



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:53 AM UTC

PDB ID : 1APN / pdb_00001apn
Title : THE CRYSTALLOGRAPHIC STRUCTURE OF METAL-FREE CON-
CANAVALLIN A AT 2.5 ANGSTROMS RESOLUTION
Authors : Bouckaert, J.; Loris, R.; Poortmans, F.; Wyns, L.
Deposited on : 1995-07-28
Resolution : 2.50 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) : 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

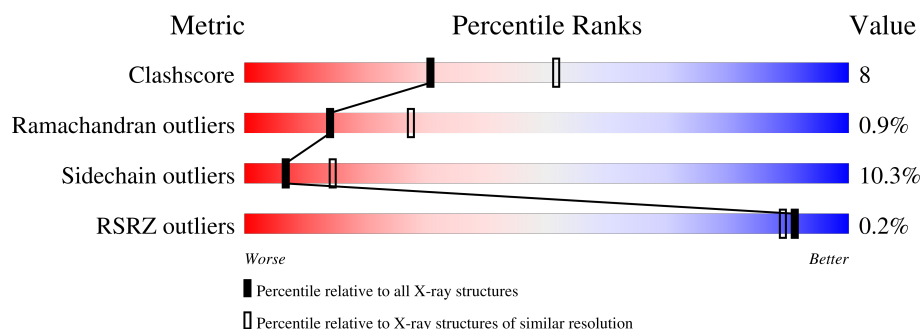
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	237	
1	B	237	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3589 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 CONCANAVALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1713	1085	286	340	2			
1	B	225	Total	C	N	O	S	0	0	0
			1708	1087	283	336	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ASP	GLU	conflict	UNP P02866
A	155	GLU	ARG	conflict	UNP P02866
B	151	ASP	GLU	conflict	UNP P02866
B	155	GLU	ARG	conflict	UNP P02866

- Molecule 2 is water.

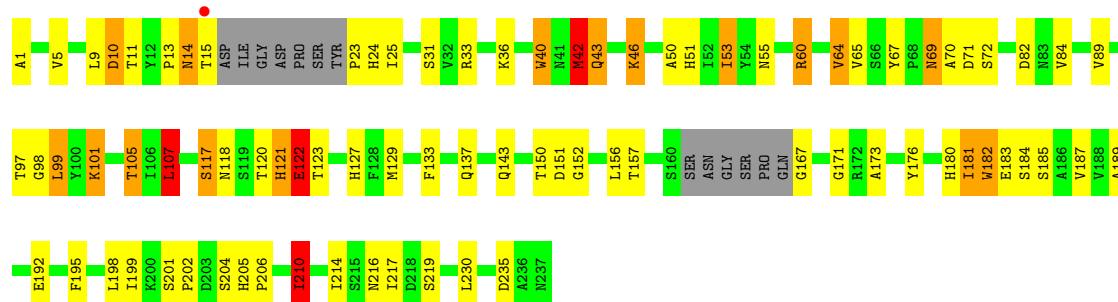
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	76	Total	O	0	0
			76	76		
2	B	92	Total	O	0	0
			92	92		

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 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.

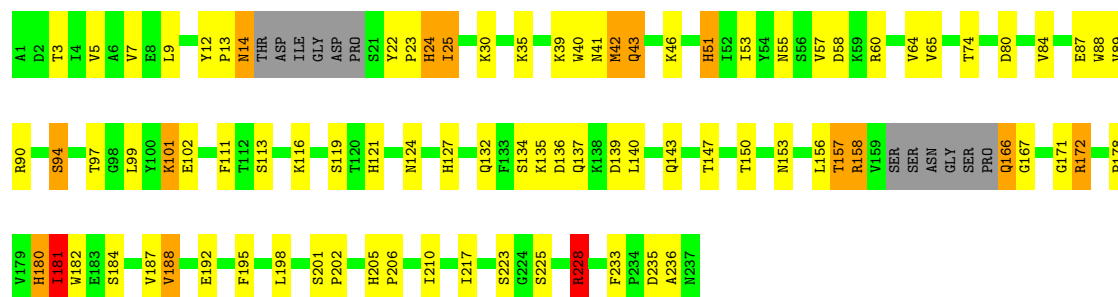
• Molecule 1: CONCAVALIN A

Chain A: 



• Molecule 1: CONCAVALIN A

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	61.36Å 85.46Å 91.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (10.00-2.50) 96.3 (10.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.00 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.180 , 0.247 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 77.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3589	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	1.24	10/1750 (0.6%)	1.97	55/2379 (2.3%)
1	B	1.19	9/1746 (0.5%)	1.93	46/2376 (1.9%)
All	All	1.22	19/3496 (0.5%)	1.95	101/4755 (2.1%)

