



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:22 PM UTC

PDB ID : 2LTN / pdb_00002ltn
Title : DESIGN, EXPRESSION, AND CRYSTALLIZATION OF RECOMBINANT LECTIN FROM THE GARDEN PEA (PISUM SATIVUM)
Authors : Suddath, F.L.; Phillips, S.R.; Einspahr, H.
Deposited on : 1990-06-26
Resolution : 1.70 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) : **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

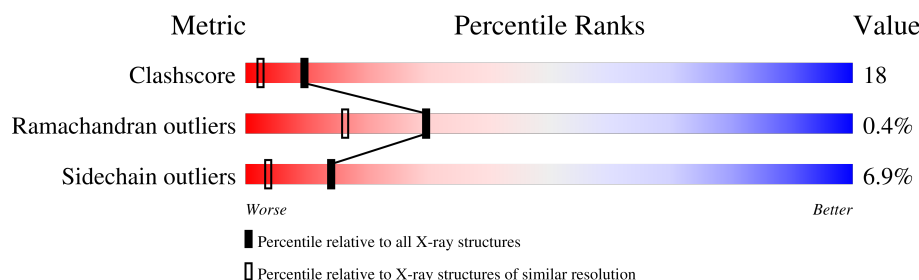
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	
1	C	181	
2	B	52	
2	D	52	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3866 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 PEA LECTIN, ALPHA CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	0	0	0
			1417	903	233	281			
1	C	181	Total	C	N	O	0	0	0
			1417	903	233	281			

- Molecule 2 is a protein called PEA LECTIN, BETA CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	48	Total	C	N	O	0	0	1
			367	236	58	73			
2	D	48	Total	C	N	O	0	0	1
			367	236	58	73			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

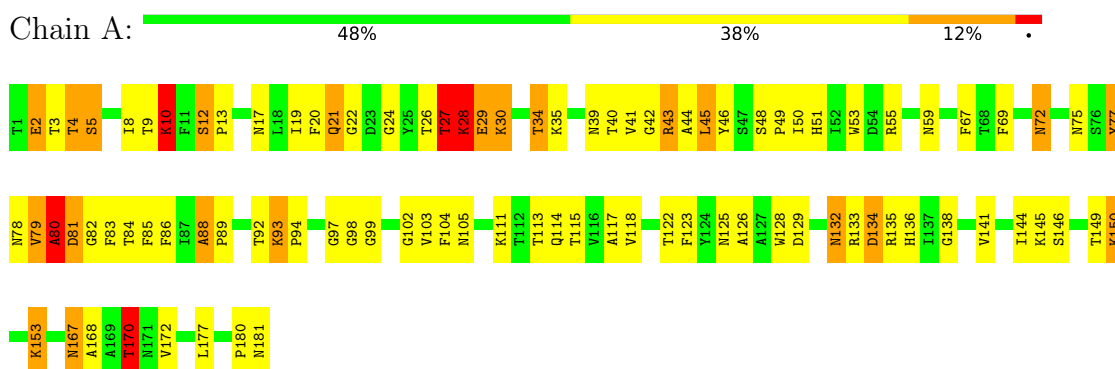
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total 120	O 120	0	0
5	B	27	Total 27	O 27	0	0
5	C	125	Total 125	O 125	0	0
5	D	22	Total 22	O 22	0	0

3 Residue-property plots [i](#)

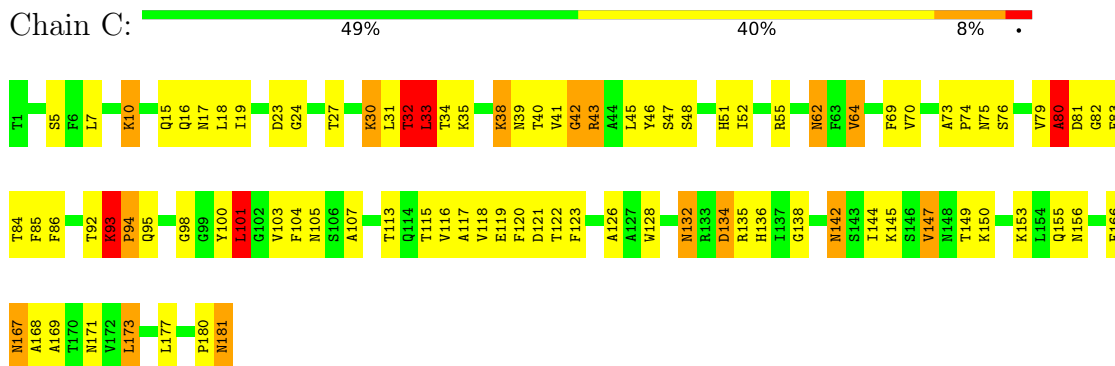
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

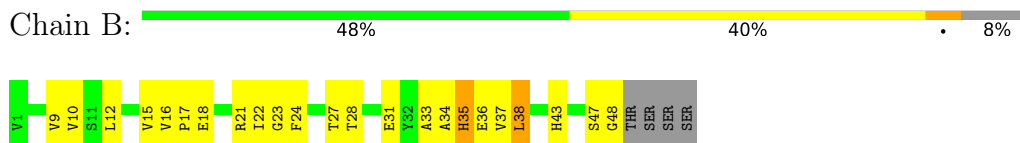
• Molecule 1: PEA LECTIN, ALPHA CHAIN



• Molecule 1: PEA LECTIN, ALPHA CHAIN



• Molecule 2: PEA LECTIN, BETA CHAIN



• Molecule 2: PEA LECTIN, BETA CHAIN



Y1	T2	S3	Y4	T5	L6	S7	D8	V9	V10	S11	L12	K13		R21	I22	G23	F24		T27		E31	Y32	A33	A34	H35	E36	V37	L38	S39	W40		H43		G48	THR	SER	SER	SER
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.73Å 61.16Å 136.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3866	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CA

