



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:13 PM UTC

PDB ID : 1LEN / pdb_00001len
Title : REFINEMENT OF TWO CRYSTAL FORMS OF LENTIL LECTIN AT 1.8
ANGSTROMS RESOLUTION
Authors : Van Overberge, D.; Loris, R.; Wyns, L.
Deposited on : 1993-11-17
Resolution : 1.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

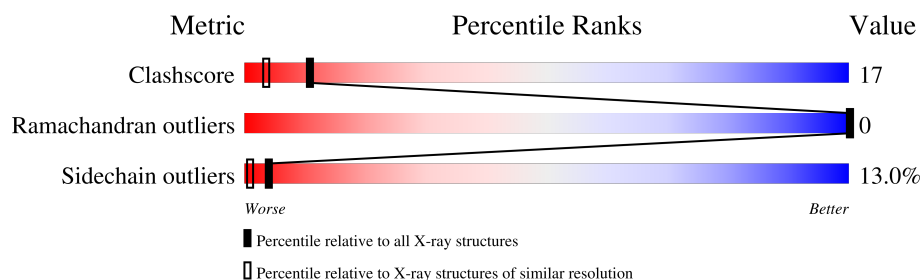
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	57% 33% 8% .
1	C	181	43% 44% 12% .
2	B	52	44% 35% 12% 10%
2	D	52	42% 35% 12% . 10%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3820 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 LECTIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	0	3	0
			1415	903	231	281			
1	C	181	Total	C	N	O	0	2	0
			1420	906	232	282			

- Molecule 2 is a protein called LECTIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	1	0
			370	238	60	72			
2	D	47	Total	C	N	O	0	1	0
			370	238	60	72			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is water.

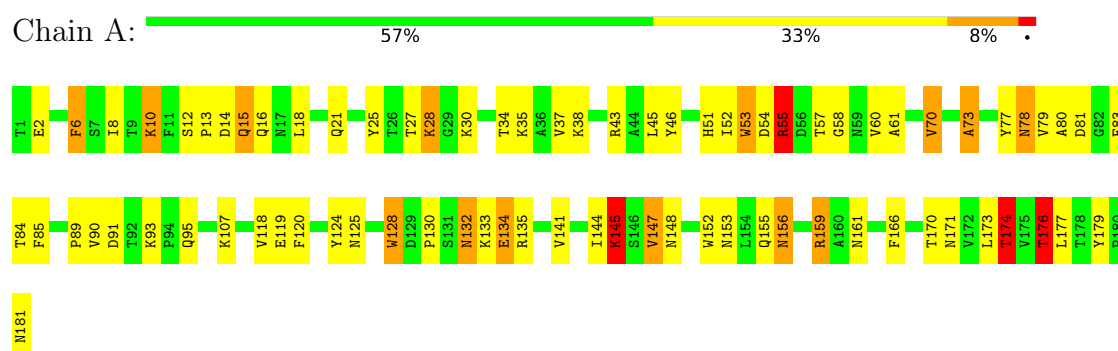
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	101	Total O 101 101	0	0
6	B	27	Total O 27 27	0	0
6	C	88	Total O 88 88	0	0
6	D	15	Total O 15 15	0	0

3 Residue-property plots

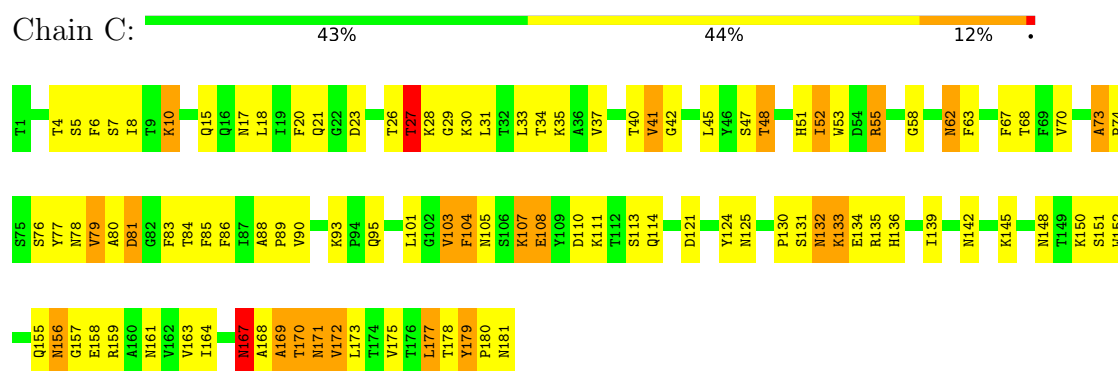
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

