



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:49 PM GMT

PDB ID : 1COL
Title : REFINED STRUCTURE OF THE PORE-FORMING DOMAIN OF COL-
ICIN A AT 2.4 ANGSTROMS RESOLUTION
Authors : Parker, M.W.; Postma, J.P.M.; Pattus, F.; Tucker, A.D.; Tsernoglou, D.
Deposited on : 1991-07-06
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

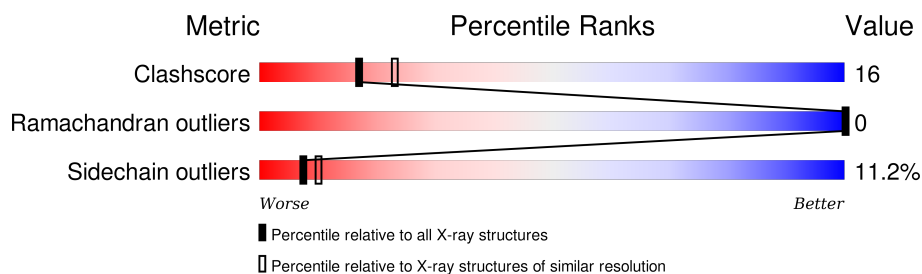
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	204	
1	B	204	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3039 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 COLICIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1478	938	251	283	6			
1	B	197	Total	C	N	O	S	0	0	0
			1478	938	251	283	6			

- Molecule 2 is water.

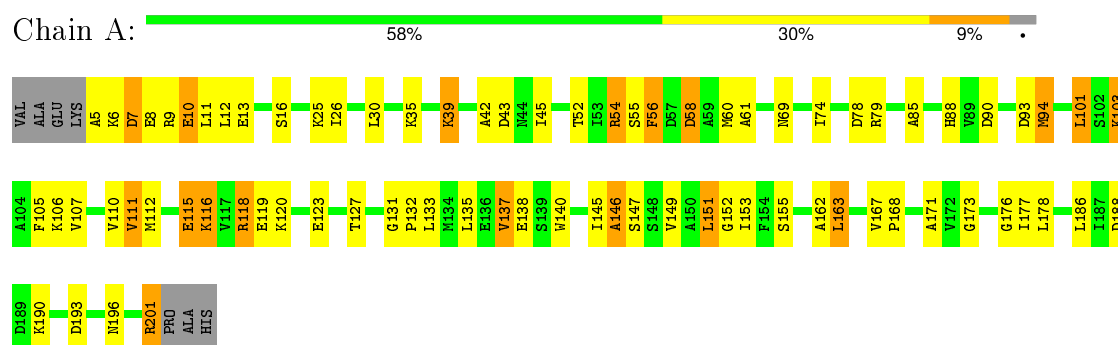
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total	O	0	0
			41	41		
2	B	42	Total	O	0	0
			42	42		

3 Residue-property plots [i](#)

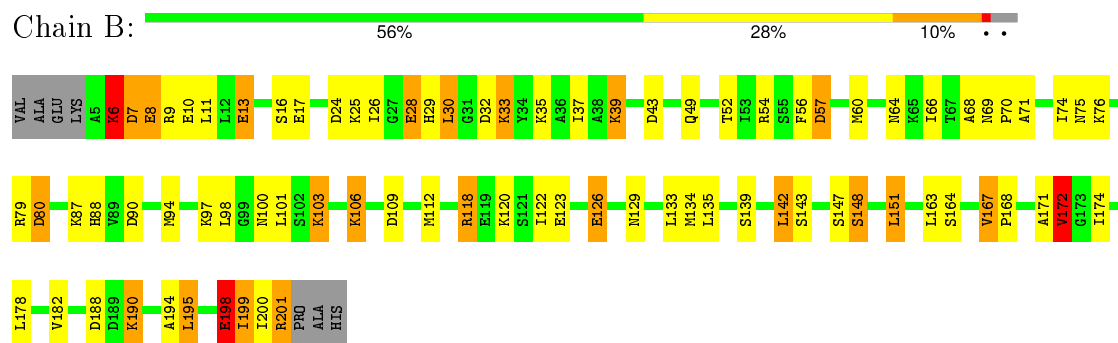
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: COLICIN A



• Molecule 1: COLICIN A



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.00 Å 73.00 Å 171.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3039	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

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	0.87	0/1496	1.96	36/2016 (1.8%)
1	B	0.89	0/1496	2.00	51/2016 (2.5%)
All	All	0.88	0/2992	1.98	87/4032 (2.2%)

There are no bond length outliers.

