



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:25 AM UTC

PDB ID : 7WGA / pdb_00007wga
Title : 2.2 ANGSTROMS RESOLUTION STRUCTURE ANALYSIS OF TWO RE-
FINED N-ACETYLNEURAMINYLLACTOSE-WHEAT GERM AGGLU-
TININ ISOLECTIN COMPLEXES
Authors : Wright, C.S.
Deposited on : 1990-04-03
Resolution : 2.00 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

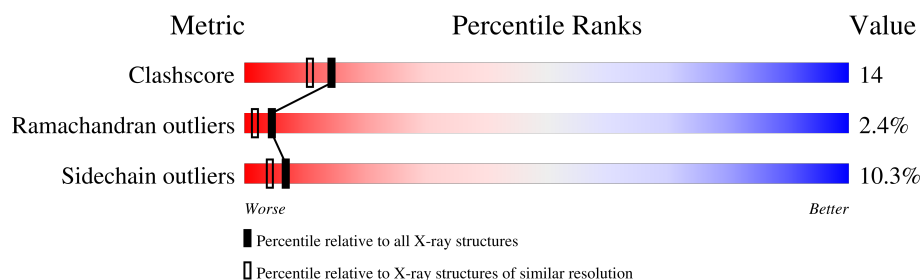
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	171	 51% 42% 5% •
1	B	171	 51% 36% 12% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2530 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 WHEAT GERM LECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1150	667	211	238	34			
1	B	171	Total	C	N	O	S	0	0	0
			1163	678	213	238	34			

- Molecule 2 is water.

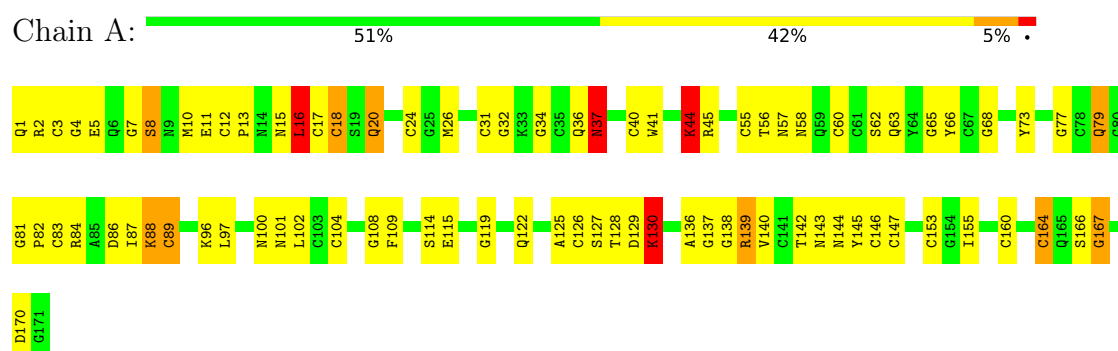
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	104	Total	O	0	0
			104	104		
2	B	113	Total	O	0	0
			113	113		

3 Residue-property plots

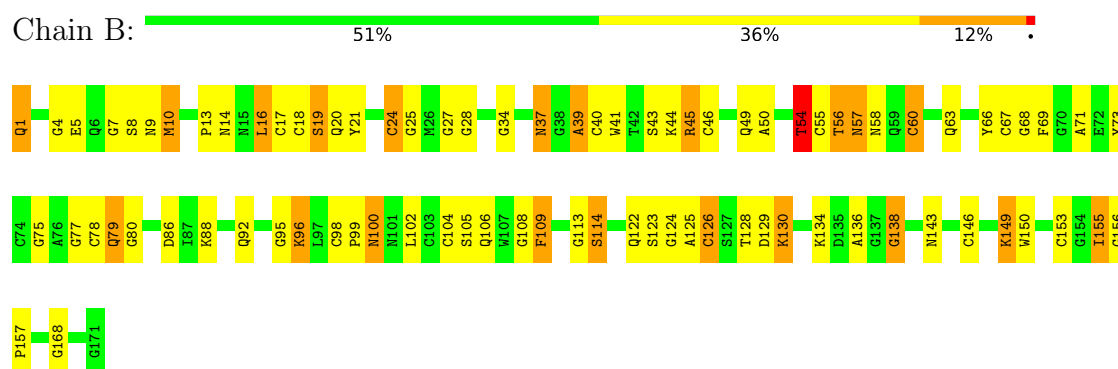
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: WHEAT GERM LECTIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	51.22Å 73.60Å 91.42Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2530	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: PCA