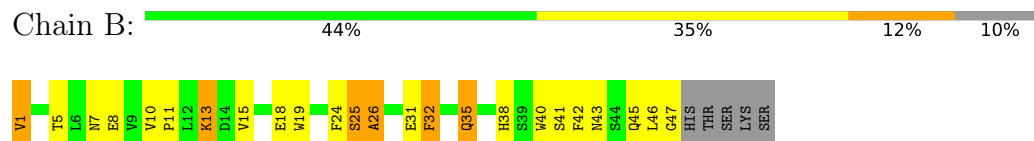
• Molecule 1: LECTIN



• Molecule 1: LECTIN



• Molecule 2: LECTIN



• Molecule 2: LECTIN





4 Data and refinement statistics

Xtriage (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	58.49Å 56.37Å 82.73Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3820	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: CA, PO4, MN

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	1.55	7/1465 (0.5%)	2.27	63/2002 (3.1%)
1	C	1.55	11/1464 (0.8%)	2.30	87/1999 (4.4%)
2	B	1.67	3/385 (0.8%)	2.40	24/527 (4.6%)
2	D	1.66	3/385 (0.8%)	2.22	19/527 (3.6%)
All	All	1.57	24/3699 (0.6%)	2.29	193/5055 (3.8%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	136	HIS	CE1-NE2	7.63	1.40	1.32
2	B	19	TRP	NE1-CE2	-7.58	1.29	1.37
1	A	51	HIS	ND1-CE1	7.27	1.39	1.32
2	D	38	HIS	ND1-CE1	7.12	1.39	1.32
1	C	51	HIS	ND1-CE1	6.90	1.39	1.32
1	A	53	TRP	NE1-CE2	-6.25	1.30	1.37
1	A	152	TRP	NE1-CE2	-6.24	1.30	1.37
2	B	38	HIS	ND1-CE1	6.08	1.38	1.32
2	B	45	GLN	CD-OE1	5.89	1.34	1.23
2	D	19	TRP	NE1-CE2	-5.67	1.31	1.37
1	C	125	ASN	CG-OD1	5.62	1.34	1.23
1	C	152	TRP	NE1-CE2	-5.53	1.31	1.37
1	C	136	HIS	ND1-CE1	5.48	1.38	1.32
1	A	176	THR	CA-CB	-5.38	1.43	1.53
1	C	52	ILE	CA-CB	-5.25	1.47	1.54
1	A	155	GLN	CD-OE1	5.25	1.33	1.23
1	C	161	ASN	CG-OD1	5.11	1.33	1.23
1	C	95	GLN	CD-OE1	5.10	1.33	1.23
1	C	114	GLN	CD-OE1	5.09	1.33	1.23
1	A	120	PHE	C-O	-5.09	1.16	1.23
2	D	45	GLN	CD-OE1	5.06	1.33	1.23
1	C	155	GLN	CD-OE1	5.06	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	105	ASN	CG-OD1	5.02	1.33	1.23
1	A	89	PRO	C-N	-5.02	1.27	1.34