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH1	14.51	127.56	120.30
1	B	118	ARG	NE-CZ-NH1	-13.94	113.33	120.30
1	A	54	ARG	NE-CZ-NH1	11.53	126.07	120.30
1	A	118	ARG	NE-CZ-NH2	11.02	125.81	120.30
1	B	190	LYS	CA-CB-CG	9.64	134.60	113.40
1	B	43	ASP	CB-CG-OD2	9.14	126.53	118.30
1	B	54	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	B	32	ASP	CB-CG-OD1	8.79	126.21	118.30
1	A	101	LEU	CA-CB-CG	8.69	135.28	115.30
1	B	28	GLU	CA-CB-CG	8.65	132.43	113.40
1	A	9	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	B	118	ARG	NH1-CZ-NH2	7.91	128.10	119.40
1	B	13	GLU	OE1-CD-OE2	7.91	132.79	123.30
1	A	115	GLU	CA-CB-CG	7.91	130.79	113.40
1	B	123	GLU	OE1-CD-OE2	7.51	132.32	123.30
1	B	54	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	B	33	LYS	CA-CB-CG	7.48	129.85	113.40
1	A	9	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	30	LEU	CB-CA-C	7.31	124.09	110.20
1	A	201	ARG	CD-NE-CZ	7.30	133.82	123.60
1	B	151	LEU	CA-CB-CG	7.29	132.07	115.30
1	B	28	GLU	CG-CD-OE2	7.21	132.72	118.30
1	A	201	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	B	8	GLU	OE1-CD-OE2	7.01	131.71	123.30
1	B	7	ASP	C-N-CA	6.99	139.17	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	HIS	CA-CB-CG	-6.98	101.74	113.60
1	A	94	MET	CA-CB-CG	-6.93	101.52	113.30
1	A	85	ALA	CB-CA-C	6.90	120.44	110.10
1	A	78	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	90	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	79	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	6	LYS	N-CA-CB	6.81	122.87	110.60
1	B	123	GLU	CG-CD-OE2	-6.74	104.81	118.30
1	B	17	GLU	OE1-CD-OE2	-6.73	115.22	123.30
1	A	93	ASP	CB-CG-OD2	6.66	124.30	118.30
1	B	90	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	198	GLU	OE1-CD-OE2	6.61	131.23	123.30
1	A	43	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	171	ALA	N-CA-CB	6.38	119.04	110.10
1	B	126	GLU	CA-CB-CG	6.38	127.43	113.40
1	B	182	VAL	CG1-CB-CG2	-6.37	100.71	110.90
1	B	120	LYS	CB-CA-C	6.34	123.09	110.40
1	B	182	VAL	CB-CA-C	6.27	123.31	111.40
1	B	198	GLU	CB-CA-C	-6.25	97.90	110.40
1	A	146	ALA	N-CA-CB	-6.24	101.36	110.10
1	A	58	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	118	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	54	ARG	NH1-CZ-NH2	-6.11	112.68	119.40
1	B	118	ARG	CD-NE-CZ	-6.08	115.09	123.60
1	B	71	ALA	CB-CA-C	-6.02	101.07	110.10
1	B	171	ALA	N-CA-CB	5.98	118.47	110.10
1	A	56	PHE	N-CA-CB	5.97	121.35	110.60
1	B	188	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	167	VAL	CA-CB-CG2	5.91	119.77	110.90
1	B	24	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	B	148	SER	CB-CA-C	-5.82	99.04	110.10
1	A	13	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	137	VAL	CB-CA-C	-5.72	100.52	111.40
1	A	116	LYS	CA-CB-CG	-5.68	100.89	113.40
1	A	151	LEU	CA-C-O	5.66	131.99	120.10
1	A	103	LYS	CA-CB-CG	5.62	125.77	113.40
1	B	112	MET	CA-CB-CG	-5.58	103.82	113.30
1	B	143	SER	CA-CB-OG	-5.57	96.16	111.20
1	B	90	ASP	CB-CG-OD2	-5.52	113.34	118.30
1	B	142	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	201	ARG	CA-C-O	-5.50	108.55	120.10
1	A	30	LEU	N-CA-CB	-5.43	99.53	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ASN	CA-CB-CG	-5.42	101.47	113.40
1	A	193	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	127	THR	CA-CB-OG1	-5.40	97.66	109.00
1	B	43	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	B	13	GLU	CG-CD-OE1	-5.38	107.53	118.30
1	B	182	VAL	CA-CB-CG2	5.38	118.98	110.90
1	B	75	ASN	CB-CA-C	5.38	121.15	110.40
1	B	129	ASN	N-CA-CB	-5.33	101.00	110.60
1	B	94	MET	CB-CA-C	5.30	121.00	110.40
1	A	111	VAL	CA-CB-CG2	5.30	118.85	110.90
1	B	52	THR	CA-CB-CG2	5.20	119.68	112.40
1	B	7	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	119	GLU	CG-CD-OE1	-5.17	107.97	118.30
1	B	57	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	39	LYS	CB-CA-C	5.10	120.60	110.40
1	B	28	GLU	OE1-CD-OE2	-5.06	117.22	123.30
1	B	134	MET	CA-CB-CG	5.06	121.90	113.30
1	B	172	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	B	164	SER	CA-C-N	5.05	128.31	117.20
1	A	6	LYS	CA-CB-CG	5.02	124.44	113.40

