1.70	0.71
1:C:145:LEU:HB2	1:C:146:PRO:HD3	1.71	0.71
2:D:89:GLU:HG3	2:D:90:PRO:HD2	1.73	0.70
1:A:102:ALA:HB2	1:A:116:LEU:HD23	1.73	0.70
1:A:216:LYS:HB3	1:A:217:PRO:HD3	1.71	0.70
1:A:159:THR:O	1:A:163:LEU:HG	1.92	0.70
1:C:88:MET:CG	1:C:92:GLU:HA	2.21	0.70
1:C:32:LEU:HD23	1:C:183:LEU:HD21	1.72	0.69
1:C:265:VAL:O	1:C:273:GLN:HB2	1.92	0.69
1:C:238:LEU:HD12	1:C:246:TYR:HD2	1.57	0.69
1:A:36:GLN:O	1:A:51:LYS:HE2	1.92	0.69
1:C:102:ALA:CB	1:C:116:LEU:HD23	2.20	0.69
1:A:262:ALA:CB	1:A:277:LEU:HD13	2.23	0.68
1:C:15:MET:HE1	2:D:55:SER:HA	1.74	0.68
1:C:262:ALA:CB	1:C:277:LEU:HA	2.22	0.68
2:D:49:VAL:HG22	2:D:68:THR:HB	1.75	0.68
1:C:186:GLN:HB3	1:C:269:SER:HB3	1.76	0.67
2:B:29:GLN:HA	2:B:61:SER:HB2	1.76	0.67
1:A:125:VAL:HG23	1:A:126:VAL:HG23	1.76	0.67
1:A:15:MET:HE1	2:B:55:SER:HA	1.75	0.66
1:A:219:TRP:HB3	1:A:266:LYS:HB3	1.76	0.66
2:D:4:THR:HG22	2:D:86:SER:HB2	1.78	0.66
1:C:211:SER:HB2	1:C:246:TYR:HD1	1.61	0.66
1:C:186:GLN:NE2	1:C:268:SER:HB2	2.09	0.66
1:C:84:LEU:HD11	1:C:146:PRO:HB3	1.77	0.66
2:D:28:THR:HG22	2:D:29:GLN:H	1.61	0.66
1:C:118:VAL:CG2	1:C:126:VAL:HB	2.26	0.65
1:C:161:GLN:O	1:C:165:ASN:HB2	1.97	0.65
1:A:118:VAL:CG2	1:A:126:VAL:HB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ASN:HA	1:C:106:MET:O	1.95	0.65
1:A:16:SER:HB3	1:A:18:PHE:CE1	2.31	0.65
1:C:127:ARG:HG2	1:C:134:GLN:HG3	1.80	0.64
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.62	0.64
1:C:133:TRP:CD1	1:C:150:LEU:HG	2.31	0.64
1:A:201:HIS:HD2	1:A:203:HIS:HB2	1.62	0.64
1:C:100:LEU:HD21	1:C:116:LEU:HD21	1.80	0.64
1:A:51:LYS:HB2	1:A:54:SER:OG	1.98	0.63
1:A:131:THR:HG22	1:A:161:GLN:CD	2.24	0.63
2:B:50:GLU:HB3	2:B:67:HIS:NE2	2.13	0.63
1:A:65:LYS:HE3	1:A:65:LYS:HA	1.80	0.62
1:A:18:PHE:HB2	1:A:96:ILE:CG1	2.29	0.62
2:B:28:THR:HG22	2:B:29:GLN:H	1.63	0.62
2:D:28:THR:HG23	2:D:63:TYR:HB3	1.81	0.62
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.35	0.62
1:C:168:CYS:HB3	1:C:169:PRO:CD	2.29	0.61
2:D:30:PHE:HZ	2:D:54:MET:CE	2.14	0.60
1:A:161:GLN:O	1:A:165:ASN:HB2	2.01	0.60
1:C:77:PHE:O	1:C:81:ILE:HG12	2.02	0.60
1:C:219:TRP:HE1	1:C:264:ARG:HG2	1.66	0.60
2:B:28:THR:HG23	2:B:63:TYR:HB3	1.84	0.60
1:A:106:MET:HG3	1:A:172:VAL:HG11	1.83	0.60
2:D:10:TYR:CE2	2:D:24:ASN:HB2	2.37	0.60