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	PRO	CA-C-N	13.74	139.21	120.38
1	C	130	PRO	C-N-CA	13.74	139.21	120.38
1	A	55	ARG	CA-C-N	13.27	138.68	120.63
1	A	55	ARG	C-N-CA	13.27	138.68	120.63
2	D	10	VAL	CA-C-O	-11.02	114.21	119.94
1	C	80	ALA	CA-C-O	-10.60	109.44	121.10
1	C	23	ASP	CA-C-N	-10.59	110.28	120.34
1	C	23	ASP	C-N-CA	-10.59	110.28	120.34
1	A	78	ASN	OD1-CG-ND2	-10.47	112.13	122.60
1	A	179	TYR	CA-C-N	10.47	130.67	119.05
1	A	179	TYR	C-N-CA	10.47	130.67	119.05
1	A	8	ILE	CA-C-O	-9.98	110.53	120.31
1	C	169	ALA	CA-C-N	9.90	139.39	122.36
1	C	169	ALA	C-N-CA	9.90	139.39	122.36
1	C	90	VAL	O-C-N	-9.73	112.35	121.89
1	C	55	ARG	CA-C-N	9.57	133.28	120.65
1	C	55	ARG	C-N-CA	9.57	133.28	120.65
1	C	173	LEU	O-C-N	-9.27	112.66	123.22
1	A	80	ALA	CA-C-O	-9.07	111.52	121.23
1	A	79	VAL	CA-CB-CG2	8.90	125.53	110.40
1	A	78	ASN	CA-CB-CG	8.84	121.44	112.60
2	B	31	GLU	CB-CG-CD	8.54	127.12	112.60
1	A	73	ALA	O-C-N	8.53	128.88	121.20
2	D	43	ASN	CA-CB-CG	-8.52	104.08	112.60
2	D	46	LEU	CA-C-O	-8.41	111.07	120.32
1	C	179	TYR	CA-C-N	8.24	128.72	119.32
1	C	179	TYR	C-N-CA	8.24	128.72	119.32
1	A	159	ARG	CA-C-O	-8.11	111.09	120.49
2	B	40	TRP	CA-C-N	7.83	135.10	122.81
2	B	40	TRP	C-N-CA	7.83	135.10	122.81
2	B	43	ASN	CB-CG-ND2	7.81	128.12	116.40
1	A	147	VAL	CA-CB-CG2	7.79	123.65	110.40
2	B	38	HIS	CA-CB-CG	-7.71	106.09	113.80
1	A	89	PRO	CA-C-N	7.70	131.38	120.53
1	A	89	PRO	C-N-CA	7.70	131.38	120.53
1	C	79	VAL	CA-CB-CG2	7.66	123.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	43	ASN	OD1-CG-ND2	-7.64	114.96	122.60
2	D	15	VAL	CA-CB-CG2	7.58	123.28	110.40
1	A	159	ARG	O-C-N	7.57	132.33	123.02
1	C	58	GLY	O-C-N	-7.55	112.80	122.39
1	C	81	ASP	CA-CB-CG	-7.52	105.08	112.60
1	C	145	LYS	CA-C-N	7.42	131.37	120.90
1	C	145	LYS	C-N-CA	7.42	131.37	120.90
1	A	54	ASP	CA-C-N	7.38	132.93	121.19
1	A	54	ASP	C-N-CA	7.38	132.93	121.19
1	C	86	PHE	CA-C-N	7.37	132.90	123.10
1	C	86	PHE	C-N-CA	7.37	132.90	123.10
1	C	21	GLN	OE1-CD-NE2	-7.36	115.24	122.60
1	A	55	ARG	O-C-N	7.27	130.99	122.20
2	B	10	VAL	CA-CB-CG2	7.15	122.56	110.40
1	A	156	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	A	10	LYS	CA-C-O	-7.12	111.46	120.14
1	C	27	THR	O-C-N	7.11	131.72	123.41
1	A	46	TYR	O-C-N	-7.09	114.20	122.93
1	C	47	SER	CA-C-O	-7.09	111.82	119.97
2	B	45	GLN	CB-CG-CD	-7.04	100.63	112.60
2	B	11	PRO	N-CA-CB	-7.04	97.87	102.65
2	B	1	VAL	CA-CB-CG1	6.98	122.26	110.40
2	B	7	ASN	OD1-CG-ND2	6.95	129.55	122.60
2	B	47	GLY	CA-C-O	6.88	135.24	120.80
2	D	32	PHE	CA-CB-CG	-6.79	107.01	113.80
1	C	163	VAL	CA-C-O	-6.77	113.35	120.39
2	D	39	SER	CA-C-O	-6.73	114.03	121.23
1	A	70	VAL	CA-C-N	-6.70	114.88	123.19