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	2.05	45/1451 (3.1%)	2.87	124/1981 (6.3%)
1	C	1.95	31/1451 (2.1%)	2.67	98/1981 (4.9%)
2	B	2.05	8/377 (2.1%)	2.51	25/517 (4.8%)
2	D	1.91	9/377 (2.4%)	2.36	23/517 (4.4%)
All	All	2.00	93/3656 (2.5%)	2.71	270/4996 (5.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	C	1	3
All	All	2	5

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	ALA	N-CA	-15.77	1.26	1.46
1	A	80	ALA	N-CA	-11.97	1.28	1.46
1	C	80	ALA	CA-CB	9.62	1.70	1.53
1	C	18	LEU	N-CA	8.82	1.56	1.45
1	C	46	TYR	N-CA	8.73	1.56	1.46
1	C	81	ASP	N-CA	-8.69	1.36	1.46
1	A	27	THR	N-CA	-8.37	1.35	1.46
1	A	82	GLY	CA-C	8.18	1.60	1.51
1	A	85	PHE	N-CA	8.15	1.55	1.46
1	C	81	ASP	CA-C	7.65	1.60	1.52
1	A	46	TYR	N-CA	7.47	1.55	1.46
1	C	45	LEU	CA-C	7.34	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	VAL	N-CA	7.28	1.54	1.46
2	D	35	HIS	ND1-CE1	7.28	1.39	1.32
1	A	44	ALA	N-CA	7.21	1.55	1.46
2	B	24	PHE	N-CA	7.12	1.54	1.45
1	C	80	ALA	C-O	-7.08	1.16	1.23
1	A	138	GLY	N-CA	-7.00	1.38	1.45
1	C	46	TYR	C-N	6.97	1.43	1.33
1	C	84	THR	CA-C	6.79	1.61	1.52
1	A	86	PHE	C-N	-6.74	1.25	1.33
2	B	34	ALA	N-CA	6.67	1.54	1.45
1	A	146	SER	C-O	6.63	1.31	1.23
1	C	116	VAL	C-O	6.63	1.31	1.24
2	D	24	PHE	N-CA	6.59	1.54	1.45
2	D	22	ILE	C-O	6.57	1.30	1.24
1	C	31	LEU	CA-C	6.57	1.60	1.52
1	C	100	TYR	CA-C	6.55	1.61	1.52
1	A	98	GLY	C-N	6.54	1.41	1.33
1	C	62	ASN	C-O	6.52	1.31	1.23
1	A	80	ALA	C-N	-6.51	1.25	1.33
1	A	81	ASP	N-CA	-6.38	1.38	1.46
1	A	135	ARG	N-CA	6.38	1.54	1.45
1	A	115	THR	CB-OG1	6.34	1.53	1.43
1	C	128	TRP	C-O	6.32	1.31	1.23
1	A	44	ALA	C-O	6.21	1.30	1.23
2	B	22	ILE	C-N	6.20	1.39	1.33
1	C	83	PHE	N-CA	6.16	1.53	1.45
2	B	36	GLU	N-CA	6.15	1.53	1.45
1	C	43	ARG	CZ-NH2	6.08	1.41	1.33
1	C	135	ARG	N-CA	6.07	1.53	1.46
1	C	142	ASN	C-N	-6.06	1.26	1.33
1	A	46	TYR	C-N	6.05	1.41	1.33
2	D	31	GLU	CA-C	6.03	1.60	1.52
1	C	85	PHE	N-CA	5.99	1.53	1.46
1	A	102	GLY	C-O	5.98	1.32	1.23
1	A	181	ASN	C-OXT	5.93	1.35	1.23
1	A	82	GLY	C-N	-5.88	1.25	1.33
2	B	27	THR	CB-OG1	5.88	1.53	1.43
1	C	43	ARG	CA-C	5.87	1.59	1.52
1	C	98	GLY	C-O	5.86	1.31	1.23
1	A	28	LYS	CA-C	5.82	1.60	1.52
2	B	35	HIS	ND1-CE1	5.77	1.38	1.32
2	D	36	GLU	N-CA	5.75	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	42	GLY	N-CA	5.70	1.53	1.45
1	A	126	ALA	C-O	5.69	1.31	1.24
1	A	5	SER	C-O	5.66	1.30	1.23
2	D	39	SER	CA-CB	5.60	1.63	1.53
1	C	149	THR	CB-OG1	5.59	1.52	1.43
1	C	118	VAL	C-N	5.57	1.41	1.33
1	A	51	HIS	CE1-NE2	-5.57	1.26	1.32
1	A	149	THR	CB-OG1	5.57	1.52	1.43
1	A	22	GLY	N-CA	5.52	1.53	1.45
1	A	141	VAL	C-O	5.50	1.30	1.24
1	A	83	PHE	C-N	5.48	1.40	1.33
2	D	35	HIS	CA-C	5.46	1.58	1.52
1	A	123	PHE	C-N	5.46	1.41	1.33
1	A	40	THR	N-CA	5.46	1.53	1.45
1	A	97	GLY	CA-C	5.44	1.59	1.51
1	C	95	GLN	N-CA	5.40	1.53	1.46
1	A	144	ILE	CA-C	5.38	1.58	1.52
1	A	88	ALA	CA-C	5.37	1.59	1.52
1	C	32	THR	N-CA	5.36	1.52	1.46
1	A	92	THR	CA-C	-5.30	1.46	1.52
1	A	134	ASP	CA-C	5.30	1.59	1.52
2	D	37	VAL	CA-C	5.29	1.59	1.52
1	A	98	GLY	N-CA	5.29	1.53	1.45
1	A	118	VAL	N-CA	5.27	1.52	1.46
1	C	123	PHE	C-N	5.23	1.41	1.33
2	B	27	THR	CA-C	5.23	1.59	1.52
1	C	70	VAL	C-O	-5.22	1.18	1.24
2	B	35	HIS	CA-C	5.21	1.58	1.52
1	A	83	PHE	N-CA	5.20	1.52	1.45
1	A	3	THR	N-CA	5.19	1.52	1.45
1	A	24	GLY	CA-C	5.17	1.58	1.52
1	A	94	PRO	N-CA	5.15	1.53	1.47
1	A	42	GLY	N-CA	5.13	1.52	1.45
1	C	82	GLY	CA-C	5.11	1.58	1.52
1	A	170	THR	CA-CB	5.10	1.61	1.54
1	A	17	ASN	CA-C	5.07	1.59	1.52
1	C	121	ASP	N-CA	5.07	1.52	1.46
2	D	34	ALA	N-CA	5.03	1.52	1.46
1	A	150	LYS	N-CA	5.01	1.52	1.46

