



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:20 AM UTC

PDB ID : 9WGA / pdb_00009wga
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 : 1990-04-20
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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

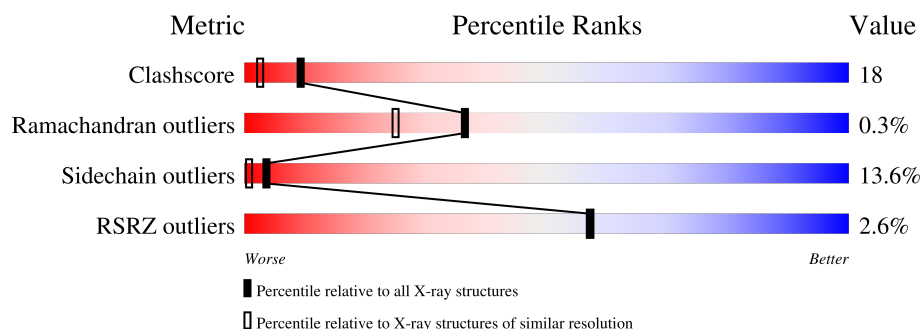
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	171	4% 54% 36% 10%
1	B	171	2% 57% 30% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2544 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
			1159	674	215	236	34			
1	B	171	Total	C	N	O	S	0	0	0
			1154	669	215	236	34			

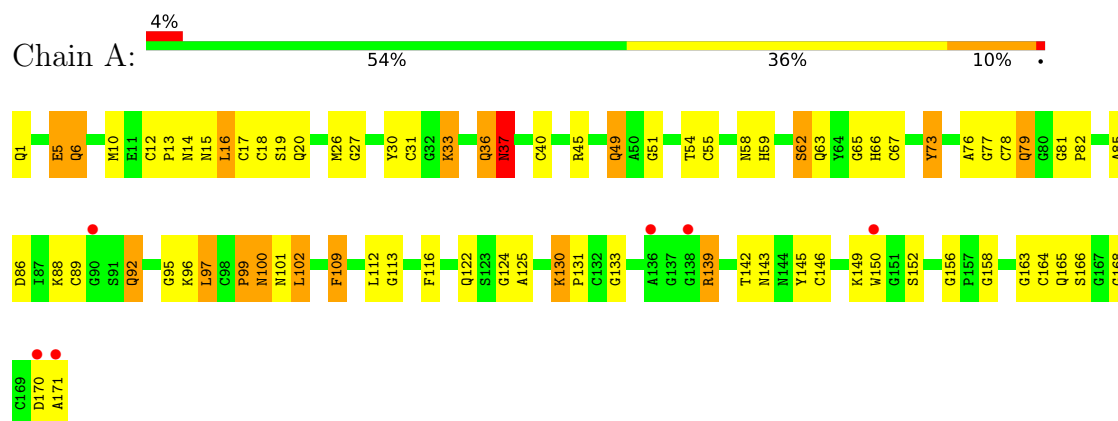
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	109	Total	O	0	0
			109	109		
2	B	122	Total	O	0	0
			122	122		

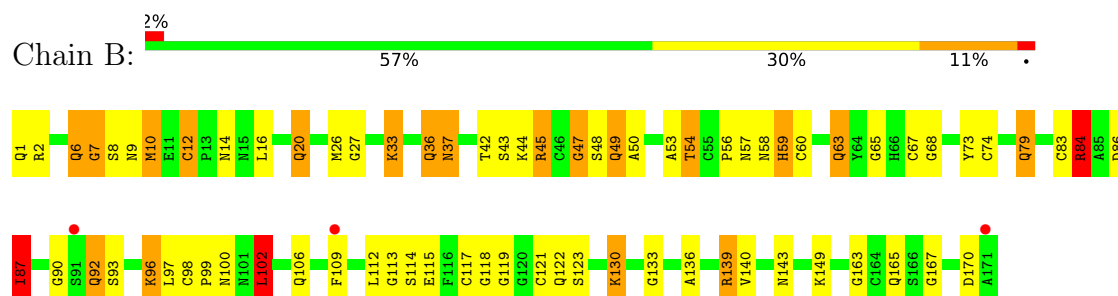
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: WHEAT GERM LECTIN



• Molecule 1: WHEAT GERM LECTIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	51.34Å 73.53Å 91.54Å 90.00° 97.59° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80 8.00 – 1.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-1.80) 97.1 (8.00-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.175 , (Not available) 0.267 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.1	EDS
L-test for twinning ¹	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.44$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2544	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.35	2/1175 (0.2%)	2.32	59/1575 (3.7%)
1	B	1.32	0/1168	2.24	55/1563 (3.5%)
All	All	1.33	2/2343 (0.1%)	2.28	114/3138 (3.6%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLY	N-CA	6.03	1.52	1.44
1	A	82	PRO	CA-C	5.12	1.58	1.53