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	1.42	3/1162 (0.3%)	2.34	64/1556 (4.1%)
1	B	1.36	2/1177 (0.2%)	2.40	80/1576 (5.1%)
All	All	1.39	5/2339 (0.2%)	2.37	144/3132 (4.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	TYR	CA-CB	5.95	1.63	1.53
1	A	81	GLY	N-CA	5.68	1.52	1.44
1	A	115	GLU	CD-OE2	5.43	1.35	1.25
1	B	156	GLY	N-CA	5.25	1.51	1.44
1	B	73	TYR	CA-CB	5.08	1.61	1.53

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	GLN	OE1-CD-NE2	12.48	135.08	122.60
1	A	20	GLN	OE1-CD-NE2	12.12	134.72	122.60
1	A	79	GLN	OE1-CD-NE2	11.82	134.42	122.60
1	B	143	ASN	CA-CB-CG	10.75	123.35	112.60
1	A	86	ASP	CA-CB-CG	-9.83	102.77	112.60
1	A	37	ASN	CA-C-O	-9.14	111.53	121.31
1	B	68	GLY	O-C-N	9.12	134.11	123.62
1	B	153	CYS	CA-C-O	-9.07	110.73	120.80
1	B	24	CYS	CA-C-O	8.55	130.20	120.54
1	B	68	GLY	CA-C-O	-8.32	112.64	121.38
1	B	155	ILE	N-CA-CB	8.31	123.65	111.52
1	A	83	CYS	CA-CB-SG	7.77	132.28	114.40
1	A	15	ASN	CA-CB-CG	-7.29	105.31	112.60
1	B	138	GLY	N-CA-C	-7.22	104.82	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	GLN	CA-CB-CG	-7.20	99.70	114.10
1	A	114	SER	O-C-N	7.13	129.68	122.12
1	B	56	THR	CA-C-O	-7.08	113.46	121.81
1	B	123	SER	CA-C-O	-7.04	113.74	121.28
1	A	36	GLN	OE1-CD-NE2	6.92	129.53	122.60
1	B	40	CYS	CA-C-N	6.91	129.42	120.44
1	B	40	CYS	C-N-CA	6.91	129.42	120.44
1	B	66	TYR	CA-C-O	-6.89	112.33	120.60
1	A	143	ASN	OD1-CG-ND2	6.78	129.38	122.60
1	B	71	ALA	CA-C-O	-6.72	113.40	120.92
1	A	57	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	101	ASN	OD1-CG-ND2	6.68	129.28	122.60
1	A	40	CYS	CA-C-N	6.67	129.22	120.28
1	A	40	CYS	C-N-CA	6.67	129.22	120.28
1	B	157	PRO	N-CA-C	-6.67	104.84	113.57
1	B	19	SER	CA-C-O	-6.65	114.56	121.87
1	A	15	ASN	OD1-CG-ND2	6.57	129.17	122.60
1	A	10	MET	CA-C-O	-6.52	114.66	122.03
1	B	67	CYS	CA-C-O	-6.44	114.06	121.47
1	B	9	ASN	CA-CB-CG	-6.44	106.16	112.60
1	A	18	CYS	CA-C-O	-6.37	113.91	120.54
1	B	69	PHE	CA-C-N	6.35	132.82	122.21
1	B	69	PHE	C-N-CA	6.35	132.82	122.21
1	B	54	THR	O-C-N	6.29	130.14	122.84
1	B	45	ARG	CD-NE-CZ	6.28	133.20	124.40
1	A	60	CYS	CA-C-O	-6.26	113.91	121.05
1	B	134	LYS	CA-C-O	-6.21	111.64	120.51
1	B	58	ASN	CA-CB-CG	6.14	118.74	112.60
1	A	16	LEU	CB-CA-C	6.13	119.90	109.72
1	B	113	GLY	N-CA-C	-6.13	104.49	111.85
1	B	58	ASN	CA-C-O	-6.13	114.48	121.65
1	A	144	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	130	LYS	CA-C-N	6.11	126.02	119.85
1	A	130	LYS	C-N-CA	6.11	126.02	119.85
1	A	82	PRO	CA-C-N	6.06	129.32	120.71
1	A	82	PRO	C-N-CA	6.06	129.32	120.71
1	B	113	GLY	CA-C-O	-6.05	116.74	122.13
1	A	142	THR	N-CA-C	-5.96	101.12	110.36
1	B	24	CYS	N-CA-C	5.94	119.33	109.46
1	A	164	CYS	CA-CB-SG	5.94	128.06	114.40
1	A	127	SER	N-CA-C	-5.94	105.22	112.88
1	A	167	GLY	N-CA-C	-5.92	103.29	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ASN	CB-CA-C	-5.87	103.55	111.89
1	B	54	THR	CA-CB-OG1	-5.84	100.84	109.60
1	A	144	ASN	OD1-CG-ND2	5.83	128.43	122.60
1	A	44	LYS	CA-C-O	-5.83	115.20	121.56
1	B	79	GLN	N-CA-CB	5.83	118.92	110.88
1	B	34	GLY	CA-C-O	-5.82	112.76	119.10
1	A	84	ARG	CA-C-N	5.82	130.75	122.72
1	A	84	ARG	C-N-CA	5.82	130.75	122.72
1	A	65	GLY	CA-C-N	5.81	131.36	122.93
1	A	65	GLY	C-N-CA	5.81	131.36	122.93