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	VAL	O-C-N	33.65	160.40	123.05
1	C	80	ALA	N-CA-C	29.59	161.06	108.69
1	C	79	VAL	O-C-N	23.41	149.04	123.05
1	A	80	ALA	N-CA-C	18.38	135.28	109.18
1	C	80	ALA	O-C-N	-17.93	101.48	123.36
1	A	26	THR	CA-C-N	15.52	151.19	121.54
1	A	26	THR	C-N-CA	15.52	151.19	121.54
1	A	80	ALA	CA-C-O	-15.21	103.85	121.49
1	A	27	THR	CA-C-N	14.95	150.08	121.54
1	A	27	THR	C-N-CA	14.95	150.08	121.54
1	A	28	LYS	N-CA-CB	14.07	134.28	110.49
1	C	45	LEU	O-C-N	13.95	140.40	123.24
1	A	170	THR	N-CA-CB	-13.89	92.43	110.90
1	A	105	ASN	OD1-CG-ND2	13.22	135.82	122.60
1	A	27	THR	CA-C-O	13.16	139.33	120.51
1	C	181	ASN	CA-CB-CG	-12.70	99.90	112.60
1	A	26	THR	CA-C-O	12.31	135.07	121.16
1	A	82	GLY	O-C-N	12.15	136.46	123.58
1	A	80	ALA	O-C-N	-11.86	106.37	122.74
2	B	35	HIS	O-C-N	11.77	137.04	123.27
1	C	80	ALA	CA-C-O	-11.55	106.08	120.28
1	C	81	ASP	N-CA-CB	11.54	130.53	110.44
1	C	181	ASN	N-CA-CB	11.43	129.94	110.50
1	A	138	GLY	O-C-N	11.28	132.37	123.23
1	A	136	HIS	O-C-N	10.97	135.15	123.42
1	C	100	TYR	O-C-N	10.90	137.89	122.41
2	B	23	GLY	O-C-N	10.85	136.10	123.62
1	C	84	THR	O-C-N	10.59	135.98	123.17
1	A	27	THR	N-CA-C	10.53	133.22	110.80
1	A	97	GLY	O-C-N	10.50	133.36	122.96
2	B	27	THR	O-C-N	10.36	135.70	123.17
1	A	134	ASP	O-C-N	10.31	135.03	122.86
1	C	75	ASN	CA-CB-CG	-10.29	102.31	112.60
1	A	24	GLY	O-C-N	10.26	133.41	122.84
2	D	35	HIS	O-C-N	10.10	134.99	123.27
1	C	80	ALA	CB-CA-C	-10.01	92.14	109.65
1	A	170	THR	OG1-CB-CG2	9.96	129.23	109.30
2	D	23	GLY	O-C-N	9.92	134.79	123.58
1	A	27	THR	O-C-N	-9.81	109.55	122.59
1	A	26	THR	O-C-N	-9.65	111.00	123.16
1	A	88	ALA	O-C-N	9.53	132.28	121.32
1	A	93	LYS	O-C-N	9.50	129.42	121.35
1	A	24	GLY	CA-C-O	-9.44	113.09	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	HIS	CA-C-O	-9.40	110.27	120.24
2	B	33	ALA	O-C-N	9.33	132.69	123.46
1	C	41	VAL	O-C-N	9.23	133.29	123.05
1	C	17	ASN	O-C-N	9.19	134.25	122.39
2	D	31	GLU	O-C-N	9.17	133.65	123.10
1	C	122	THR	O-C-N	9.13	133.75	122.34
1	C	45	LEU	CA-C-O	-9.10	110.46	121.11
1	A	105	ASN	O-C-N	9.07	132.12	122.23
1	A	81	ASP	N-CA-C	9.01	120.87	111.14
1	A	40	THR	CA-CB-OG1	-8.95	96.17	109.60
2	B	31	GLU	O-C-N	8.91	133.34	123.10
2	B	15	VAL	O-C-N	8.90	129.90	121.98
1	C	31	LEU	O-C-N	8.89	133.35	123.13
1	C	15	GLN	OE1-CD-NE2	8.87	131.47	122.60
1	A	43	ARG	O-C-N	8.82	133.84	123.17
1	C	45	LEU	CA-C-N	-8.79	108.39	120.87
1	C	45	LEU	C-N-CA	-8.79	108.39	120.87
1	C	93	LYS	O-C-N	8.77	128.39	121.55
2	D	37	VAL	O-C-N	8.71	132.66	123.26
1	A	81	ASP	N-CA-CB	8.58	122.52	110.07
2	D	35	HIS	CA-C-O	-8.55	111.15	120.30
1	A	75	ASN	CA-CB-CG	8.54	121.14	112.60
1	A	84	THR	O-C-N	8.42	133.36	123.17
2	D	9	VAL	N-CA-CB	8.39	119.86	110.72
1	A	39	ASN	O-C-N	8.29	133.05	122.86
1	A	17	ASN	O-C-N	8.25	133.75	122.37
2	D	33	ALA	O-C-N	8.19	131.57	123.46
1	C	24	GLY	O-C-N	8.19	131.27	122.84
1	C	32	THR	CB-CA-C	8.08	123.44	110.19
1	A	114	GLN	OE1-CD-NE2	8.03	130.63	122.60
1	C	136	HIS	O-C-N	7.89	131.86	123.42
1	C	16	GLN	OE1-CD-NE2	7.87	130.47	122.60
2	D	39	SER	CA-CB-OG	-7.83	95.43	111.10
1	C	134	ASP	O-C-N	7.80	132.06	122.86
2	B	37	VAL	O-C-N	7.77	131.65	123.26
1	C	80	ALA	CA-C-N	7.71	136.33	122.46
1	C	80	ALA	C-N-CA	7.71	136.33	122.46
1	C	83	PHE	N-CA-CB	-7.67	97.26	111.53
1	A	17	ASN	CA-C-O	-7.51	110.19	119.28
1	A	105	ASN	CA-C-O	-7.49	110.57	119.03
1	A	2	GLU	CG-CD-OE2	-7.48	101.19	118.40
1	A	80	ALA	CA-C-N	7.44	130.56	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ALA	C-N-CA	7.44	130.56	120.44
1	C	105	ASN	O-C-N	7.41	129.82	122.19
1	A	45	LEU	O-C-N	7.40	132.81	123.19
1	C	43	ARG	NE-CZ-NH1	7.35	128.85	121.50
1	C	135	ARG	N-CA-C	-7.34	100.36	110.35
1	C	138	GLY	CA-C-O	-7.24	114.95	121.47
1	A	117	ALA	O-C-N	7.24	131.66	123.27
1	A	41	VAL	O-C-N	7.23	131.48	123.09