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	0	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	VAL	CA-CB	7.28	1.64	1.54
1	B	127	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	180	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	121	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	127	HIS	CD2-NE2	-6.76	1.30	1.37
1	B	180	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	205	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	24	HIS	CD2-NE2	-6.74	1.30	1.37
1	B	24	HIS	CD2-NE2	-6.72	1.30	1.37
1	B	205	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	121	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	129	MET	CA-CB	-6.30	1.43	1.53
1	B	188	VAL	CA-CB	6.00	1.62	1.54
1	A	69	ASN	CA-CB	5.57	1.62	1.53
1	B	51	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	210	ILE	CA-CB	5.21	1.63	1.54
1	B	24	HIS	CG-ND1	-5.17	1.32	1.38
1	A	219	SER	CA-CB	-5.12	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	VAL	CA-CB	5.06	1.61	1.54

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASP	CA-CB-CG	11.23	123.83	112.60
1	A	137	GLN	OE1-CD-NE2	-10.76	111.84	122.60
1	A	123	THR	N-CA-C	10.29	125.30	109.96
1	B	236	ALA	N-CA-C	-9.73	98.24	111.96
1	B	51	HIS	CB-CG-CD2	-8.37	120.32	131.20
1	B	51	HIS	CB-CG-ND1	8.22	135.03	122.70
1	A	118	ASN	N-CA-C	-8.18	102.33	111.82
1	A	70	ALA	CA-C-N	-8.11	111.98	122.77
1	A	70	ALA	C-N-CA	-8.11	111.98	122.77
1	A	43	GLN	OE1-CD-NE2	-8.03	114.58	122.60
1	A	84	VAL	N-CA-C	-7.98	105.42	112.12
1	B	228	ARG	CA-CB-CG	7.91	129.92	114.10
1	A	230	LEU	N-CA-C	7.62	121.92	112.47
1	B	172	ARG	CB-CG-CD	-7.61	93.80	111.30
1	A	122	GLU	N-CA-C	7.49	126.75	110.80
1	B	127	HIS	CB-CG-CD2	-7.45	121.52	131.20
1	A	64	VAL	CB-CA-C	-7.43	99.06	110.50
1	B	14	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	A	216	ASN	CB-CG-ND2	7.04	126.95	116.40
1	A	127	HIS	CB-CG-CD2	-6.96	122.14	131.20
1	A	210	ILE	CB-CA-C	-6.92	100.94	110.90
1	B	181	ILE	CB-CG1-CD1	-6.92	99.27	113.80
1	A	204	SER	N-CA-C	6.83	118.81	111.36
1	B	192	GLU	CA-CB-CG	6.83	127.75	114.10
1	A	71	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	122	GLU	CA-CB-CG	6.76	127.63	114.10
1	B	153	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	B	167	GLY	N-CA-C	-6.74	103.91	112.54
1	B	84	VAL	CB-CA-C	-6.71	104.85	111.30
1	B	134	SER	CA-CB-OG	6.70	124.50	111.10
1	B	195	PHE	CA-CB-CG	6.69	120.49	113.80
1	A	107	LEU	CD1-CG-CD2	-6.61	96.27	110.80
1	B	184	SER	CA-CB-OG	-6.60	97.89	111.10
1	A	182	TRP	CA-CB-CG	6.53	126.00	113.60
1	A	60	ARG	CB-CG-CD	-6.47	96.43	111.30
1	A	183	GLU	CA-CB-CG	6.46	127.03	114.10
1	B	88	TRP	CG-CD2-CE3	6.43	140.33	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ALA	CA-C-N	6.36	133.15	121.70
1	B	236	ALA	C-N-CA	6.36	133.15	121.70
1	A	121	HIS	CA-C-O	6.22	128.80	121.40
1	B	136	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	51	HIS	CB-CG-ND1	6.18	131.96	122.70