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASN	CA-C-O	-12.31	108.14	121.31
1	A	170	ASP	N-CA-C	-11.93	98.21	113.12
1	A	109	PHE	CA-CB-CG	-10.75	103.05	113.80
1	A	113	GLY	N-CA-C	-10.21	101.02	111.85
1	B	14	ASN	OD1-CG-ND2	10.08	132.68	122.60
1	B	14	ASN	CA-CB-CG	-9.79	102.81	112.60
1	B	84	ARG	CD-NE-CZ	9.00	137.00	124.40
1	B	113	GLY	N-CA-C	-8.91	102.40	111.85
1	A	86	ASP	CA-CB-CG	-8.87	103.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ASN	OD1-CG-ND2	8.54	131.14	122.60
1	A	36	GLN	OE1-CD-NE2	8.35	130.95	122.60
1	B	43	SER	CA-C-O	-8.34	112.19	121.87
1	B	60	CYS	O-C-N	8.34	132.40	123.06
1	B	57	ASN	CA-CB-CG	7.82	120.42	112.60
1	A	15	ASN	OD1-CG-ND2	-7.71	114.89	122.60
1	B	139	ARG	CA-CB-CG	7.46	129.02	114.10
1	A	17	CYS	O-C-N	7.25	131.56	123.01
1	B	60	CYS	CA-C-O	-7.18	112.75	121.36
1	B	100	ASN	CA-C-O	-7.10	112.21	121.08
1	A	66	HIS	CA-CB-CG	-7.06	106.74	113.80
1	B	9	ASN	OD1-CG-ND2	6.95	129.55	122.60
1	A	14	ASN	N-CA-C	6.85	120.86	111.54
1	A	30	TYR	O-C-N	6.81	131.22	122.10
1	B	14	ASN	CB-CG-ND2	-6.81	106.19	116.40
1	B	84	ARG	NE-CZ-NH1	6.62	128.12	121.50
1	A	89	CYS	O-C-N	6.58	129.87	123.29
1	B	73	TYR	CA-CB-CG	-6.55	102.10	113.90
1	B	9	ASN	CA-CB-CG	-6.55	106.05	112.60
1	A	27	GLY	N-CA-C	-6.49	104.17	111.63
1	A	130	LYS	CA-C-N	6.35	126.69	119.83
1	A	130	LYS	C-N-CA	6.35	126.69	119.83
1	A	166	SER	CA-C-O	-6.30	114.20	121.26
1	A	36	GLN	CA-C-O	-6.30	112.43	120.31
1	A	142	THR	N-CA-C	-6.28	101.49	110.59
1	A	55	CYS	N-CA-CB	6.18	118.63	110.29
1	B	59	HIS	ND1-CE1-NE2	6.17	114.57	108.40
1	A	170	ASP	N-CA-CB	6.16	119.84	110.42
1	A	13	PRO	CB-CA-C	6.08	118.99	110.60
1	A	143	ASN	OD1-CG-ND2	6.04	128.64	122.60
1	A	73	TYR	O-C-N	5.96	131.06	122.13
1	B	167	GLY	N-CA-C	-5.96	102.05	112.53
1	A	139	ARG	CB-CA-C	5.95	119.56	109.50
1	A	51	GLY	N-CA-C	5.94	123.45	114.61
1	A	150	TRP	N-CA-C	5.92	120.34	113.18
1	A	40	CYS	CA-C-N	5.91	128.79	120.28
1	A	40	CYS	C-N-CA	5.91	128.79	120.28
1	A	112	LEU	O-C-N	5.88	130.44	123.33
1	A	156	GLY	O-C-N	5.88	127.65	121.77
1	B	56	PRO	CA-C-O	-5.86	114.42	122.15
1	A	116	PHE	O-C-N	5.85	130.75	122.20
1	B	20	GLN	CB-CG-CD	-5.83	102.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ILE	CA-C-O	5.82	126.80	120.57
1	B	86	ASP	CA-CB-CG	-5.81	106.79	112.60
1	B	20	GLN	OE1-CD-NE2	5.60	128.20	122.60
1	A	133	GLY	CA-C-N	5.60	128.05	120.38
1	A	133	GLY	C-N-CA	5.60	128.05	120.38
1	A	85	ALA	CB-CA-C	-5.58	100.32	109.53
1	B	12	CYS	CA-C-N	5.57	125.54	120.03
1	B	12	CYS	C-N-CA	5.57	125.54	120.03
1	A	97	LEU	N-CA-CB	-5.57	101.55	110.63
1	A	113	GLY	O-C-N	5.56	128.15	123.43
1	B	53	ALA	CA-C-N	5.55	130.30	122.09
1	B	53	ALA	C-N-CA	5.55	130.30	122.09
1	A	59	HIS	ND1-CE1-NE2	5.49	113.89	108.40
1	B	130	LYS	CA-C-N	5.49	125.39	119.85
1	B	130	LYS	C-N-CA	5.49	125.39	119.85
1	B	63	GLN	OE1-CD-NE2	5.48	128.08	122.60