1	A	72	ASN	CA-CB-CG	-7.23	105.37	112.60
1	A	8	ILE	O-C-N	7.20	130.01	123.03
1	C	100	TYR	CA-C-O	-7.16	110.66	119.18
1	A	27	THR	CA-CB-OG1	-7.14	98.89	109.60
1	C	69	PHE	O-C-N	7.09	132.37	123.15
1	A	181	ASN	CB-CG-ND2	-7.06	105.81	116.40
1	A	136	HIS	CA-C-O	-7.00	113.73	121.23
2	B	23	GLY	CA-C-O	-7.00	114.03	121.38
1	A	4	THR	CA-C-O	-6.99	111.69	120.28
2	D	37	VAL	CA-C-O	-6.95	113.09	120.39
1	C	31	LEU	CA-C-O	-6.92	112.68	120.43
1	C	120	PHE	CA-CB-CG	-6.91	106.89	113.80
1	C	81	ASP	CA-C-O	6.88	127.86	119.81
1	A	181	ASN	OD1-CG-ND2	6.88	129.48	122.60
1	A	75	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	135	ARG	N-CA-C	-6.82	101.53	110.53
1	C	147	VAL	CG1-CB-CG2	6.80	125.75	110.80
1	A	79	VAL	N-CA-C	-6.78	98.42	108.45
1	A	85	PHE	N-CA-C	-6.77	98.69	109.59
1	A	115	THR	O-C-N	6.73	131.47	123.33
1	C	48	SER	O-C-N	6.71	130.76	121.64
2	D	35	HIS	CA-C-N	-6.70	112.16	122.62
2	D	35	HIS	C-N-CA	-6.70	112.16	122.62
1	C	121	ASP	OD1-CG-OD2	6.66	138.88	122.90
2	B	47	SER	CB-CA-C	6.65	122.74	110.10
1	C	64	VAL	CB-CA-C	-6.61	99.27	110.71
1	A	138	GLY	CA-C-O	-6.60	115.19	121.19
1	A	35	LYS	O-C-N	6.58	130.98	122.23
2	B	10	VAL	CA-C-O	-6.56	113.65	120.27
1	C	117	ALA	CA-C-O	-6.55	113.47	121.06
1	A	82	GLY	CA-C-O	-6.53	115.07	121.86
1	C	17	ASN	CA-C-O	-6.52	111.55	119.43
1	A	8	ILE	CA-C-O	-6.50	113.94	120.31
1	A	39	ASN	CA-C-O	-6.47	114.12	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	THR	CA-CB-OG1	-6.44	99.94	109.60
1	A	128	TRP	CA-C-O	-6.42	111.33	120.51
1	C	64	VAL	N-CA-CB	6.42	121.98	111.45
1	C	43	ARG	O-C-N	6.42	130.71	123.27
1	C	23	ASP	O-C-N	6.37	130.60	122.39
1	C	104	PHE	O-C-N	6.35	131.64	122.94
1	C	142	ASN	CA-C-O	-6.35	112.83	120.32
2	B	21	ARG	CA-C-O	-6.32	113.97	121.11
1	A	19	ILE	CA-C-O	-6.29	113.81	120.48
1	C	81	ASP	CA-C-N	-6.28	113.67	121.83
1	C	81	ASP	C-N-CA	-6.28	113.67	121.83
1	C	84	THR	CA-C-N	-6.24	113.89	122.93
1	C	84	THR	C-N-CA	-6.24	113.89	122.93
1	C	85	PHE	N-CA-C	-6.21	99.60	109.59
2	D	13	LYS	CA-CB-CG	6.20	126.50	114.10
1	C	31	LEU	CA-C-N	-6.19	114.38	123.05
1	C	31	LEU	C-N-CA	-6.19	114.38	123.05
1	A	134	ASP	CA-C-O	-6.19	114.81	121.56
1	A	21	GLN	O-C-N	6.18	130.84	123.24
1	A	75	ASN	CA-C-O	-6.17	114.07	120.99
1	A	72	ASN	OD1-CG-ND2	6.16	128.76	122.60
1	A	20	PHE	CA-C-O	6.16	127.24	120.71
1	C	145	LYS	O-C-N	6.15	130.49	122.68
1	C	94	PRO	O-C-N	6.14	130.46	123.03
2	D	27	THR	O-C-N	6.08	130.53	123.17
1	A	102	GLY	O-C-N	-6.07	114.94	122.34
1	C	86	PHE	CA-C-O	-6.07	114.55	121.40
1	A	86	PHE	CA-C-O	-6.04	114.57	121.40
1	C	82	GLY	O-C-N	6.04	132.00	123.67
2	B	10	VAL	O-C-N	6.03	129.45	123.18
1	C	19	ILE	CA-C-O	-6.02	114.10	120.48
1	C	138	GLY	O-C-N	6.01	128.71	123.36
2	D	8	ASP	CA-CB-CG	-6.01	106.59	112.60
1	A	67	PHE	O-C-N	5.99	129.83	123.42
1	A	167	ASN	OD1-CG-ND2	-5.98	116.62	122.60
2	B	35	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	A	129	ASP	OD1-CG-OD2	5.96	137.20	122.90
1	A	10	LYS	CA-CB-CG	5.94	125.99	114.10
1	A	35	LYS	N-CA-C	-5.93	102.17	110.35
2	B	21	ARG	O-C-N	5.93	130.89	123.19
1	A	28	LYS	N-CA-C	-5.89	98.26	110.80
2	B	35	HIS	CA-C-N	-5.86	113.48	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	HIS	C-N-CA	-5.86	113.48	122.62
1	C	35	LYS	N-CA-C	-5.85	102.11	110.59
1	C	43	ARG	NH1-CZ-NH2	-5.85	111.69	119.30
1	A	29	GLU	O-C-N	5.83	127.99	121.87
1	A	26	THR	CA-CB-OG1	-5.83	100.86	109.60
1	C	51	HIS	CA-CB-CG	-5.83	107.97	113.80
1	A	168	ALA	CA-C-O	-5.83	113.52	120.10
1	A	45	LEU	CA-C-O	-5.82	114.53	121.11
1	C	48	SER	CA-C-O	-5.81	114.31	120.23
1	A	34	THR	CA-CB-OG1	-5.80	100.89	109.60
1	C	180	PRO	CA-C-O	5.80	128.81	119.64
1	A	81	ASP	CA-C-O	5.77	126.64	120.70
1	C	64	VAL	CA-CB-CG1	5.77	120.20	110.40
2	D	6	LEU	CA-C-O	-5.76	113.45	120.54
1	A	43	ARG	CA-C-O	-5.75	114.90	121.40