1:A:41:SER:HB2	1:A:43:ASP:OD1	2.02	0.60
1:A:264:ARG:HG2	1:A:264:ARG:NH1	2.16	0.59
1:C:15:MET:O	1:C:26:THR:HA	2.01	0.59
1:C:39:ARG:HH11	1:C:39:ARG:HB3	1.66	0.59
1:C:116:LEU:HD12	1:C:133:TRP:CH2	2.37	0.59
2:D:70:PHE:HB2	2:D:78:TYR:CE2	2.36	0.59
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.84	0.59
1:C:265:VAL:HB	1:C:274:ASP:OD1	2.03	0.59
1:C:157:SER:O	1:C:161:GLN:HG3	2.03	0.59
1:C:30:VAL:HG22	1:C:38:HIS:HB2	1.85	0.58
2:D:44:LYS:HB2	2:D:44:LYS:NZ	2.18	0.58
2:B:2:GLN:OE1	2:B:2:GLN:N	2.36	0.58
1:A:47:ILE:CD1	1:A:67:GLN:HG3	2.34	0.58
1:A:100:LEU:HD21	1:A:116:LEU:HD21	1.86	0.58
1:C:84:LEU:CD1	1:C:146:PRO:HB3	2.33	0.58
2:D:35:ILE:HD11	2:D:82:VAL:CG1	2.35	0.57
1:C:264:ARG:HH21	1:C:275:ILE:HD11	1.68	0.57
2:D:97:ARG:O	2:D:97:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ARG:HB3	1:C:39:ARG:NH1	2.19	0.57
1:A:179:GLY:O	1:A:181:SER:N	2.37	0.57
1:A:237:PHE:HB3	1:A:245:TRP:CE3	2.40	0.56
1:A:240:ASN:OD1	2:B:12:ARG:HG2	2.06	0.56
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.87	0.56
1:C:69:MET:SD	1:C:163:LEU:HD21	2.45	0.56
2:D:17:ASN:OD1	2:D:74:GLU:HG3	2.06	0.56
1:A:13:LEU:HB3	2:B:56:PHE:CE2	2.40	0.55
1:C:106:MET:HG3	1:C:172:VAL:CG1	2.36	0.55
1:A:123:LYS:HD3	1:A:124:TYR:O	2.06	0.55
1:A:203:HIS:ND1	1:A:254:GLU:HG3	2.20	0.55
1:A:265:VAL:CG2	1:A:274:ASP:HB2	2.34	0.55
1:C:29:VAL:HG23	1:C:36:GLN:NE2	2.21	0.55
1:C:79:ARG:HG3	1:C:80:ASP:N	2.20	0.55
2:B:36:GLU:OE1	2:B:36:GLU:HA	2.06	0.55
1:A:222:TRP:HD1	1:A:232:THR:HG23	1.73	0.54
1:A:15:MET:O	1:A:26:THR:HA	2.07	0.54
1:A:142:TRP:O	1:A:146:PRO:HD2	2.07	0.54
1:A:83:GLU:O	1:A:87:MET:SD	2.66	0.54
1:A:94:TYR:O	1:A:94:TYR:CD1	2.60	0.54
1:C:29:VAL:CG2	1:C:36:GLN:NE2	2.70	0.54
2:B:9:VAL:HG11	2:B:95:TRP:HB2	1.89	0.53
2:D:87:MET:HE2	2:D:87:MET:HA	1.90	0.53
2:D:73:THR:OG1	2:D:76:ASP:HB2	2.08	0.53
1:A:94:TYR:O	1:A:96:ILE:N	2.41	0.53
1:A:263:CYS:O	1:A:275:ILE:HA	2.07	0.53
1:C:257:GLU:C	1:C:259:ALA:H	2.15	0.53
1:C:29:VAL:HG11	2:D:55:SER:OG	2.09	0.53
1:A:60:ASN:OD1	1:A:60:ASN:N	2.41	0.53
1:A:136:VAL:HG22	1:A:137:PRO:HD2	1.91	0.53
1:A:18:PHE:HB2	1:A:96:ILE:HG12	1.88	0.53
1:A:94:TYR:O	1:A:94:TYR:HD1	1.92	0.53
1:C:118:VAL:HG21	1:C:126:VAL:HB	1.90	0.53
1:C:116:LEU:HD12	1:C:133:TRP:CZ3	2.44	0.52
1:C:224:ARG:NH2	1:C:259:ALA:O	2.42	0.52