1	A	121	HIS	CA-C-N	6.18	133.34	121.54
1	A	121	HIS	C-N-CA	6.18	133.34	121.54
1	A	51	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	B	166	GLN	CA-CB-CG	5.97	126.03	114.10
1	A	183	GLU	N-CA-C	-5.94	98.60	108.75
1	B	121	HIS	CA-CB-CG	5.90	119.70	113.80
1	A	214	ILE	N-CA-C	-5.89	99.63	108.12
1	B	124	ASN	O-C-N	-5.84	116.36	123.19
1	B	58	ASP	N-CA-C	5.83	117.71	111.36
1	B	55	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	B	205	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	B	147	THR	CA-C-O	-5.78	115.09	121.33
1	A	184	SER	N-CA-C	5.71	118.44	111.82
1	B	201	SER	O-C-N	-5.70	117.83	121.88
1	A	205	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	121	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	A	173	ALA	O-C-N	-5.65	116.58	123.30
1	B	25	ILE	O-C-N	-5.65	116.94	122.93
1	B	101	LYS	N-CA-C	-5.62	100.14	109.46
1	A	5	VAL	N-CA-C	-5.58	100.43	108.53
1	A	180	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	A	210	ILE	N-CA-CB	5.57	121.83	112.47
1	A	14	ASN	O-C-N	5.52	129.93	122.59
1	A	216	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	A	127	HIS	CB-CG-ND1	5.50	130.96	122.70
1	B	41	ASN	CA-CB-CG	-5.50	107.10	112.60
1	A	105	THR	CA-C-O	-5.48	114.62	120.92
1	B	180	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	B	80	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	14	ASN	CB-CG-ND2	5.41	124.52	116.40
1	B	7	VAL	N-CA-C	-5.41	99.37	107.37
1	B	236	ALA	O-C-N	5.39	128.56	122.19
1	A	217	ILE	CB-CG1-CD1	-5.36	102.55	113.80
1	A	82	ASP	CB-CA-C	-5.34	100.42	110.67
1	A	60	ARG	N-CA-CB	-5.29	101.92	110.81
1	A	185	SER	CA-CB-OG	-5.28	100.55	111.10
1	A	101	LYS	N-CA-C	-5.28	100.57	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ALA	N-CA-C	-5.25	101.60	109.95
1	B	43	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	64	VAL	N-CA-CB	5.20	119.96	111.44
1	A	117	SER	N-CA-C	5.19	116.80	110.41
1	B	235	ASP	N-CA-C	5.19	116.41	108.52
1	A	201	SER	CA-C-N	5.19	124.80	119.56
1	A	201	SER	C-N-CA	5.19	124.80	119.56
1	A	42	MET	CG-SD-CE	-5.16	89.56	100.90
1	B	88	TRP	CB-CG-CD1	-5.16	119.17	126.90
1	A	137	GLN	CG-CD-NE2	5.15	124.13	116.40
1	B	57	VAL	N-CA-C	-5.15	105.58	110.42
1	B	188	VAL	CA-C-O	5.13	126.13	120.64
1	A	55	ASN	CB-CG-ND2	5.13	124.09	116.40
1	B	182	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	B	5	VAL	N-CA-C	-5.09	100.32	107.75
1	A	40	TRP	CA-C-O	5.08	126.19	120.70
1	A	143	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	143	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	139	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	228	ARG	N-CA-CB	-5.01	102.75	110.46
1	A	98	GLY	O-C-N	-5.00	116.19	122.70
1	B	42	MET	CG-SD-CE	-5.00	89.89	100.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	HIS	Mainchain
1	A	122	GLU	Peptide
1	A	67	TYR	Sidechain