1	C	17	ASN	CA-C-N	-5.72	113.83	122.81
1	C	17	ASN	C-N-CA	-5.72	113.83	122.81
1	A	122	THR	O-C-N	5.70	129.46	122.34
1	C	113	THR	CA-CB-OG1	-5.67	101.09	109.60
1	C	147	VAL	N-CA-CB	-5.67	98.92	111.50
1	A	93	LYS	CA-CB-CG	5.66	125.43	114.10
1	A	79	VAL	CA-C-O	-5.65	114.54	120.76
1	A	97	GLY	CA-C-O	-5.64	116.00	121.92
1	A	27	THR	CA-CB-CG2	5.64	120.08	110.50
1	C	19	ILE	O-C-N	5.64	129.10	123.18
2	B	38	LEU	CA-C-O	-5.63	113.04	119.41
1	A	28	LYS	CA-CB-CG	-5.62	102.86	114.10
1	A	79	VAL	N-CA-CB	-5.60	102.27	111.45
1	A	180	PRO	O-C-N	5.58	129.81	122.27
1	A	93	LYS	CB-CG-CD	5.57	124.12	111.30
1	A	92	THR	N-CA-CB	-5.53	101.48	109.83
1	C	74	PRO	N-CA-C	-5.52	105.58	113.47
1	A	146	SER	N-CA-C	5.51	117.40	110.24
1	A	12	SER	CA-C-N	5.46	125.29	119.28
1	A	12	SER	C-N-CA	5.46	125.29	119.28
1	C	69	PHE	CA-C-O	-5.46	115.05	121.44
1	A	180	PRO	CA-C-O	-5.45	111.33	119.34
1	A	113	THR	O-C-N	5.42	127.87	122.12
1	A	125	ASN	O-C-N	5.41	129.49	123.05
1	A	170	THR	CA-CB-CG2	5.40	119.69	110.50
2	B	37	VAL	CA-C-O	-5.40	114.72	120.39
1	A	67	PHE	CA-C-O	-5.39	115.47	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	THR	CA-C-O	-5.38	115.31	121.40
1	A	84	THR	CA-C-N	-5.38	115.13	122.93
1	A	84	THR	C-N-CA	-5.38	115.13	122.93
1	A	80	ALA	N-CA-CB	5.38	119.72	111.22
1	C	119	GLU	OE1-CD-OE2	5.37	135.79	122.90
1	C	84	THR	CA-C-O	-5.37	115.34	121.40
1	C	92	THR	O-C-N	-5.36	116.28	122.87
1	A	113	THR	CA-CB-OG1	-5.36	101.57	109.60
2	B	31	GLU	CA-C-O	-5.35	114.97	121.28
1	C	47	SER	N-CA-C	5.34	117.11	111.28
1	C	126	ALA	CA-C-N	5.34	127.97	120.28
1	C	126	ALA	C-N-CA	5.34	127.97	120.28
1	C	33	LEU	O-C-N	5.29	128.57	122.17
2	D	21	ARG	NE-CZ-NH1	5.29	126.78	121.50
1	C	17	ASN	N-CA-CB	5.28	118.13	110.47
1	A	69	PHE	O-C-N	5.26	129.54	123.17
1	C	93	LYS	CA-C-O	-5.26	115.43	120.64
1	A	133	ARG	CD-NE-CZ	5.26	131.76	124.40
2	D	2	THR	CA-C-O	-5.25	114.68	120.24
1	C	95	GLN	OE1-CD-NE2	-5.23	117.37	122.60
2	D	40	TRP	CA-C-O	-5.22	113.16	120.21
1	C	107	ALA	N-CA-C	-5.21	106.43	112.89
1	A	83	PHE	N-CA-CB	-5.21	101.85	111.53
1	A	78	ASN	O-C-N	5.20	130.87	122.96
2	B	21	ARG	NE-CZ-NH1	5.20	126.70	121.50
2	D	39	SER	N-CA-CB	-5.20	101.86	111.52
2	B	15	VAL	N-CA-C	5.17	116.01	111.56
2	D	40	TRP	O-C-N	5.15	129.78	123.44
1	A	10	LYS	N-CA-CB	5.15	119.27	110.57
1	A	17	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	2	GLU	OE1-CD-OE2	5.12	135.20	122.90
1	C	75	ASN	OD1-CG-ND2	5.12	127.72	122.60
2	D	11	SER	N-CA-CB	5.12	118.07	110.49
1	C	62	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	145	LYS	CA-CB-CG	-5.11	103.88	114.10
1	A	86	PHE	O-C-N	5.11	129.35	123.17
1	A	138	GLY	CA-C-N	-5.11	116.36	122.90
1	A	138	GLY	C-N-CA	-5.11	116.36	122.90
1	C	34	THR	CA-C-O	5.10	126.98	121.06
1	C	180	PRO	CA-C-N	5.10	130.88	121.70
1	C	180	PRO	C-N-CA	5.10	130.88	121.70
2	B	28	THR	CA-CB-CG2	5.10	119.17	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	LEU	CA-C-O	-5.10	114.33	119.78
2	B	9	VAL	CA-C-O	5.10	126.47	120.71
1	C	39	ASN	N-CA-C	5.09	118.27	111.24
1	A	94	PRO	CA-C-O	5.09	126.67	121.23
1	C	75	ASN	CA-C-O	-5.07	114.74	120.32
1	A	9	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	129	ASP	O-C-N	5.07	128.32	121.12
1	A	28	LYS	O-C-N	5.07	129.33	122.59
2	B	35	HIS	ND1-CG-CD2	5.06	111.16	106.10
1	C	86	PHE	O-C-N	5.06	129.29	123.17
1	C	173	LEU	CB-CA-C	5.04	118.07	109.75
1	C	149	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	99	GLY	N-CA-C	5.03	119.98	114.40
2	D	10	VAL	CA-C-O	-5.03	115.19	120.27
2	D	23	GLY	CA-C-O	-5.02	115.45	121.08
1	A	46	TYR	CA-C-O	5.02	126.78	121.16
1	A	181	ASN	CB-CA-C	-5.01	100.58	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	27	THR	CA
1	C	80	ALA	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	ALA	Peptide,Mainchain
1	C	43	ARG	Sidechain
1	C	80	ALA	Peptide,Mainchain