1	A	70	VAL	C-N-CA	-6.70	114.88	123.19
1	C	139	ILE	CA-C-N	6.70	132.25	123.00
1	C	139	ILE	C-N-CA	6.70	132.25	123.00
2	B	15	VAL	CA-CB-CG2	6.70	121.79	110.40
1	C	108	GLU	O-C-N	6.69	130.56	123.06
1	A	156	ASN	CB-CG-ND2	6.68	126.42	116.40
1	A	58	GLY	N-CA-C	-6.65	106.05	115.30
1	C	81	ASP	CA-C-N	-6.62	113.22	121.83
1	C	81	ASP	C-N-CA	-6.62	113.22	121.83
1	C	164	ILE	CA-C-O	-6.62	113.50	120.39
1	C	58	GLY	N-CA-C	-6.61	106.57	115.36
1	C	84	THR	O-C-N	6.60	131.16	123.17
1	C	142	ASN	CA-C-O	-6.59	112.54	120.32
1	C	148	ASN	OD1-CG-ND2	-6.57	116.03	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	A	61	ALA	CA-C-O	-6.50	114.48	121.56
1	C	103	VAL	CA-CB-CG2	6.46	121.37	110.40
1	A	181	ASN	CA-CB-CG	-6.42	106.18	112.60
1	A	34	THR	O-C-N	6.38	130.67	123.27
1	C	67	PHE	O-C-N	6.36	130.23	123.42
1	C	35	LYS	CA-C-O	-6.35	113.62	121.88
2	B	25	SER	O-C-N	6.33	130.62	123.27
1	A	6	PHE	O-C-N	6.29	130.53	123.48
1	C	101	LEU	CA-C-O	-6.26	112.94	120.32
2	D	1	VAL	CA-CB-CG1	6.26	121.04	110.40
1	A	141	VAL	CA-CB-CG2	6.23	121.00	110.40
1	C	171	ASN	CA-C-N	-6.18	114.39	122.37
1	C	171	ASN	C-N-CA	-6.18	114.39	122.37
1	C	170	THR	OG1-CB-CG2	6.15	121.60	109.30
1	C	108	GLU	CA-C-O	-6.12	114.02	121.36
1	C	177	LEU	CA-C-O	-6.12	113.76	120.36
1	A	176	THR	CA-CB-OG1	6.08	118.72	109.60
1	C	83	PHE	O-C-N	-6.07	116.23	123.27
1	C	58	GLY	CA-C-O	6.06	125.75	119.02
1	A	51	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	C	8	ILE	CA-C-O	-6.03	113.85	120.48
1	A	148	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	C	34	THR	CA-C-N	-6.03	111.97	122.64
1	C	34	THR	C-N-CA	-6.03	111.97	122.64
1	A	130	PRO	CA-C-N	6.02	130.24	120.60
1	A	130	PRO	C-N-CA	6.02	130.24	120.60
2	D	9	VAL	CA-C-O	-6.02	113.99	120.85
1	C	15	GLN	CA-C-O	-5.99	114.88	121.58
1	A	119	GLU	CA-C-N	5.98	132.45	123.24
1	A	119	GLU	C-N-CA	5.98	132.45	123.24
2	B	26	ALA	CA-C-O	-5.95	114.34	120.89
1	C	104	PHE	CA-C-O	-5.92	114.71	121.58
1	A	85	PHE	CA-C-O	-5.90	114.05	120.36
1	C	21	GLN	CG-CD-NE2	5.90	125.24	116.40
2	B	32	PHE	CA-CB-CG	-5.87	107.93	113.80
2	D	6	LEU	CA-C-N	5.86	132.00	122.81
2	D	6	LEU	C-N-CA	5.86	132.00	122.81
1	C	83	PHE	CA-CB-CG	5.85	119.65	113.80
1	C	157	GLY	CA-C-O	5.83	125.49	119.02
1	A	15	GLN	CB-CG-CD	5.81	122.48	112.60
1	A	166	PHE	CA-CB-CG	-5.81	107.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	11	PRO	N-CA-CB	-5.80	98.50	102.73
1	C	121	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	8	ILE	O-C-N	5.74	128.60	123.03
1	A	176	THR	CA-CB-CG2	5.74	120.25	110.50
1	C	29	GLY	N-CA-C	-5.74	107.73	115.36
2	D	21	ARG	CA-C-O	-5.73	114.64	121.11
1	C	51	HIS	CA-C-N	5.73	129.71	120.55
1	C	51	HIS	C-N-CA	5.73	129.71	120.55
1	A	6	PHE	CA-C-O	-5.70	114.61	120.89