1	B	58	ASN	OD1-CG-ND2	5.47	128.07	122.60
1	A	37	ASN	O-C-N	5.46	128.84	122.99
1	A	156	GLY	CA-C-N	5.46	125.54	119.32
1	A	156	GLY	C-N-CA	5.46	125.54	119.32
1	A	76	ALA	CA-C-O	5.40	127.08	120.92
1	B	54	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	79	GLN	CA-C-O	-5.39	113.21	119.14
1	A	124	GLY	CA-C-N	5.38	131.82	121.54
1	A	124	GLY	C-N-CA	5.38	131.82	121.54
1	A	78	CYS	CA-C-O	-5.37	115.58	120.95
1	B	42	THR	CA-CB-OG1	-5.35	101.57	109.60
1	A	19	SER	CA-C-O	5.32	128.11	120.51
1	A	66	HIS	ND1-CG-CD2	5.32	111.42	106.10
1	B	123	SER	N-CA-CB	-5.30	102.16	111.49
1	A	36	GLN	N-CA-C	5.29	119.66	112.04
1	B	143	ASN	CA-CB-CG	5.26	117.86	112.60
1	B	48	SER	O-C-N	5.25	128.15	122.11
1	B	67	CYS	CA-C-O	-5.25	114.89	120.92
1	B	68	GLY	O-C-N	5.24	128.94	123.92
1	B	57	ASN	O-C-N	5.23	130.45	122.03
1	B	106	GLN	OE1-CD-NE2	5.21	127.81	122.60
1	B	102	LEU	CA-C-N	5.20	128.25	120.87
1	B	102	LEU	C-N-CA	5.20	128.25	120.87
1	B	7	GLY	CA-C-N	-5.18	114.78	122.35
1	B	7	GLY	C-N-CA	-5.18	114.78	122.35
1	B	47	GLY	CA-C-N	5.18	128.60	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	GLY	C-N-CA	5.18	128.60	120.82
1	B	73	TYR	O-C-N	5.17	128.29	122.19
1	A	100	ASN	CA-C-O	-5.16	114.41	120.81
1	B	7	GLY	O-C-N	5.16	129.41	122.70
1	B	84	ARG	CG-CD-NE	5.14	123.32	112.00
1	B	143	ASN	CA-C-O	-5.14	114.25	120.32
1	A	112	LEU	CA-C-O	-5.14	114.43	120.60
1	B	27	GLY	CA-C-N	5.13	125.68	119.98
1	B	27	GLY	C-N-CA	5.13	125.68	119.98
1	A	165	GLN	OE1-CD-NE2	5.12	127.72	122.60
1	B	36	GLN	CA-C-O	-5.12	113.63	119.41
1	B	68	GLY	CA-C-O	-5.10	115.99	121.35
1	B	113	GLY	CA-C-O	-5.10	118.20	122.33
1	A	145	TYR	N-CA-C	-5.09	103.76	110.43
1	B	170	ASP	CB-CG-OD1	5.09	130.10	118.40
1	A	31	CYS	O-C-N	5.07	129.41	122.46
1	A	67	CYS	N-CA-C	5.07	117.50	109.24
1	A	102	LEU	O-C-N	5.07	128.68	122.75
1	A	97	LEU	CA-C-O	-5.06	115.31	121.28
1	A	99	PRO	N-CD-CG	-5.06	95.61	103.20
1	A	62	SER	CA-CB-OG	-5.04	101.03	111.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	45	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1159	0	972	34	0
1	B	1154	0	975	44	0
2	A	109	0	0	4	0
2	B	122	0	0	10	0
All	All	2544	0	1947	77	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 (77) 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:16:LEU:HD12	1:A:26:MET:HE2	1.32	1.08
1:B:49:GLN:NE2	1:B:79:GLN:HE22	1.60	0.99
1:B:92:GLN:HE22	1:B:122:GLN:HE22	1.28	0.79
1:B:7:GLY:O	1:B:8:SER:HB2	1.84	0.78
1:B:49:GLN:HE22	1:B:79:GLN:HE22	1.32	0.76
1:A:16:LEU:HD12	1:A:26:MET:CE	2.14	0.76
1:A:49:GLN:H	1:A:49:GLN:HE21	1.34	0.75
1:A:5:GLU:HG2	2:A:274:HOH:O	1.87	0.74
1:A:49:GLN:HE22	1:A:79:GLN:HE22	1.34	0.72
1:A:49:GLN:H	1:A:49:GLN:NE2	1.88	0.71
1:A:92:GLN:HE22	1:A:122:GLN:HE22	1.39	0.70
1:B:7:GLY:O	1:B:10:MET:HB2	1.93	0.68
1:A:6:GLN:HE21	1:A:6:GLN:H	1.44	0.64
1:A:92:GLN:NE2	1:A:92:GLN:H	1.95	0.64
1:B:59:HIS:ND1	2:B:183:HOH:O	2.30	0.63