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	1478	0	1521	44	0
1	B	1478	0	1521	54	1
2	A	41	0	0	1	1
2	B	42	0	0	3	0
All	All	3039	0	3042	98	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 16.

All (98) 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:76:LYS:HG2	1:B:79:ARG:NH1	1.93	0.83
1:A:5:ALA:HB3	1:A:8:GLU:HG3	1.62	0.82
1:B:6:LYS:HD2	1:B:9:ARG:NH1	1.98	0.77
1:B:76:LYS:HG2	1:B:79:ARG:HH11	1.50	0.77
1:B:9:ARG:NH1	1:B:49:GLN:NE2	2.33	0.76
1:B:6:LYS:HG3	1:B:9:ARG:HD2	1.68	0.75
1:B:6:LYS:CD	1:B:9:ARG:HH11	2.06	0.68
1:B:9:ARG:NH1	1:B:49:GLN:HE22	1.92	0.68
1:B:194:ALA:O	1:B:198:GLU:HG3	1.94	0.67
1:A:107:VAL:HG22	1:A:110:VAL:HB	1.77	0.67
1:B:6:LYS:HG3	1:B:9:ARG:HG3	1.76	0.67
1:A:167:VAL:HB	1:A:168:PRO:HD2	1.77	0.67
1:A:146:ALA:HB3	1:A:149:VAL:HG23	1.78	0.65
1:A:167:VAL:HB	1:A:168:PRO:CD	2.28	0.63
1:A:35:LYS:O	1:A:39:LYS:HG3	1.99	0.62
1:A:140:TRP:HB3	1:A:145:ILE:HD13	1.81	0.62
1:A:173:GLY:O	1:A:177:ILE:HG13	2.00	0.61
1:A:103:LYS:HA	1:A:106:LYS:HE2	1.81	0.61
1:B:6:LYS:HG3	1:B:9:ARG:CD	2.30	0.60
1:A:149:VAL:O	1:A:153:ILE:HD12	2.02	0.59
1:B:6:LYS:CD	1:B:9:ARG:NH1	2.63	0.59
1:B:6:LYS:HG3	1:B:9:ARG:HH11	1.67	0.59
1:A:54:ARG:HG3	1:A:186:LEU:O	2.03	0.59
1:B:6:LYS:CG	1:B:9:ARG:HD2	2.32	0.58
1:A:103:LYS:O	1:A:106:LYS:HB2	2.04	0.57
1:B:66:ILE:HD12	1:B:200:ILE:HD11	1.85	0.57
1:B:6:LYS:HG3	1:B:9:ARG:CG	2.35	0.56
1:A:10:GLU:OE1	1:A:10:GLU:HA	2.06	0.56
1:B:98:LEU:O	1:B:101:LEU:HB2	2.05	0.56
1:A:39:LYS:HB3	2:A:234:HOH:O	2.06	0.56
1:B:56:PHE:O	1:B:60:MET:HG2	2.06	0.56
1:B:26:ILE:CG2	1:B:30:LEU:HD22	2.36	0.55
1:B:109:ASP:HA	2:B:235:HOH:O	2.06	0.55
1:A:107:VAL:HG11	1:A:153:ILE:HD11	1.89	0.55
1:B:29:HIS:HD2	1:B:172:VAL:HG11	1.71	0.55
1:B:37:ILE:HG21	1:B:195:LEU:HD13	1.89	0.55
1:B:6:LYS:CG	1:B:9:ARG:HH11	2.20	0.54
1:A:149:VAL:HG12	1:A:153:ILE:CD1	2.38	0.53
1:B:29:HIS:CD2	1:B:172:VAL:HG11	2.44	0.53
1:A:58:ASP:O	1:A:61:ALA:HB3	2.09	0.52
1:A:74:ILE:HD11	1:A:178:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLU:C	1:B:199:ILE:HG12	2.30	0.51
1:B:26:ILE:HG13	1:B:172:VAL:HG22	1.92	0.51
1:B:194:ALA:O	1:B:198:GLU:CG	2.58	0.51
1:B:76:LYS:CG	1:B:79:ARG:NH1	2.72	0.50
1:B:35:LYS:O	1:B:39:LYS:HD3	2.12	0.50
1:A:26:ILE:HG21	1:A:176:GLY:HA3	1.93	0.50