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	1417	0	1365	76	0
1	C	1417	0	1366	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	367	0	349	10	0
2	D	367	0	349	9	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	120	0	0	5	0
5	B	27	0	0	0	0
5	C	125	0	0	0	0
5	D	22	0	0	0	0
All	All	3866	0	3429	124	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 18.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HZ3	1:A:153:LYS:CB	1.35	1.30
1:A:153:LYS:HB2	1:A:153:LYS:NZ	1.18	1.25
1:A:27:THR:HG23	1:A:29:GLU:N	1.62	1.11
1:A:28:LYS:HE3	1:A:30:LYS:HE2	1.33	1.09
1:A:27:THR:CG2	1:A:29:GLU:H	1.74	1.01
1:A:27:THR:HG23	1:A:29:GLU:H	0.85	0.99
1:A:29:GLU:C	1:A:30:LYS:NZ	2.22	0.98
1:A:29:GLU:HB2	1:A:30:LYS:HZ1	1.29	0.95
1:C:73:ALA:H	1:C:156:ASN:HD21	1.19	0.90
1:A:28:LYS:CE	1:A:30:LYS:HE2	2.03	0.89
1:A:29:GLU:HB2	1:A:30:LYS:NZ	1.92	0.84
1:C:38:LYS:HE3	2:D:32:TYR:CE1	2.17	0.80
1:A:30:LYS:N	1:A:30:LYS:HZ3	1.80	0.79
1:A:27:THR:HG23	1:A:28:LYS:H	1.46	0.79
1:A:27:THR:CG2	1:A:28:LYS:N	2.44	0.79
1:C:167:ASN:HD22	1:C:167:ASN:C	1.92	0.78
1:A:21:GLN:HE22	1:A:43:ARG:HH11	1.32	0.78
1:A:30:LYS:NZ	1:A:30:LYS:N	2.32	0.77
1:A:170:THR:HG23	1:A:172:VAL:HG23	1.66	0.77
1:A:153:LYS:CB	1:A:153:LYS:NZ	2.04	0.77
1:C:5:SER:OG	2:D:43:HIS:HD2	1.67	0.77
1:A:28:LYS:HE3	1:A:30:LYS:CE	2.15	0.76
1:C:38:LYS:HZ2	1:C:38:LYS:H	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:C	1:A:30:LYS:HZ3	1.94	0.73
1:C:55:ARG:HB3	1:C:55:ARG:CZ	2.18	0.73
1:A:132:ASN:HD22	1:A:134:ASP:H	1.36	0.73
1:A:77:TYR:HE1	5:A:624:HOH:O	1.73	0.71
1:C:153:LYS:HE2	2:D:4:TYR:OH	1.90	0.71
1:C:38:LYS:H	1:C:38:LYS:NZ	1.89	0.71
1:A:27:THR:HG23	1:A:28:LYS:N	2.06	0.70
1:C:132:ASN:HD22	1:C:134:ASP:H	1.39	0.70
1:A:27:THR:CG2	1:A:28:LYS:H	2.02	0.70
1:C:55:ARG:HG2	1:C:55:ARG:HH21	1.57	0.69
1:C:27:THR:O	1:C:30:LYS:HG2	1.92	0.69
1:C:155:GLN:HE22	1:C:181:ASN:C	2.03	0.66
1:A:21:GLN:NE2	1:A:43:ARG:HE	1.93	0.66
1:C:27:THR:HG22	1:C:32:THR:CG2	2.28	0.64
1:A:10:LYS:C	1:A:10:LYS:HD3	2.21	0.64
1:A:28:LYS:NZ	1:A:29:GLU:OE2	2.31	0.63
1:C:27:THR:HG22	1:C:32:THR:HG23	1.81	0.62
1:C:167:ASN:ND2	1:C:169:ALA:H	1.98	0.62
1:A:53:TRP:O	2:B:18:GLU:HG3	2.00	0.61
1:A:29:GLU:CB	1:A:30:LYS:HZ1	2.09	0.61
1:A:28:LYS:O	1:A:30:LYS:NZ	2.35	0.60
1:C:132:ASN:ND2	1:C:134:ASP:H	1.98	0.60
1:A:4:THR:HG21	1:A:50:ILE:CD1	2.32	0.60
1:C:167:ASN:HD22	1:C:169:ALA:H	1.50	0.60
1:A:79:VAL:O	5:A:407:HOH:O	2.17	0.59
1:A:170:THR:HG23	1:A:172:VAL:CG2	2.32	0.59
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.52	0.57
1:A:77:TYR:CD1	1:A:77:TYR:N	2.71	0.57
1:C:167:ASN:HD21	1:C:169:ALA:HB3	1.68	0.57
1:C:80:ALA:HB3	2:D:31:GLU:HB2	1.87	0.57
1:C:103:VAL:CG1	1:C:115:THR:HG21	2.35	0.56
1:A:5:SER:OG	2:B:43:HIS:HD2	1.90	0.54
1:A:28:LYS:HE3	1:A:28:LYS:O	2.08	0.54
1:A:28:LYS:O	1:A:28:LYS:HG2	2.05	0.54
1:A:59:ASN:HD22	2:B:48:GLY:N	2.06	0.53
1:A:28:LYS:O	1:A:28:LYS:CG	2.57	0.53
1:C:177:LEU:C	1:C:177:LEU:HD23	2.33	0.53
1:A:34:THR:OG1	2:B:35:HIS:HD2	1.92	0.53