1:B:16:LEU:HD23	1:B:26:MET:CE	2.28	0.63
1:A:99:PRO:O	1:A:102:LEU:HD13	1.98	0.63
1:A:20:GLN:HE22	1:A:33:LYS:NZ	1.98	0.62
1:B:90:GLY:C	1:B:92:GLN:H	2.08	0.62
1:B:2:ARG:NH2	2:B:284:HOH:O	2.32	0.61
1:B:16:LEU:HD23	1:B:26:MET:HE3	1.83	0.61
1:B:6:GLN:NE2	1:B:6:GLN:H	1.99	0.60
1:A:45:ARG:NH1	1:A:65:GLY:O	2.34	0.60
1:A:6:GLN:HE22	1:A:36:GLN:HE22	1.50	0.58
1:B:49:GLN:HG2	1:B:65:GLY:HA3	1.85	0.58
1:A:62:SER:HB3	1:A:73:TYR:CD1	2.40	0.56
1:B:90:GLY:C	1:B:92:GLN:N	2.64	0.56
1:B:63:GLN:NE2	2:B:242:HOH:O	2.38	0.55
1:B:49:GLN:CG	1:B:65:GLY:HA3	2.37	0.55
1:A:49:GLN:NE2	1:A:79:GLN:HE22	2.05	0.54
1:A:92:GLN:H	1:A:92:GLN:HE21	1.55	0.54
1:B:20:GLN:HG2	2:B:265:HOH:O	2.07	0.53
1:B:63:GLN:NE2	2:B:187:HOH:O	2.37	0.53
1:A:18:CYS:HB3	1:A:36:GLN:HB2	1.91	0.53
1:B:6:GLN:HE22	1:B:36:GLN:HE22	1.56	0.53
1:A:12:CYS:HB2	2:A:218:HOH:O	2.09	0.53
1:A:37:ASN:HD22	1:A:37:ASN:C	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HH12	1:A:49:GLN:HB2	1.74	0.52
1:B:47:GLY:HA2	2:B:209:HOH:O	2.10	0.51
1:B:49:GLN:NE2	1:B:49:GLN:H	2.08	0.51
1:A:20:GLN:HE22	1:A:33:LYS:HZ1	1.58	0.51
1:B:96:LYS:HD3	2:B:208:HOH:O	2.10	0.51
1:A:45:ARG:HH12	1:A:49:GLN:CB	2.25	0.49
1:B:74:CYS:O	1:B:84:ARG:HB2	2.13	0.49
1:B:2:ARG:O	1:B:7:GLY:HA3	2.12	0.49
1:A:20:GLN:NE2	2:A:276:HOH:O	2.46	0.49
1:A:149:LYS:HA	1:A:163:GLY:O	2.14	0.47
1:B:37:ASN:ND2	2:B:213:HOH:O	2.46	0.47
1:A:49:GLN:NE2	1:A:49:GLN:N	2.59	0.47
1:B:98:CYS:HB2	1:B:102:LEU:O	2.15	0.46
1:B:118:GLY:O	1:B:119:GLY:C	2.58	0.46
1:B:130:LYS:HB3	1:B:130:LYS:HE2	1.82	0.46
1:A:95:GLY:HA3	1:B:165:GLN:O	2.16	0.46
1:A:164:CYS:HB3	1:A:171:ALA:OXT	2.15	0.45
1:A:146:CYS:SG	1:A:168:GLY:O	2.75	0.45
1:A:130:LYS:HA	1:A:131:PRO:HD3	1.76	0.45
1:A:63:GLN:HB3	1:A:77:GLY:HA3	1.99	0.44
1:B:45:ARG:HA	1:B:65:GLY:O	2.16	0.44
1:B:92:GLN:H	1:B:92:GLN:HE21	1.66	0.44
1:B:83:CYS:HB2	1:B:87:ILE:HD11	1.99	0.44
1:B:33:LYS:H	1:B:33:LYS:HG3	1.59	0.44
1:B:45:ARG:HA	1:B:45:ARG:HD2	1.85	0.43
1:B:133:GLY:HA2	2:B:231:HOH:O	2.19	0.43
1:A:100:ASN:O	1:A:101:ASN:HB2	2.18	0.43
1:B:115:GLU:HG3	2:B:256:HOH:O	2.18	0.43
1:A:88:LYS:HG3	1:A:109:PHE:CE1	2.54	0.43
1:B:149:LYS:HB3	1:B:163:GLY:O	2.19	0.42
1:B:12:CYS:HB3	1:B:16:LEU:HB2	2.01	0.42
1:B:49:GLN:H	1:B:49:GLN:CD	2.27	0.41
1:B:109:PHE:HD1	1:B:109:PHE:HA	1.65	0.41
1:A:158:GLY:HA3	2:A:238:HOH:O	2.20	0.41
1:B:87:ILE:O	1:B:109:PHE:HA	2.21	0.41
1:A:88:LYS:HG3	1:A:109:PHE:HE1	1.86	0.41
1:B:133:GLY:O	1:B:136:ALA:N	2.40	0.41
1:B:45:ARG:HB3	1:B:50:ALA:HB2	2.02	0.41
1:B:97:LEU:HD23	1:B:97:LEU:HA	1.91	0.40
1:B:117:CYS:O	1:B:121:CYS:HB2	2.21	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	169/171 (99%)	155 (92%)	13 (8%)	1 (1%)	21	11
1	B	169/171 (99%)	158 (94%)	11 (6%)	0	100	100
All	All	338/342 (99%)	313 (93%)	24 (7%)	1 (0%)	36	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	ALA