1:A:156:THR:O	1:A:160:VAL:HG23	2.08	0.52
2:B:69:GLU:H	2:B:69:GLU:CD	2.16	0.52
1:A:13:LEU:HB3	2:B:56:PHE:CZ	2.44	0.52
1:A:219:TRP:HZ2	1:A:228:GLU:OE2	1.93	0.52
1:C:88:MET:HG3	1:C:88:MET:O	2.09	0.52
1:C:140:PRO:O	1:C:143:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LEU:O	1:C:149:VAL:HG23	2.10	0.52
2:B:35:ILE:HD11	2:B:82:VAL:HG13	1.92	0.51
1:A:47:ILE:HD13	1:A:67:GLN:HG3	1.92	0.51
1:C:107:TYR:HB2	1:C:110:ASN:HB2	1.91	0.51
1:C:211:SER:HB2	1:C:246:TYR:CD1	2.42	0.51
1:C:53:TRP:HB2	1:C:178:ALA:HB1	1.91	0.51
1:C:220:VAL:H	1:C:234:ARG:HH21	1.57	0.51
1:C:32:LEU:CD2	1:C:183:LEU:HD21	2.40	0.51
1:A:135:THR:HG23	1:A:139:ALA:HB3	1.93	0.51
1:C:20:ASN:C	1:C:22:SER:H	2.18	0.51
1:C:219:TRP:CD1	1:C:219:TRP:C	2.88	0.51
1:C:227:GLN:HG2	1:C:228:GLU:O	2.11	0.51
1:A:218:VAL:HG23	1:A:267:HIS:HB2	1.93	0.51
2:B:48:LYS:HE3	2:B:50:GLU:OE1	2.10	0.51
2:B:28:THR:HG22	2:B:29:GLN:N	2.26	0.51
1:C:116:LEU:CD1	1:C:133:TRP:CH2	2.94	0.51
1:C:220:VAL:HG22	1:C:265:VAL:HG13	1.93	0.50
1:A:90:PRO:O	1:A:92:GLU:N	2.38	0.50
2:D:22:ILE:HG23	2:D:68:THR:O	2.11	0.50
1:A:206:LEU:HB3	1:A:222:TRP:CH2	2.47	0.50
2:B:35:ILE:HG13	2:B:83:LYS:O	2.12	0.50
1:C:7:ASN:OD1	1:C:7:ASN:N	2.44	0.50
1:A:198:SER:OG	1:A:203:HIS:O	2.30	0.50
1:C:79:ARG:HH11	1:C:79:ARG:HG2	1.77	0.49
1:A:77:PHE:O	1:A:81:ILE:HG12	2.12	0.49
1:C:267:HIS:ND1	1:C:269:SER:OG	2.45	0.49
2:D:41:LYS:O	2:D:44:LYS:HE3	2.11	0.49
1:C:238:LEU:HD12	1:C:246:TYR:CD2	2.44	0.49
2:B:51:MET:HG2	2:B:66:ALA:HA	1.94	0.49
1:C:94:TYR:O	1:C:96:ILE:N	2.45	0.49
1:A:237:PHE:CE1	1:A:247:LEU:HD22	2.48	0.49
1:C:123:LYS:HD3	1:C:124:TYR:O	2.13	0.49
1:C:242:ASP:OD2	2:D:12:ARG:NH1	2.45	0.49
1:C:257:GLU:C	1:C:259:ALA:N	2.71	0.49
1:A:18:PHE:HB2	1:A:96:ILE:HG13	1.94	0.48
1:A:107:TYR:HB2	1:A:111:ALA:O	2.13	0.48
1:A:166:ASP:O	1:A:169:PRO:HD2	2.12	0.48
2:D:33:PRO:HB3	2:D:62:PHE:CE2	2.48	0.48
1:A:200:ALA:O	1:A:201:HIS:HB3	2.12	0.48
1:A:202:GLY:O	1:A:203:HIS:ND1	2.46	0.48
1:A:224:ARG:O	1:A:227:GLN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:CD1	1:A:94:TYR:C	2.91	0.48
2:B:73:THR:HG22	2:B:75:THR:H	1.77	0.48
1:C:118:VAL:HG22	1:C:126:VAL:HB	1.96	0.48
1:A:266:LYS:HE3	1:A:273:GLN:NE2	2.29	0.48
1:A:35:LEU:HD21	1:A:214:TYR:CE2	2.48	0.48
1:A:47:ILE:HD12	1:A:47:ILE:H	1.78	0.48