1	A	37	ASN	OD1-CG-ND2	5.81	128.41	122.60
1	B	25	GLY	CA-C-N	5.77	132.30	122.37
1	B	25	GLY	C-N-CA	5.77	132.30	122.37
1	A	84	ARG	CD-NE-CZ	-5.76	116.33	124.40
1	B	109	PHE	CA-CB-CG	5.76	119.56	113.80
1	B	17	CYS	CA-C-O	-5.75	114.86	121.47
1	A	55	CYS	N-CA-CB	5.75	119.78	110.41
1	A	109	PHE	N-CA-CB	5.72	120.87	111.08
1	B	143	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	89	CYS	O-C-N	5.68	128.60	123.26
1	B	28	GLY	CA-C-N	5.65	128.90	120.31
1	B	28	GLY	C-N-CA	5.65	128.90	120.31
1	B	73	TYR	CA-CB-CG	-5.65	103.73	113.90
1	B	14	ASN	CA-C-O	-5.65	115.29	121.84
1	A	129	ASP	CA-CB-CG	-5.63	106.97	112.60
1	A	8	SER	CB-CA-C	-5.62	102.67	111.39
1	B	57	ASN	OD1-CG-ND2	5.58	128.18	122.60
1	B	27	GLY	CA-C-O	-5.58	117.59	122.16
1	B	136	ALA	CA-C-N	5.57	132.32	121.41
1	B	136	ALA	C-N-CA	5.57	132.32	121.41
1	A	68	GLY	CA-C-N	5.55	131.20	122.21
1	A	68	GLY	C-N-CA	5.55	131.20	122.21
1	B	57	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	58	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	B	130	LYS	CA-C-N	5.51	125.27	119.76
1	B	130	LYS	C-N-CA	5.51	125.27	119.76
1	A	37	ASN	O-C-N	5.50	128.87	122.99
1	A	97	LEU	CA-C-O	-5.50	114.95	121.16
1	A	3	CYS	N-CA-CB	-5.49	102.31	111.20
1	A	145	TYR	N-CA-C	-5.46	102.81	110.50
1	B	100	ASN	OD1-CG-ND2	5.44	128.04	122.60
1	B	104	CYS	CA-C-O	-5.43	114.35	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	ALA	CA-C-O	-5.43	112.75	120.51
1	B	114	SER	CB-CA-C	-5.41	101.80	110.79
1	A	11	GLU	CA-C-N	5.41	128.90	120.68
1	A	11	GLU	C-N-CA	5.41	128.90	120.68
1	A	101	ASN	CB-CG-ND2	-5.40	108.30	116.40
1	A	153	CYS	O-C-N	5.40	129.37	123.27
1	B	69	PHE	CA-CB-CG	5.38	119.18	113.80
1	B	126	CYS	N-CA-CB	5.35	118.20	109.69
1	A	166	SER	CA-C-O	-5.33	115.57	121.28
1	B	134	LYS	CA-C-N	-5.32	113.41	122.56
1	B	134	LYS	C-N-CA	-5.32	113.41	122.56
1	A	155	ILE	N-CA-CB	5.32	119.29	111.52
1	A	17	CYS	CA-C-N	-5.31	115.93	122.84
1	A	17	CYS	C-N-CA	-5.31	115.93	122.84
1	B	56	THR	CA-C-N	-5.31	115.45	124.31
1	B	56	THR	C-N-CA	-5.31	115.45	124.31
1	B	18	CYS	O-C-N	5.30	129.90	123.01
1	A	24	CYS	N-CA-C	5.30	118.26	109.46
1	A	126	CYS	N-CA-C	-5.22	103.25	110.35
1	B	95	GLY	CA-C-N	5.22	131.51	121.54
1	B	95	GLY	C-N-CA	5.22	131.51	121.54
1	B	128	THR	CA-C-O	5.21	125.38	119.18
1	A	166	SER	O-C-N	5.17	128.46	123.29
1	B	4	GLY	O-C-N	5.16	128.35	122.67
1	A	20	GLN	CA-CB-CG	-5.16	103.79	114.10
1	B	58	ASN	O-C-N	5.14	128.75	122.58
1	B	20	GLN	CG-CD-NE2	-5.14	108.69	116.40
1	B	14	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	100	ASN	N-CA-CB	-5.12	104.21	111.84
1	B	153	CYS	O-C-N	5.11	129.16	123.19
1	A	62	SER	CA-CB-OG	-5.10	100.90	111.10
1	A	4	GLY	CA-C-O	-5.09	115.95	122.01
1	B	41	TRP	O-C-N	5.09	127.31	122.07
1	B	157	PRO	CB-CA-C	5.08	119.52	112.11
1	B	17	CYS	O-C-N	5.06	128.68	122.96
1	B	10	MET	CA-CB-CG	5.04	124.19	114.10
1	B	43	SER	CA-C-O	-5.04	115.99	121.44
1	B	134	LYS	O-C-N	5.04	129.30	122.59
1	B	79	GLN	CA-CB-CG	5.04	124.17	114.10
1	A	101	ASN	N-CA-C	5.03	119.00	112.86
1	B	55	CYS	N-CA-C	-5.02	101.96	109.95
1	A	115	GLU	CB-CG-CD	5.02	121.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	PRO	CA-C-O	-5.02	115.74	121.86
1	B	54	THR	CA-C-O	-5.01	115.53	121.89
1	B	60	CYS	CA-C-O	-5.01	115.71	121.47
1	B	114	SER	N-CA-C	5.01	116.74	111.28