1:C:38:LYS:CE	2:D:32:TYR:CE1	2.91	0.53
1:C:155:GLN:NE2	1:C:181:ASN:OXT	2.35	0.52
1:A:30:LYS:HZ2	1:A:30:LYS:CA	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:GLN:OE1	1:C:181:ASN:O	2.29	0.51
1:A:29:GLU:C	1:A:30:LYS:HZ2	2.15	0.51
1:C:55:ARG:HH21	1:C:55:ARG:CG	2.22	0.51
1:C:55:ARG:HG2	1:C:55:ARG:NH2	2.25	0.50
1:C:10:LYS:O	1:C:10:LYS:HG3	2.10	0.50
1:A:30:LYS:HG3	2:B:38:LEU:HD22	1.94	0.50
2:B:16:VAL:HB	2:B:17:PRO:HD2	1.93	0.49
1:A:30:LYS:CG	2:B:38:LEU:CD2	2.90	0.49
1:A:80:ALA:HB1	1:A:81:ASP:HA	1.94	0.49
1:C:55:ARG:CG	1:C:55:ARG:NH2	2.75	0.49
1:C:132:ASN:HD22	1:C:132:ASN:C	2.21	0.49
1:C:166:PHE:HZ	1:C:171:ASN:HD22	1.59	0.49
1:A:28:LYS:CE	1:A:28:LYS:O	2.62	0.47
1:C:101:LEU:HD22	1:C:144:ILE:HD11	1.96	0.47
1:A:88:ALA:HB1	1:A:89:PRO:CD	2.44	0.47
1:A:28:LYS:O	1:A:30:LYS:CE	2.62	0.47
1:A:30:LYS:CG	2:B:38:LEU:HD22	2.43	0.47
1:C:62:ASN:ND2	1:C:168:ALA:H	2.12	0.47
1:A:132:ASN:ND2	1:A:134:ASP:H	2.06	0.47
1:C:167:ASN:HD21	1:C:169:ALA:CB	2.28	0.47
1:A:21:GLN:HE22	1:A:43:ARG:NH1	2.06	0.46
1:C:38:LYS:HE3	2:D:32:TYR:CD1	2.50	0.46
1:A:29:GLU:CB	1:A:30:LYS:NZ	2.72	0.46
1:A:55:ARG:HD3	5:A:683:HOH:O	2.15	0.46
1:A:29:GLU:C	1:A:30:LYS:HZ1	2.21	0.46
1:A:10:LYS:HD3	1:A:10:LYS:O	2.16	0.46
1:A:30:LYS:HG2	2:B:38:LEU:CD2	2.46	0.46
1:A:27:THR:HG23	1:A:28:LYS:CA	2.45	0.45
1:A:30:LYS:N	1:A:30:LYS:HZ2	2.14	0.45
1:A:177:LEU:C	1:A:177:LEU:HD23	2.42	0.44
1:A:88:ALA:HB1	1:A:89:PRO:HD2	1.99	0.44
1:A:167:ASN:HB3	1:A:170:THR:HG22	1.99	0.44
1:C:115:THR:H	1:C:142:ASN:ND2	2.14	0.44
1:A:2:GLU:HA	1:C:7:LEU:O	2.18	0.44
1:A:28:LYS:O	1:A:29:GLU:HB2	2.19	0.43
1:A:132:ASN:HD22	1:A:132:ASN:C	2.27	0.43
1:C:153:LYS:HE2	1:C:153:LYS:HB2	1.73	0.43
1:A:28:LYS:C	1:A:30:LYS:HZ3	2.26	0.43
5:A:538:HOH:O	1:C:10:LYS:HE3	2.18	0.42
1:A:153:LYS:NZ	1:A:153:LYS:CA	2.80	0.42
1:C:93:LYS:HG2	1:C:94:PRO:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ASN:ND2	1:C:169:ALA:HB3	2.34	0.42
1:A:30:LYS:HG3	2:B:38:LEU:CD2	2.50	0.42
1:C:33:LEU:O	1:C:42:GLY:HA3	2.20	0.42
1:C:5:SER:OG	2:D:43:HIS:CD2	2.58	0.41
1:C:153:LYS:CE	2:D:4:TYR:OH	2.66	0.41
1:C:167:ASN:C	1:C:167:ASN:ND2	2.64	0.41
1:A:48:SER:HA	1:A:49:PRO:HD3	1.92	0.41
1:A:153:LYS:HD2	5:A:548:HOH:O	2.19	0.41
1:A:153:LYS:CB	1:A:153:LYS:HZ2	2.21	0.41
1:A:29:GLU:O	1:A:30:LYS:NZ	2.50	0.41
1:A:150:LYS:HB2	1:A:150:LYS:HE3	1.62	0.41
2:D:31:GLU:OE2	2:D:31:GLU:HA	2.21	0.41
1:A:12:SER:HA	1:A:13:PRO:HD3	1.84	0.41
1:C:103:VAL:HG13	1:C:115:THR:HG21	2.01	0.41
1:C:93:LYS:HG2	1:C:94:PRO:HD2	2.03	0.40
1:A:30:LYS:NZ	1:A:30:LYS:CA	2.84	0.40
1:C:27:THR:CG2	1:C:32:THR:CG2	2.98	0.40
1:A:28:LYS:O	1:A:30:LYS:HE2	2.22	0.40
1:A:103:VAL:HG23	1:A:104:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	179/181 (99%)	172 (96%)	5 (3%)	2 (1%)	11	3
1	C	179/181 (99%)	176 (98%)	3 (2%)	0	100	100
2	B	46/52 (88%)	46 (100%)	0	0	100	100
2	D	46/52 (88%)	46 (100%)	0	0	100	100
All	All	450/466 (97%)	440 (98%)	8 (2%)	2 (0%)	30	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	27	THR