1:C:70:PHE:HA	1:C:73:TYR:HB3	1.95	0.48
1:C:206:LEU:HB3	1:C:222:TRP:CH2	2.49	0.48
2:D:28:THR:HG23	2:D:63:TYR:CB	2.41	0.48
1:A:131:THR:HG22	1:A:161:GLN:NE2	2.28	0.48
1:C:112:SER:OG	1:C:169:PRO:HG3	2.14	0.48
1:C:254:GLU:HG2	1:C:255:ALA:N	2.29	0.48
2:D:19:LYS:O	2:D:72:PRO:HD2	2.14	0.48
1:C:50:THR:O	1:C:51:LYS:HG3	2.13	0.47
1:A:59:SER:O	1:A:60:ASN:C	2.56	0.47
1:A:106:MET:HG3	1:A:172:VAL:CG1	2.43	0.47
1:A:135:THR:CG2	1:A:139:ALA:HB3	2.44	0.47
2:B:54:MET:HE3	2:B:54:MET:HB2	1.72	0.47
1:C:219:TRP:HD1	1:C:219:TRP:O	1.98	0.47
1:C:266:LYS:HE3	1:C:273:GLN:NE2	2.29	0.47
1:A:81:ILE:O	1:A:85:VAL:HG23	2.14	0.47
1:C:188:LYS:HB3	1:C:188:LYS:HE3	1.60	0.47
1:A:216:LYS:HE2	1:A:237:PHE:CG	2.50	0.47
1:A:216:LYS:HD2	1:A:245:TRP:CE2	2.50	0.47
1:C:174:GLY:O	1:C:177:GLU:HB3	2.15	0.47
1:C:219:TRP:CD1	1:C:219:TRP:O	2.68	0.47
1:A:107:TYR:HE2	1:A:113:GLU:HG3	1.80	0.46
1:C:16:SER:HB3	1:C:18:PHE:HE1	1.79	0.46
1:C:108:PRO:HG2	1:C:109:GLY:H	1.80	0.46
1:C:220:VAL:N	1:C:234:ARG:HH21	2.12	0.46
2:D:64:ILE:HG13	2:D:65:LEU:H	1.80	0.46
2:D:68:THR:OG1	2:D:69:GLU:N	2.48	0.46
2:B:10:TYR:CE2	2:B:24:ASN:HB2	2.51	0.46
2:B:74:GLU:HG2	2:B:75:THR:HG23	1.98	0.46
1:C:219:TRP:CD1	1:C:266:LYS:HG3	2.50	0.46
1:A:29:VAL:CG2	1:A:36:GLN:NE2	2.79	0.46
1:A:238:LEU:HD12	1:A:246:TYR:HD2	1.81	0.46
1:C:61:GLN:HA	1:C:64:GLU:HG2	1.98	0.46
2:D:35:ILE:HD11	2:D:82:VAL:HG11	1.97	0.46
1:A:140:PRO:CG	1:A:143:LEU:HD23	2.42	0.46
2:B:27:VAL:HG11	2:B:35:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:HIS:NE2	1:C:203:HIS:HB2	2.31	0.46
1:C:192:TRP:CE3	2:D:14:PRO:HD3	2.51	0.46
1:C:264:ARG:NE	1:C:273:GLN:OE1	2.48	0.46
1:C:267:HIS:HD1	1:C:269:SER:H	1.63	0.46
2:D:30:PHE:CZ	2:D:54:MET:HE2	2.40	0.46
2:D:84:HIS:HD2	2:D:86:SER:OG	1.98	0.46
1:A:53:TRP:CE2	1:A:179:GLY:HA2	2.51	0.45
2:D:42:ASN:ND2	2:D:76:ASP:OD1	2.49	0.45
1:C:200:ALA:O	1:C:201:HIS:HB3	2.15	0.45
1:A:208:CYS:O	1:A:248:GLN:HA	2.17	0.45
2:B:96:ASP:O	2:B:98:ASP:N	2.45	0.45
1:C:191:ALA:HA	1:C:209:HIS:O	2.16	0.45
1:A:65:LYS:HA	1:A:65:LYS:CE	2.44	0.45
2:B:58:LYS:HD2	2:B:58:LYS:HA	1.80	0.45
1:C:142:TRP:O	1:C:144:ASP:N	2.49	0.45
1:C:201:HIS:CE1	1:C:203:HIS:HB2	2.51	0.45
1:C:273:GLN:HE21	1:C:273:GLN:HB3	1.61	0.45
2:B:9:VAL:HG12	2:B:95:TRP:HD1	1.82	0.45
1:A:238:LEU:HB2	1:A:246:TYR:HB3	1.98	0.45