1	A	128	TRP	CA-C-O	-5.70	112.36	120.51
1	C	156	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	A	45	LEU	CA-C-O	-5.68	114.69	120.71
1	A	51	HIS	CA-CB-CG	-5.62	108.18	113.80
1	C	103	VAL	O-C-N	-5.60	115.57	122.57
1	C	67	PHE	CA-C-O	-5.59	115.25	121.23
2	D	4	TYR	CA-C-O	-5.59	113.40	120.28
1	C	15	GLN	CA-C-N	5.58	128.31	120.28
1	C	15	GLN	C-N-CA	5.58	128.31	120.28
1	C	181	ASN	CA-CB-CG	-5.55	107.05	112.60
1	A	144	ILE	CA-C-O	5.55	126.30	119.58
1	A	84	THR	CA-C-N	5.54	130.14	122.77
1	A	84	THR	C-N-CA	5.54	130.14	122.77
1	C	5	SER	CA-CB-OG	-5.52	100.06	111.10
1	C	78	ASN	OD1-CG-ND2	-5.49	117.11	122.60
2	B	35[A]	GLN	CB-CG-CD	5.44	121.85	112.60
2	B	35[B]	GLN	CB-CG-CD	5.44	121.85	112.60
1	C	37	VAL	CA-CB-CG2	5.44	119.65	110.40
1	A	58	GLY	CA-C-O	5.44	125.76	119.13
1	C	52	ILE	N-CA-C	5.42	116.91	111.00
1	C	107	LYS	CA-C-O	5.41	125.62	119.18
1	A	174	THR	CA-CB-OG1	5.41	117.72	109.60
1	C	62	ASN	CA-C-O	-5.40	114.71	120.92
1	C	172	VAL	CA-C-N	5.40	129.95	122.77
1	C	172	VAL	C-N-CA	5.40	129.95	122.77
2	B	45	GLN	CA-C-O	-5.39	113.63	120.20
2	B	24	PHE	CG-CD1-CE1	5.38	129.84	120.70
1	C	156	ASN	CB-CG-ND2	5.37	124.46	116.40
2	D	27	THR	CA-C-N	5.37	131.03	122.59
2	D	27	THR	C-N-CA	5.37	131.03	122.59
1	A	153	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	83	PHE	CA-CB-CG	5.35	119.15	113.80
2	D	3	SER	CA-C-N	5.33	131.28	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	SER	C-N-CA	5.33	131.28	122.33
1	A	173	LEU	O-C-N	-5.32	117.01	123.13
1	C	135	ARG	CA-C-N	-5.31	111.91	121.62
1	C	135	ARG	C-N-CA	-5.31	111.91	121.62
1	A	118	VAL	CA-C-O	-5.30	114.45	120.66
1	C	175	VAL	CA-CB-CG2	5.30	119.41	110.40
1	C	23	ASP	CA-C-O	-5.30	113.02	119.43
2	B	46	LEU	CA-C-O	-5.28	114.72	120.36
1	A	145	LYS	CA-C-O	-5.26	115.30	120.98
1	A	25	TYR	CA-C-O	-5.25	115.81	121.38
1	A	176	THR	N-CA-CB	5.24	119.87	110.80
1	C	73	ALA	CA-C-N	5.24	125.29	119.32
1	C	73	ALA	C-N-CA	5.24	125.29	119.32
2	B	25	SER	CA-CB-OG	-5.21	100.68	111.10
2	D	45	GLN	O-C-N	5.20	129.84	123.44
1	C	63	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	148	ASN	CB-CG-ND2	5.18	124.18	116.40
2	D	18	GLU	O-C-N	5.18	127.61	122.12
2	B	31	GLU	OE1-CD-OE2	-5.17	110.49	122.90
1	C	167	ASN	CA-C-N	5.15	127.70	120.28
1	C	167	ASN	C-N-CA	5.15	127.70	120.28
1	A	2	GLU	CA-CB-CG	5.13	124.36	114.10
1	A	53	TRP	CA-C-O	-5.11	115.63	121.40
2	B	7	ASN	CA-C-O	-5.09	115.15	121.06
1	C	17	ASN	O-C-N	-5.09	115.85	122.37
1	C	85	PHE	CA-C-O	-5.09	114.72	120.32
1	A	85	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	125	ASN	CA-CB-CG	-5.04	107.56	112.60
1	C	167	ASN	CA-CB-CG	-5.03	107.57	112.60
1	C	53	TRP	CA-C-O	-5.02	115.91	121.33
1	C	155	GLN	O-C-N	-5.00	116.72	122.87