1:B:25:LYS:O	1:B:28:GLU:HG3	2.13	0.49
1:A:123:GLU:OE2	1:A:132:PRO:HG2	2.12	0.49
1:B:7:ASP:OD2	2:B:225:HOH:O	2.19	0.49
1:A:149:VAL:HG12	1:A:153:ILE:HD12	1.94	0.49
1:B:37:ILE:HD11	1:B:198:GLU:HG3	1.94	0.48
1:A:118:ARG:HG2	1:A:118:ARG:HH11	1.79	0.48
1:A:55:SER:O	1:A:56:PHE:C	2.51	0.48
1:A:69:ASN:C	1:A:69:ASN:OD1	2.52	0.48
1:B:167:VAL:HB	1:B:168:PRO:CD	2.44	0.47
1:B:8:GLU:OE1	1:B:49:GLN:HG3	2.14	0.47
1:A:140:TRP:HB3	1:A:145:ILE:CD1	2.43	0.47
1:A:16:SER:HB2	1:A:42:ALA:O	2.14	0.47
1:B:122:ILE:O	1:B:126:GLU:HG2	2.14	0.47
1:B:69:ASN:OD1	1:B:70:PRO:HD2	2.14	0.46
1:B:198:GLU:HB2	1:B:199:ILE:HG12	1.98	0.46
1:A:8:GLU:O	1:A:12:LEU:HG	2.16	0.46
1:A:151:LEU:O	1:A:155:SER:HB2	2.16	0.46
1:B:167:VAL:HB	1:B:168:PRO:HD2	1.97	0.46
1:B:9:ARG:HG2	1:B:49:GLN:HE21	1.80	0.45
1:B:87:LYS:HA	1:B:118:ARG:HH21	1.81	0.45
1:B:57:ASP:O	2:B:214:HOH:O	2.21	0.45
1:B:64:ASN:O	1:B:68:ALA:HB3	2.16	0.45
1:B:10:GLU:O	1:B:13:GLU:HB3	2.17	0.45
1:A:25:LYS:HE2	1:A:162:ALA:O	2.17	0.45
1:B:66:ILE:HD12	1:B:200:ILE:CD1	2.48	0.44
1:A:112:MET:O	1:A:116:LYS:HG3	2.17	0.44
1:A:45:ILE:HG21	1:A:45:ILE:HD13	1.66	0.43
1:A:146:ALA:HB3	1:A:149:VAL:CG2	2.46	0.43
1:B:97:LYS:O	1:B:100:ASN:HB2	2.18	0.43
1:B:103:LYS:HA	1:B:106:LYS:CD	2.48	0.43
1:A:111:VAL:O	1:A:115:GLU:HB2	2.19	0.43
1:A:151:LEU:HA	1:A:151:LEU:HD12	1.84	0.42
1:B:103:LYS:HA	1:B:106:LYS:HD2	2.01	0.42
1:B:6:LYS:HA	1:B:9:ARG:HG3	2.02	0.42
1:B:13:GLU:O	1:B:16:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD11	1:A:105:PHE:CD1	2.54	0.42
1:A:5:ALA:HB1	1:A:7:ASP:H	1.84	0.42
1:A:60:MET:HE2	1:A:131:GLY:HA2	2.02	0.42
1:A:94:MET:CG	1:A:94:MET:O	2.68	0.41
1:B:9:ARG:CG	1:B:49:GLN:HE21	2.33	0.41
1:B:74:ILE:HG12	1:B:174:ILE:HG21	2.03	0.41
1:B:76:LYS:HE2	1:B:79:ARG:HH12	1.84	0.41
1:A:111:VAL:HG12	1:A:111:VAL:O	2.19	0.41
1:B:79:ARG:HG2	1:B:80:ASP:N	2.35	0.41
1:A:116:LYS:O	1:A:120:LYS:HG3	2.21	0.41
1:A:54:ARG:O	1:A:138:GLU:OE2	2.39	0.41
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.81	0.40
1:B:69:ASN:OD1	1:B:70:PRO:CD	2.69	0.40
1:A:151:LEU:O	1:A:152:GLY:C	2.60	0.40
1:B:118:ARG:HD3	1:B:118:ARG:HH11	1.54	0.40
1:A:188:ASP:OD1	1:A:190:LYS:HB2	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:57:ASP:OD2	2:A:216:HOH:O[4_455]	2.12	0.08