1:C:16:SER:HB3	1:C:18:PHE:CE1	2.52	0.45
2:D:10:TYR:HB3	2:D:99:MET:HE2	1.98	0.45
2:D:30:PHE:CZ	2:D:54:MET:CE	2.99	0.45
1:A:213:PHE:HE2	1:A:216:LYS:O	2.00	0.45
1:C:138:GLY:O	1:C:140:PRO:HD3	2.17	0.45
1:C:142:TRP:O	1:C:146:PRO:HD2	2.17	0.45
1:A:264:ARG:HD3	1:A:275:ILE:HG12	1.99	0.45
1:A:179:GLY:C	1:A:181:SER:N	2.75	0.45
2:D:39:MET:HB2	2:D:49:VAL:HG21	1.99	0.45
1:A:61:GLN:CD	1:A:61:GLN:H	2.23	0.44
2:B:50:GLU:HB3	2:B:67:HIS:CE1	2.52	0.44
1:C:278:TYR:O	1:C:279:TRP:HB2	2.16	0.44
1:A:140:PRO:HG2	1:A:143:LEU:CD2	2.45	0.44
1:A:235:GLY:O	1:A:247:LEU:HD11	2.17	0.44
1:C:136:VAL:HB	1:C:137:PRO:HD2	1.99	0.44
2:D:23:LEU:HB2	2:D:70:PHE:CD1	2.52	0.44
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.86	0.44
1:A:66:LEU:O	1:A:69:MET:HB2	2.18	0.44
1:A:69:MET:HE2	1:A:69:MET:HB3	1.90	0.44
1:A:262:ALA:CB	1:A:277:LEU:HA	2.47	0.44
1:A:265:VAL:O	1:A:273:GLN:HB2	2.18	0.44
1:A:102:ALA:HB2	1:A:116:LEU:CD2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:C	1:A:177:GLU:N	2.73	0.44
2:D:9:VAL:HG12	2:D:23:LEU:HD11	1.99	0.44
1:C:146:PRO:O	1:C:149:VAL:HB	2.18	0.43
1:A:193:LEU:HG	1:A:276:ILE:HG21	1.99	0.43
2:B:3:LYS:HE2	2:B:31:HIS:CB	2.48	0.43
2:B:9:VAL:HG12	2:B:95:TRP:CD1	2.53	0.43
1:A:39:ARG:HH11	1:A:39:ARG:HB3	1.82	0.43
1:A:267:HIS:HB3	1:A:270:LEU:HD13	1.99	0.43
1:C:79:ARG:O	1:C:83:GLU:HG3	2.17	0.43
1:C:207:VAL:HG22	1:C:250:THR:HG22	2.01	0.43
1:C:266:LYS:HE3	1:C:273:GLN:HE22	1.82	0.43
1:A:58:LEU:HD12	1:A:63:TRP:HE3	1.83	0.43
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.29	0.43
2:B:22:ILE:HG23	2:B:68:THR:O	2.17	0.43
1:C:19:ALA:HB3	1:C:23:TRP:HB3	2.00	0.43
1:A:107:TYR:HA	1:A:108:PRO:HD3	1.84	0.43
2:D:9:VAL:HG23	2:D:93:VAL:CG2	2.48	0.43
1:A:216:LYS:HB3	1:A:217:PRO:CD	2.46	0.43
1:C:238:LEU:O	1:C:246:TYR:N	2.52	0.43
2:B:23:LEU:HD23	2:B:39:MET:HE3	2.00	0.43
2:B:32:PRO:O	2:B:84:HIS:HE1	2.02	0.43
1:A:49:PHE:CE2	1:A:55:GLN:HB2	2.54	0.43
1:A:60:ASN:O	1:A:63:TRP:N	2.52	0.42
1:C:47:ILE:N	1:C:47:ILE:HD12	2.34	0.42
1:A:168:CYS:HB3	1:A:169:PRO:HD3	2.00	0.42
1:A:129:TRP:HA	1:A:129:TRP:CE3	2.53	0.42
1:A:142:TRP:O	1:A:144:ASP:N	2.52	0.42
2:B:7:ILE:HD11	2:B:82:VAL:HB	2.02	0.42
1:C:67:GLN:O	1:C:67:GLN:HG2	2.18	0.42
2:B:13:HIS:HB3	2:B:14:PRO:HD2	2.02	0.42