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	1415	0	1363	38	0
1	C	1420	0	1368	63	0
2	B	370	0	354	17	0
2	D	370	0	354	11	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	101	0	0	4	0
6	B	27	0	0	0	0
6	C	88	0	0	2	0
6	D	15	0	0	0	0
All	All	3820	0	3439	117	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 17.

All (117) 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)
2:D:43:ASN:HD22	2:D:43:ASN:C	1.64	1.03
2:D:43:ASN:C	2:D:43:ASN:ND2	2.20	0.96
1:A:55:ARG:HH11	1:A:55:ARG:HG2	1.34	0.91
1:C:73:ALA:H	1:C:156:ASN:HD21	1.10	0.90
1:C:170:THR:HG23	1:C:172:VAL:HG23	1.53	0.88
1:A:132:ASN:HD22	1:A:134:GLU:H	1.20	0.85
1:A:73:ALA:H	1:A:156:ASN:HD21	1.23	0.85
1:C:10:LYS:NZ	1:C:10:LYS:HB2	1.95	0.82
2:D:43:ASN:ND2	2:D:44:SER:N	2.29	0.80
1:C:132:ASN:ND2	1:C:134:GLU:H	1.80	0.77
1:C:167:ASN:HD22	1:C:167:ASN:C	1.91	0.77
1:C:132:ASN:HD22	1:C:133:LYS:N	1.83	0.76
2:B:13:LYS:NZ	2:B:13:LYS:CB	2.48	0.76
1:C:177:LEU:C	1:C:177:LEU:HD23	2.11	0.76
1:A:21:GLN:HE22	1:A:43:ARG:HH21	1.33	0.76
1:C:132:ASN:HD22	1:C:132:ASN:C	1.95	0.75
1:A:132:ASN:ND2	1:A:134:GLU:H	1.87	0.73
1:C:170:THR:HG23	1:C:172:VAL:CG2	2.19	0.72
1:A:55:ARG:HG2	1:A:55:ARG:NH1	2.02	0.72
1:A:128:TRP:HB2	1:A:145:LYS:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:273:HOH:O	1:C:48:THR:HG23	1.91	0.71
1:C:27:THR:O	1:C:27:THR:CG2	2.40	0.70
1:C:76:SER:OG	1:C:77[B]:TYR:HD1	1.75	0.70
1:C:158:GLU:HG3	1:C:159:ARG:N	2.07	0.69
1:C:73:ALA:H	1:C:156:ASN:ND2	1.89	0.69
1:A:27:THR:O	1:A:27:THR:HG23	1.93	0.67
1:C:55:ARG:HB2	2:D:18:GLU:OE2	1.93	0.67
2:B:26:ALA:HB1	2:B:35[B]:GLN:HG3	1.77	0.66
1:A:77[B]:TYR:HD1	1:A:78:ASN:N	1.92	0.66
1:C:76:SER:OG	1:C:77[B]:TYR:CD1	2.48	0.65
1:A:77[B]:TYR:CD1	1:A:78:ASN:N	2.66	0.64
1:A:132:ASN:ND2	1:A:134:GLU:HB2	2.13	0.64
2:B:13:LYS:NZ	2:B:13:LYS:HB2	2.13	0.62
1:C:159:ARG:HD3	2:D:38:HIS:ND1	2.16	0.61
1:A:73:ALA:H	1:A:156:ASN:ND2	1.97	0.61
1:C:27:THR:O	1:C:27:THR:HG22	2.00	0.60
2:D:43:ASN:HD22	2:D:44:SER:N	1.95	0.60
1:A:174:THR:HG23	6:A:230:HOH:O	2.01	0.59
1:C:68:THR:HG21	1:C:159:ARG:HD2	1.84	0.59
2:B:13:LYS:HB2	2:B:13:LYS:HZ1	1.67	0.59
1:C:170:THR:CG2	1:C:172:VAL:HB	2.34	0.58
1:C:167:ASN:ND2	1:C:169:ALA:H	2.02	0.57
1:A:147:VAL:HG23	2:B:8:GLU:HG2	1.86	0.57
1:C:180:PRO:HD2	6:C:238:HOH:O	2.03	0.57
1:C:73:ALA:HB2	1:C:79:VAL:HG13	1.86	0.56
1:C:10:LYS:HB2	1:C:10:LYS:HZ2	1.70	0.56
1:A:176:THR:HG23	6:A:246:HOH:O	2.05	0.56
1:C:20:PHE:HE1	1:C:31:LEU:CD1	2.19	0.56
1:C:167:ASN:C	1:C:167:ASN:ND2	2.60	0.55
1:A:38:LYS:HG2	2:B:32:PHE:CD2	2.42	0.54
1:C:170:THR:HG22	1:C:172:VAL:H	1.72	0.54
1:C:177:LEU:HD23	1:C:178:THR:N	2.22	0.54
1:C:40:THR:HG22	2:D:28:THR:OG1	2.09	0.53
1:C:70:VAL:CG2	1:C:159:ARG:HG3	2.40	0.52
1:A:147:VAL:CG2	2:B:8:GLU:HG2	2.40	0.52
1:C:158:GLU:HG3	1:C:159:ARG:H	1.72	0.52
1:C:70:VAL:HG23	1:C:159:ARG:HG2	1.92	0.51
1:C:73:ALA:N	1:C:156:ASN:HD21	1.93	0.51