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	195/204 (96%)	184 (94%)	11 (6%)	0	100	100
1	B	195/204 (96%)	186 (95%)	9 (5%)	0	100	100
All	All	390/408 (96%)	370 (95%)	20 (5%)	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	152/157 (97%)	141 (93%)	11 (7%)	18	28
1	B	152/157 (97%)	129 (85%)	23 (15%)	3	4
All	All	304/314 (97%)	270 (89%)	34 (11%)	7	10

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	GLU
1	A	52	THR
1	A	88	HIS
1	A	101	LEU
1	A	133	LEU
1	A	135	LEU
1	A	137	VAL
1	A	147	SER
1	A	163	LEU
1	A	201	ARG
1	B	6	LYS
1	B	11	LEU
1	B	30	LEU
1	B	33	LYS
1	B	39	LYS
1	B	80	ASP
1	B	103	LYS
1	B	106	LYS
1	B	133	LEU
1	B	135	LEU
1	B	139	SER
1	B	142	LEU
1	B	147	SER
1	B	148	SER

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Mol	Chain	Res	Type
1	B	151	LEU
1	B	163	LEU
1	B	172	VAL
1	B	178	LEU
1	B	190	LYS
1	B	195	LEU
1	B	198	GLU
1	B	199	ILE
1	B	201	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	197	ASN
1	B	29	HIS
1	B	49	GLN
1	B	96	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.