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	1713	0	1673	26	0
1	B	1708	0	1657	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	76	0	0	1	0
2	B	92	0	0	2	0
All	All	3589	0	3330	56	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 8.

All (56) 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:B:9:LEU:HD21	1:B:65:VAL:HG21	1.58	0.84
1:B:64:VAL:HG13	1:B:74:THR:HG22	1.67	0.76
1:B:158:ARG:HG2	1:B:166:GLN:HB3	1.71	0.72
1:B:25:ILE:HD12	1:B:65:VAL:HG23	1.71	0.72
1:B:22:TYR:HD1	1:B:23:PRO:O	1.80	0.65
1:A:117:SER:H	1:A:122:GLU:HB3	1.65	0.61
1:A:210:ILE:HD13	1:A:210:ILE:N	2.16	0.60
1:A:117:SER:N	1:A:122:GLU:HB3	2.17	0.60
1:B:3:THR:HG23	1:B:30:LYS:HD3	1.84	0.60
1:B:156:LEU:O	1:B:171:GLY:HA3	2.02	0.59
1:A:53:ILE:HG22	1:A:192:GLU:HG3	1.85	0.58
1:B:23:PRO:HB2	1:B:40:TRP:O	2.04	0.57
1:A:43:GLN:HB3	1:A:46:LYS:HG3	1.87	0.57
1:A:25:ILE:HD12	1:A:65:VAL:HG23	1.88	0.55
1:A:199:ILE:HD11	1:A:210:ILE:HD11	1.88	0.55
1:B:43:GLN:HE21	1:B:46:LYS:HG3	1.72	0.55
1:A:11:THR:HG22	1:A:23:PRO:HB3	1.88	0.54
1:A:99:LEU:HD23	1:A:167:GLY:HA3	1.90	0.53
1:B:22:TYR:CE1	1:B:39:LYS:HA	2.44	0.52
1:A:11:THR:HG21	1:A:42:MET:HE2	1.93	0.51
1:A:199:ILE:HD11	1:A:210:ILE:CD1	2.41	0.50
1:A:50:ALA:HB3	1:A:195:PHE:CE1	2.47	0.50
1:A:25:ILE:HD12	1:A:65:VAL:CG2	2.42	0.50
1:B:22:TYR:CE1	1:B:24:HIS:HB3	2.46	0.50
1:A:101:LYS:O	1:A:202:PRO:HD2	2.13	0.49
1:B:101:LYS:HD2	1:B:202:PRO:HD3	1.96	0.48
1:B:25:ILE:HD12	1:B:65:VAL:CG2	2.42	0.48
1:B:94:SER:OG	1:B:172:ARG:HG2	2.14	0.47
1:B:23:PRO:HD2	2:B:281:HOH:O	2.15	0.46
1:A:181:ILE:HD12	1:A:182:TRP:CD1	2.51	0.46
1:A:97:THR:HG23	1:A:157:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:O	1:A:171:GLY:HA3	2.16	0.45
1:B:64:VAL:HG13	1:B:74:THR:CG2	2.43	0.45
1:A:42:MET:HE1	1:A:206:PRO:HD2	1.99	0.45
1:B:228:ARG:HG2	1:B:228:ARG:HH11	1.82	0.45
1:A:133:PHE:O	1:A:152:GLY:HA2	2.17	0.44
1:B:90:ARG:HD2	1:B:217:ILE:O	2.18	0.44
1:B:51:HIS:CD2	2:B:291:HOH:O	2.71	0.44
1:B:101:LYS:HD2	1:B:202:PRO:CD	2.48	0.44
1:A:65:VAL:O	1:A:72:SER:HA	2.18	0.43
1:A:89:VAL:CG2	1:A:181:ILE:HG12	2.48	0.43
1:A:33:ARG:HD3	1:A:33:ARG:HA	1.81	0.43
1:A:176:TYR:CD2	1:B:178:PRO:HD3	2.54	0.43
1:A:1:ALA:HB1	2:A:300:HOH:O	2.19	0.43
1:B:137:GLN:HG2	1:B:140:LEU:HD12	2.01	0.43
1:B:111:PHE:CE2	1:B:113:SER:HB2	2.54	0.42
1:B:225:SER:HB3	1:B:233:PHE:O	2.19	0.42
1:B:43:GLN:NE2	1:B:46:LYS:HG3	2.33	0.42
1:B:35:LYS:HA	1:B:35:LYS:HD3	1.88	0.42
1:B:102:GLU:OE1	1:B:206:PRO:HB2	2.20	0.42
1:A:23:PRO:HB2	1:A:40:TRP:O	2.21	0.41
1:B:97:THR:HG23	1:B:157:THR:HG21	2.02	0.41
1:B:12:TYR:HA	1:B:13:PRO:HD2	1.94	0.40
1:B:87:GLU:HG2	1:B:180:HIS:CD2	2.56	0.40
1:A:105:THR:HG22	1:A:107:LEU:HD13	2.04	0.40
1:B:89:VAL:CG2	1:B:181:ILE:HG12	2.52	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	218/237 (92%)	204 (94%)	10 (5%)	4 (2%)	6 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	219/237 (92%)	208 (95%)	11 (5%)	0	100	100
All	All	437/474 (92%)	412 (94%)	21 (5%)	4 (1%)	14	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	14	ASN
1	A	150	THR
1	A	122	GLU

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	191/203 (94%)	171 (90%)	20 (10%)	6	14
1	B	187/203 (92%)	168 (90%)	19 (10%)	7	15
All	All	378/406 (93%)	339 (90%)	39 (10%)	7	14

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	ASP
1	A	13	PRO
1	A	15	THR
1	A	31	SER
1	A	36	LYS
1	A	42	MET
1	A	46	LYS
1	A	53	ILE
1	A	60	ARG
1	A	64	VAL
1	A	99	LEU

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Mol	Chain	Res	Type
1	A	107	LEU
1	A	120	THR
1	A	122	GLU
1	A	151	ASP
1	A	181	ILE
1	A	198	LEU
1	A	210	ILE
1	A	235	ASP
1	B	14	ASN
1	B	42	MET
1	B	53	ILE
1	B	60	ARG
1	B	94	SER
1	B	99	LEU
1	B	116	LYS
1	B	119	SER
1	B	132	GLN
1	B	135	LYS
1	B	150	THR
1	B	157	THR
1	B	158	ARG
1	B	181	ILE
1	B	188	VAL
1	B	198	LEU
1	B	210	ILE
1	B	223	SER
1	B	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	B	14	ASN
1	B	43	GLN
1	B	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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($\text{\AA}^2$)	Q<0.9
1	A	224/237 (94%)	-0.87	1 (0%) 88 86	10, 23, 65, 100	0
1	B	225/237 (94%)	-0.76	0 100 100	11, 27, 73, 125	0
All	All	449/474 (94%)	-0.82	1 (0%) 91 89	10, 24, 69, 125	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	THR	2.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.