1:A:27:THR:O	1:A:27:THR:CG2	2.58	0.51
1:A:12:SER:HB2	1:A:15:GLN:OE1	2.12	0.50
1:C:6:PHE:C	1:C:6:PHE:CD1	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.60	0.50
1:C:76:SER:C	1:C:77[B]:TYR:HD1	2.19	0.49
2:D:26:ALA:HB1	2:D:35[B]:GLN:HG3	1.94	0.49
1:C:132:ASN:ND2	1:C:132:ASN:C	2.60	0.49
1:A:177:LEU:C	1:A:177:LEU:HD23	2.38	0.49
1:C:88:ALA:HB1	1:C:89:PRO:HD2	1.95	0.48
1:C:33:LEU:O	1:C:42:GLY:HA3	2.13	0.48
2:D:43:ASN:HD21	2:D:45:GLN:HG3	1.79	0.48
2:B:13:LYS:NZ	2:B:13:LYS:HB3	2.26	0.48
1:C:10:LYS:HB3	1:C:10:LYS:HE2	1.64	0.48
1:C:177:LEU:C	1:C:177:LEU:CD2	2.81	0.48
1:A:13:PRO:HD2	1:A:14:ASP:H	1.79	0.47
2:B:13:LYS:HB3	2:B:13:LYS:HZ2	1.80	0.47
1:A:38:LYS:HG2	2:B:32:PHE:HD2	1.80	0.47
1:C:167:ASN:HD21	1:C:169:ALA:HB3	1.79	0.46
1:A:55:ARG:NH1	1:A:55:ARG:CG	2.76	0.46
1:A:161:ASN:HB3	6:A:253:HOH:O	2.16	0.46
1:A:124:TYR:CD1	1:A:133:LYS:HA	2.50	0.46
1:C:28:LYS:HB3	1:C:28:LYS:HE2	1.59	0.45
1:C:103:VAL:HG23	1:C:104:PHE:CD2	2.52	0.45
1:C:170:THR:CG2	1:C:172:VAL:H	2.29	0.45
1:A:70:VAL:HG22	1:A:159:ARG:HA	1.99	0.45
1:C:62:ASN:HD22	1:C:168:ALA:H	1.65	0.45
1:C:132:ASN:HD22	1:C:134:GLU:H	1.63	0.45
1:C:170:THR:O	1:C:171:ASN:HB2	2.17	0.45
1:A:28:LYS:HB2	1:A:28:LYS:HE3	1.39	0.44
1:C:70:VAL:HG23	1:C:159:ARG:CG	2.48	0.44
1:A:132:ASN:HD22	1:A:132:ASN:C	2.25	0.44
1:A:176:THR:HG22	2:B:5:THR:HG23	2.00	0.43
2:D:28:THR:HB	2:D:32:PHE:HB3	2.00	0.43
1:C:73:ALA:HB1	1:C:74:PRO:HD2	2.00	0.43
1:C:41:VAL:HB	2:D:27:THR:HG22	2.01	0.43
1:C:88:ALA:HB1	1:C:89:PRO:CD	2.47	0.43
1:C:179:TYR:HA	1:C:180:PRO:HD3	1.62	0.43
2:B:13:LYS:CB	2:B:13:LYS:HZ2	2.27	0.43
1:C:124:TYR:CD1	1:C:133:LYS:HA	2.53	0.43
1:A:135:ARG:HH11	1:A:135:ARG:HD2	1.66	0.43
1:C:70:VAL:CG2	1:C:159:ARG:CG	2.97	0.42
1:A:53:TRP:CD2	2:B:13:LYS:HG3	2.53	0.42
1:A:55:ARG:HB2	2:B:18:GLU:OE2	2.20	0.42
1:C:167:ASN:HD22	1:C:169:ALA:H	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LYS:CB	2:B:13:LYS:HZ1	2.24	0.42
1:C:124:TYR:CE2	1:C:133:LYS:HD3	2.55	0.42
1:C:170:THR:CG2	1:C:172:VAL:CB	2.98	0.42
1:C:124:TYR:HD1	6:C:195:HOH:O	2.03	0.42
1:A:60:VAL:CG2	2:B:13:LYS:HE3	2.50	0.41
1:A:170:THR:O	1:A:171:ASN:HB2	2.21	0.41
1:A:21:GLN:NE2	1:A:43:ARG:HH21	2.09	0.41
1:A:21:GLN:NE2	1:A:43:ARG:HE	2.18	0.41
1:C:20:PHE:CZ	1:C:26:THR:HG23	2.56	0.41
1:C:76:SER:C	1:C:77[B]:TYR:CD1	2.98	0.41
1:A:6:PHE:CD1	1:A:6:PHE:C	2.99	0.40
1:C:110:ASP:C	1:C:110:ASP:OD1	2.64	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	182/181 (101%)	179 (98%)	3 (2%)	0	100	100
1	C	181/181 (100%)	176 (97%)	5 (3%)	0	100	100
2	B	46/52 (88%)	46 (100%)	0	0	100	100
2	D	46/52 (88%)	45 (98%)	1 (2%)	0	100	100
All	All	455/466 (98%)	446 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	158/156 (101%)	137 (87%)	21 (13%)	4	1
1	C	158/156 (101%)	136 (86%)	22 (14%)	3	1
2	B	41/45 (91%)	37 (90%)	4 (10%)	7	2
2	D	41/45 (91%)	36 (88%)	5 (12%)	5	1
All	All	398/402 (99%)	346 (87%)	52 (13%)	4	1