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	1150	0	969	27	0
1	B	1163	0	988	33	1
2	A	104	0	0	1	0
2	B	113	0	0	9	0
All	All	2530	0	1957	60	1

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 14.

All (60) 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:37:ASN:HA	1:A:44:LYS:HZ2	1.34	0.91
1:B:149:LYS:HE2	1:B:150:TRP:CE2	2.19	0.77
1:A:7:GLY:O	1:A:8:SER:HB2	1.86	0.76
1:B:44:LYS:NZ	2:B:180:HOH:O	2.19	0.74
1:A:44:LYS:NZ	1:A:56:THR:OG1	2.23	0.71
1:A:37:ASN:HA	1:A:44:LYS:NZ	2.07	0.70
1:B:150:TRP:CD1	2:B:253:HOH:O	2.47	0.67
1:B:124:GLY:O	1:B:126:CYS:N	2.24	0.67
1:B:92:GLN:NE2	1:B:106:GLN:O	2.29	0.65
1:B:150:TRP:HD1	2:B:253:HOH:O	1.78	0.63
1:B:88:LYS:HG3	1:B:109:PHE:CD1	2.35	0.61
1:A:31:CYS:HB3	1:A:41:TRP:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ASP:HA	2:B:239:HOH:O	2.03	0.59
1:B:77:GLY:O	1:B:78:CYS:C	2.49	0.56
1:B:7:GLY:O	1:B:8:SER:HB2	2.05	0.56
1:B:7:GLY:O	1:B:10:MET:HB2	2.06	0.55
1:A:104:CYS:HB3	1:A:122:GLN:HB2	1.89	0.55
1:B:98:CYS:HB3	1:B:102:LEU:HB2	1.88	0.55
1:A:139:ARG:NH2	2:A:221:HOH:O	2.28	0.54
1:B:138:GLY:HA3	2:B:173:HOH:O	2.08	0.53
1:B:146:CYS:SG	1:B:168:GLY:O	2.67	0.53
1:A:63:GLN:HB3	1:A:77:GLY:HA3	1.90	0.52
1:B:88:LYS:HG3	1:B:109:PHE:HD1	1.74	0.52
1:B:105:SER:O	1:B:122:GLN:NE2	2.32	0.52
1:B:60:CYS:HA	1:B:80:GLY:O	2.10	0.51
1:A:20:GLN:HB3	1:A:34:GLY:HA3	1.93	0.50
1:B:88:LYS:HA	1:B:108:GLY:O	2.11	0.50
1:A:136:ALA:C	1:A:138:GLY:H	2.20	0.50
1:A:147:CYS:O	1:A:164:CYS:HA	2.12	0.49
1:A:146:CYS:HA	1:A:167:GLY:HA3	1.94	0.48
1:A:89:CYS:O	1:A:108:GLY:HA2	2.14	0.48
1:A:128:THR:OG1	1:A:130:LYS:HE3	2.13	0.48
1:A:16:LEU:HD12	1:A:26:MET:CE	2.44	0.47
1:A:2:ARG:HA	1:A:2:ARG:HD2	1.66	0.47
1:B:54:THR:HG21	1:B:100:ASN:OD1	2.16	0.46
1:A:12:CYS:HB3	1:A:13:PRO:HD2	1.97	0.46
1:A:88:LYS:HA	1:A:108:GLY:O	2.15	0.46
1:B:37:ASN:HA	1:B:44:LYS:NZ	2.31	0.45
1:B:46:CYS:CA	1:B:50:ALA:HB3	2.46	0.45
1:A:136:ALA:C	1:A:138:GLY:N	2.75	0.45
1:B:130:LYS:HB3	1:B:130:LYS:HE2	1.66	0.45
1:A:18:CYS:HB2	1:A:37:ASN:ND2	2.32	0.45
1:A:18:CYS:HB2	1:A:37:ASN:HD21	1.82	0.44
1:A:136:ALA:O	1:A:138:GLY:N	2.51	0.44
1:B:88:LYS:HG3	1:B:109:PHE:CE1	2.52	0.44
1:A:37:ASN:HD22	1:A:37:ASN:C	2.26	0.44
1:A:160:CYS:O	1:A:170:ASP:N	2.36	0.44