1:C:133:TRP:O	1:C:147:ILE:HD12	2.19	0.42
1:C:220:VAL:H	1:C:234:ARG:NH2	2.17	0.42
1:A:39:ARG:HG2	1:A:40:TRP:N	2.35	0.42
1:A:49:PHE:HE1	1:A:63:TRP:CZ2	2.38	0.42
1:C:224:ARG:NH1	1:C:257:GLU:HG3	2.34	0.42
1:A:76:SER:HA	1:A:79:ARG:HG2	2.00	0.42
1:C:140:PRO:HB3	1:C:142:TRP:CZ3	2.54	0.42
1:C:262:ALA:CB	1:C:277:LEU:HD13	2.50	0.42
1:A:9:THR:HG23	1:A:105:GLU:HG2	2.01	0.42
1:A:74:ARG:C	1:A:76:SER:N	2.78	0.42
2:D:83:LYS:CG	2:D:90:PRO:HG3	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASP:OD2	2:B:12:ARG:NH1	2.52	0.41
1:C:76:SER:O	1:C:77:PHE:C	2.62	0.41
1:C:112:SER:OG	1:C:169:PRO:CG	2.67	0.41
1:A:74:ARG:O	1:A:75:VAL:C	2.61	0.41
1:A:39:ARG:HB3	1:A:39:ARG:NH1	2.36	0.41
1:C:79:ARG:HG2	1:C:79:ARG:NH1	2.34	0.41
1:C:218:VAL:HG22	1:C:219:TRP:N	2.35	0.41
1:A:34:ASP:O	1:A:35:LEU:HD23	2.20	0.41
2:B:23:LEU:HD23	2:B:39:MET:CE	2.51	0.41
1:C:53:TRP:HB2	1:C:178:ALA:CB	2.50	0.41
1:C:221:MET:HB2	1:C:221:MET:HE2	1.74	0.41
1:C:90:PRO:O	1:C:92:GLU:HG2	2.21	0.41
1:A:94:TYR:O	1:A:96:ILE:HG23	2.19	0.41
1:A:126:VAL:HG12	1:A:127:ARG:N	2.36	0.41
2:B:3:LYS:HE2	2:B:31:HIS:HB3	2.03	0.41
2:B:12:ARG:HE	2:B:13:HIS:CE1	2.38	0.41
1:A:262:ALA:HB2	1:A:277:LEU:HA	2.01	0.41
1:A:238:LEU:HD12	1:A:246:TYR:CD2	2.55	0.41
2:B:68:THR:OG1	2:B:69:GLU:N	2.53	0.41
1:C:18:PHE:HB2	1:C:96:ILE:HG12	2.00	0.41
1:A:50:THR:O	1:A:51:LYS:HD3	2.21	0.41
1:A:143:LEU:HD13	1:A:143:LEU:HA	1.85	0.41
1:C:49:PHE:HE1	1:C:63:TRP:CZ2	2.38	0.41
1:C:134:GLN:HA	1:C:147:ILE:HD12	2.02	0.40
1:C:262:ALA:HB2	1:C:277:LEU:HD13	2.03	0.40
1:A:265:VAL:O	1:A:273:GLN:HG3	2.21	0.40
1:C:128:PHE:CD1	1:C:160:VAL:HG11	2.56	0.40
1:C:187:GLU:HB2	1:C:214:TYR:HB3	2.02	0.40
1:C:231:GLY:O	1:C:233:HIS:ND1	2.53	0.40
1:A:17:SER:O	1:A:24:SER:HA	2.22	0.40
1:C:192:TRP:CZ3	2:D:14:PRO:HD3	2.57	0.40
2:D:95:TRP:CE2	2:D:96:ASP:O	2.74	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	271/315 (86%)	229 (84%)	33 (12%)	9 (3%)	3	6
1	C	271/315 (86%)	232 (86%)	33 (12%)	6 (2%)	5	12
2	B	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	3	7
2	D	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	5	13
All	All	736/828 (89%)	635 (86%)	81 (11%)	20 (3%)	4	9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
1	A	199	SER
2	B	97	ARG
2	D	29	GLN
1	A	91	LYS
1	A	108	PRO