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	118/120 (98%)	105 (89%)	13 (11%)	6	1
1	B	118/120 (98%)	99 (84%)	19 (16%)	2	0
All	All	236/240 (98%)	204 (86%)	32 (14%)	3	1

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	6	GLN
1	A	10	MET
1	A	16	LEU
1	A	33	LYS

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Mol	Chain	Res	Type
1	A	37	ASN
1	A	49	GLN
1	A	54	THR
1	A	92	GLN
1	A	96	LYS
1	A	97	LEU
1	A	139	ARG
1	A	152	SER
1	B	6	GLN
1	B	10	MET
1	B	33	LYS
1	B	37	ASN
1	B	44	LYS
1	B	49	GLN
1	B	54	THR
1	B	79	GLN
1	B	84	ARG
1	B	87	ILE
1	B	92	GLN
1	B	93	SER
1	B	96	LYS
1	B	99	PRO
1	B	102	LEU
1	B	112	LEU
1	B	114	SER
1	B	139	ARG
1	B	140	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	9	ASN
1	A	20	GLN
1	A	37	ASN
1	A	49	GLN
1	A	63	GLN
1	A	92	GLN
1	A	101	ASN
1	B	6	GLN
1	B	9	ASN
1	B	14	ASN

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Mol	Chain	Res	Type
1	B	37	ASN
1	B	49	GLN
1	B	92	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	1.04	1 (14%)	9,10,12	1.88	3 (33%)
1	PCA	B	1	1	7,8,9	0.85	0	9,10,12	1.49	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	A	1	PCA	O-C	2.50	1.29	1.20

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1	PCA	CB-CA-C	3.91	118.02	112.66
1	B	1	PCA	O-C-CA	-3.15	116.67	124.77
1	A	1	PCA	O-C-CA	-3.11	116.78	124.77
1	B	1	PCA	CB-CA-C	2.57	116.19	112.66
1	A	1	PCA	CB-CG-CD	-2.09	101.18	104.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	170/171 (99%)	0.26	6 (3%) 47 47	7, 18, 40, 57	0
1	B	170/171 (99%)	0.21	3 (1%) 67 68	7, 19, 37, 53	0
All	All	340/342 (99%)	0.24	9 (2%) 57 57	7, 19, 40, 57	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	ALA	6.1
1	A	150	TRP	4.0
1	B	171	ALA	3.9
1	A	136	ALA	2.6
1	A	138	GLY	2.5
1	A	170	ASP	2.4
1	A	90	GLY	2.4
1	B	109	PHE	2.2
1	B	91	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PCA	B	1	8/9	0.65	0.14	38,41,41,42	0
1	PCA	A	1	8/9	0.84	0.10	36,39,40,41	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.