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	16	GLN
1	A	18	LEU
1	A	28	LYS
1	A	30	LYS
1	A	35	LYS
1	A	37[A]	VAL
1	A	37[B]	VAL
1	A	52	ILE
1	A	55	ARG
1	A	57	THR
1	A	81	ASP
1	A	90	VAL
1	A	91	ASP
1	A	93	LYS
1	A	107	LYS
1	A	132	ASN
1	A	134	GLU
1	A	145	LYS
1	A	174	THR
1	A	176	THR
2	B	1	VAL
2	B	13	LYS
2	B	25	SER
2	B	41	SER
1	C	4	THR
1	C	7	SER
1	C	10	LYS

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Mol	Chain	Res	Type
1	C	18	LEU
1	C	27	THR
1	C	30	LYS
1	C	41	VAL
1	C	45	LEU
1	C	48	THR
1	C	52	ILE
1	C	81	ASP
1	C	93	LYS
1	C	107	LYS
1	C	108	GLU
1	C	111	LYS
1	C	113	SER
1	C	131	SER
1	C	132	ASN
1	C	133	LYS
1	C	150	LYS
1	C	151	SER
1	C	167	ASN
2	D	1	VAL
2	D	5	THR
2	D	13	LYS
2	D	41	SER
2	D	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	59	ASN
1	A	78	ASN
1	A	105	ASN
1	A	132	ASN
1	A	142	ASN
1	A	156	ASN
1	A	161	ASN
1	A	171	ASN
2	B	43	ASN
1	C	62	ASN
1	C	105	ASN
1	C	132	ASN
1	C	142	ASN

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Mol	Chain	Res	Type
1	C	156	ASN
1	C	161	ASN
1	C	167	ASN
2	D	43	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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	C	182	-	4,4,4	0.91	0	6,6,6	0.23	0
3	PO4	A	182	-	4,4,4	0.84	0	6,6,6	0.32	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.