1	A	200	ALA
1	C	21	ARG
1	C	92	GLU
1	C	143	LEU
1	A	143	LEU
1	C	141	SER
1	A	21	ARG
1	A	95	PRO
2	B	60	TRP
1	C	198	SER
1	C	108	PRO
1	A	217	PRO
2	B	47	PRO
2	D	15	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/274 (87%)	198 (83%)	40 (17%)	2	5
1	C	238/274 (87%)	197 (83%)	41 (17%)	2	5
2	B	94/94 (100%)	82 (87%)	12 (13%)	4	9
2	D	94/94 (100%)	82 (87%)	12 (13%)	4	9
All	All	664/736 (90%)	559 (84%)	105 (16%)	2	6

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	12	CYS
1	A	13	LEU
1	A	26	THR
1	A	30	VAL
1	A	44	SER
1	A	59	SER
1	A	60	ASN
1	A	65	LYS
1	A	75	VAL
1	A	77	PHE
1	A	83	GLU
1	A	84	LEU
1	A	87	MET
1	A	89	SER
1	A	91	LYS
1	A	93	ASP
1	A	99	GLN
1	A	116	LEU
1	A	118	VAL
1	A	134	GLN
1	A	136	VAL
1	A	137	PRO
1	A	142	TRP
1	A	143	LEU
1	A	145	LEU
1	A	146	PRO
1	A	149	VAL
1	A	154	GLN
1	A	167	THR
1	A	170	LEU
1	A	185	LYS
1	A	196	VAL

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Mol	Chain	Res	Type
1	A	206	LEU
1	A	209	HIS
1	A	220	VAL
1	A	221	MET
1	A	264	ARG
1	A	265	VAL
1	A	274	ASP
2	B	6	GLN
2	B	12	ARG
2	B	28	THR
2	B	35	ILE
2	B	44	LYS
2	B	50	GLU
2	B	69	GLU
2	B	70	PHE
2	B	71	THR
2	B	73	THR
2	B	90	PRO
2	B	93	VAL
1	C	7	ASN
1	C	12	CYS
1	C	13	LEU
1	C	15	MET
1	C	21	ARG
1	C	26	THR
1	C	28	SER
1	C	30	VAL
1	C	51	LYS
1	C	61	GLN
1	C	62	GLN
1	C	65	LYS
1	C	68	HIS
1	C	79	ARG
1	C	85	VAL
1	C	87	MET
1	C	91	LYS
1	C	92	GLU
1	C	116	LEU
1	C	118	VAL
1	C	135	THR
1	C	140	PRO
1	C	141	SER

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Mol	Chain	Res	Type
1	C	143	LEU
1	C	146	PRO
1	C	150	LEU
1	C	154	GLN
1	C	167	THR
1	C	170	LEU
1	C	188	LYS
1	C	201	HIS
1	C	206	LEU
1	C	219	TRP
1	C	224	ARG
1	C	252	ASP
1	C	261	LEU
1	C	268	SER
1	C	273	GLN
1	C	274	ASP
1	C	276	ILE
1	C	277	LEU
2	D	2	GLN
2	D	6	GLN
2	D	12	ARG
2	D	28	THR
2	D	36	GLU
2	D	39	MET
2	D	44	LYS
2	D	57	SER
2	D	64	ILE
2	D	87	MET
2	D	91	LYS
2	D	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	110	ASN
1	A	161	GLN
2	B	13	HIS
2	B	31	HIS
2	B	84	HIS
1	C	7	ASN
1	C	14	GLN

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Mol	Chain	Res	Type
1	C	36	GLN
1	C	99	GLN
1	C	117	HIS
1	C	186	GLN
1	C	201	HIS
1	C	227	GLN
2	D	31	HIS
2	D	84	HIS

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

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.