1:B:146:CYS:SG	1:B:168:GLY:C	3.01	0.43
1:A:16:LEU:HD12	1:A:26:MET:HE3	2.00	0.43
1:B:63:GLN:HB3	1:B:77:GLY:HA3	2.01	0.43
1:B:1:PCA:N	2:B:198:HOH:O	2.52	0.43
1:B:106:GLN:N	2:B:220:HOH:O	2.25	0.42
1:A:45:ARG:HD3	1:A:66:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:HB3	2:B:265:HOH:O	2.19	0.42
1:B:149:LYS:HE2	1:B:150:TRP:CZ2	2.53	0.41
1:B:56:THR:O	1:B:57:ASN:HB2	2.19	0.41
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.85	0.41
1:B:45:ARG:HD2	1:B:45:ARG:HA	1.85	0.41
1:A:2:ARG:NH1	1:A:2:ARG:HG3	2.35	0.41
1:B:24:CYS:HB2	2:B:219:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:TYR:OH	1:B:86:ASP:OD2[3_455]	2.13	0.07

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	169/171 (99%)	152 (90%)	13 (8%)	4 (2%)	4	2
1	B	169/171 (99%)	147 (87%)	18 (11%)	4 (2%)	4	2
All	All	338/342 (99%)	299 (88%)	31 (9%)	8 (2%)	4	2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	ALA
1	B	75	GLY
1	B	96	LYS
1	A	125	ALA
1	A	137	GLY
1	B	39	ALA

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Mol	Chain	Res	Type
1	A	119	GLY
1	A	32	GLY

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	116/119 (98%)	104 (90%)	12 (10%)	7	4
1	B	118/119 (99%)	106 (90%)	12 (10%)	7	4
All	All	234/238 (98%)	210 (90%)	24 (10%)	7	4

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	16	LEU
1	A	37	ASN
1	A	44	LYS
1	A	79	GLN
1	A	87	ILE
1	A	88	LYS
1	A	96	LYS
1	A	102	LEU
1	A	130	LYS
1	A	139	ARG
1	A	140	VAL
1	B	5	GLU
1	B	16	LEU
1	B	19	SER
1	B	37	ASN
1	B	49	GLN
1	B	54	THR
1	B	79	GLN
1	B	96	LYS
1	B	99	PRO

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Mol	Chain	Res	Type
1	B	114	SER
1	B	149	LYS
1	B	155	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	14	ASN
1	A	37	ASN
1	A	59	GLN
1	A	100	ASN
1	B	9	ASN
1	B	20	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	0.91	0	9,10,12	1.44	1 (11%)
1	PCA	B	1	1	7,8,9	0.96	1 (14%)	9,10,12	2.26	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	PCA	O-C	2.43	1.29	1.20

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PCA	CB-CA-C	6.06	120.96	112.66
1	A	1	PCA	O-C-CA	-3.88	114.79	124.77
1	B	1	PCA	O-C-CA	-2.89	117.35	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	PCA	1	0

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.