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	156/156 (100%)	146 (94%)	10 (6%)	16	4
1	C	156/156 (100%)	141 (90%)	15 (10%)	8	1
2	B	41/45 (91%)	40 (98%)	1 (2%)	43	26
2	D	41/45 (91%)	40 (98%)	1 (2%)	43	26
All	All	394/402 (98%)	367 (93%)	27 (7%)	14	4

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	30	LYS
1	A	45	LEU
1	A	72	ASN
1	A	77	TYR
1	A	93	LYS
1	A	111	LYS
1	A	132	ASN
1	A	153	LYS
1	A	170	THR
2	B	12	LEU
1	C	10	LYS
1	C	30	LYS
1	C	32	THR
1	C	33	LEU
1	C	38	LYS
1	C	52	ILE
1	C	64	VAL

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Mol	Chain	Res	Type
1	C	76	SER
1	C	93	LYS
1	C	101	LEU
1	C	132	ASN
1	C	147	VAL
1	C	150	LYS
1	C	167	ASN
1	C	173	LEU
2	D	9	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	21	GLN
1	A	59	ASN
1	A	72	ASN
1	A	132	ASN
1	A	142	ASN
1	A	155	GLN
1	A	161	ASN
1	A	171	ASN
2	B	35	HIS
2	B	43	HIS
1	C	62	ASN
1	C	132	ASN
1	C	142	ASN
1	C	155	GLN
1	C	156	ASN
1	C	167	ASN
1	C	171	ASN
2	D	43	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.