



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:52 PM UTC

PDB ID : 2R90 / pdb_00002r90
Title : Crystal structure of cameline peptidoglycan recognition protein at 2.8Å resolution
Authors : Sharma, P.; Singh, N.; Sinha, M.; Sharma, S.; Kaur, P.; Srinivasan, A.; Singh, T.P.
Deposited on : 2007-09-12
Resolution : 2.80 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
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

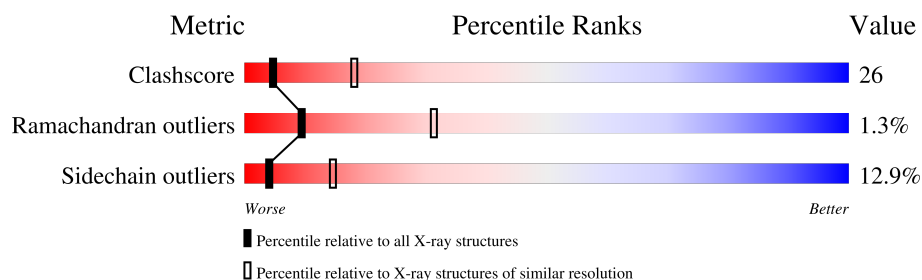
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	171	57% 32% 8% .
1	B	171	57% 30% 10% .
1	C	171	48% 42% 8% .
1	D	171	43% 43% 11% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5513 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 Peptidoglycan recognition protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1337	834	254	241	8			
1	B	171	Total	C	N	O	S	0	0	0
			1337	834	254	241	8			
1	C	171	Total	C	N	O	S	0	0	0
			1337	834	254	241	8			
1	D	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			

- Molecule 2 is water.

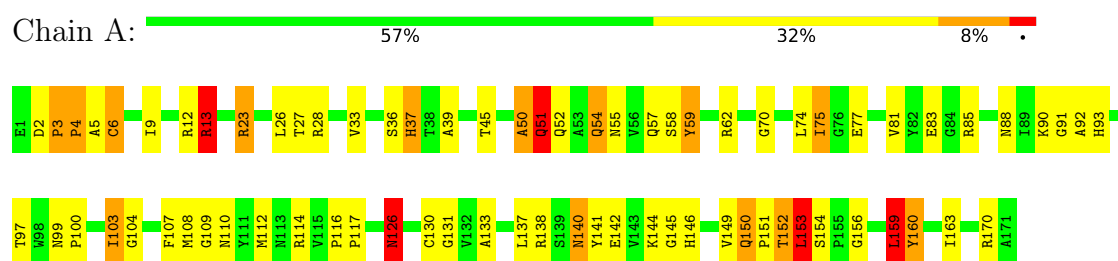
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total	O	0	0
			32	32		
2	B	40	Total	O	0	0
			40	40		
2	C	44	Total	O	0	0
			44	44		
2	D	50	Total	O	0	0
			50	50		

3 Residue-property plots

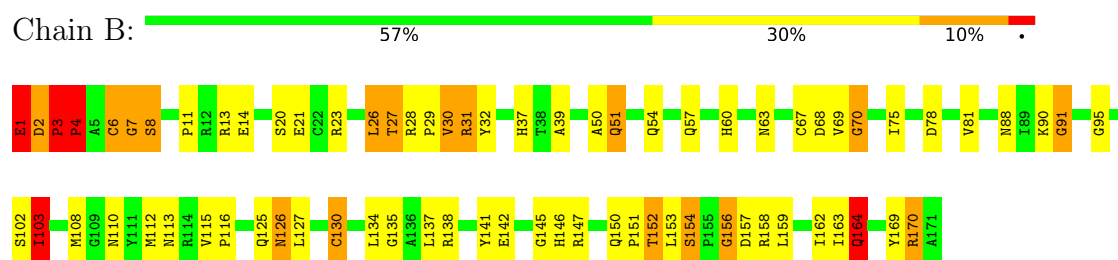
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: Peptidoglycan recognition protein

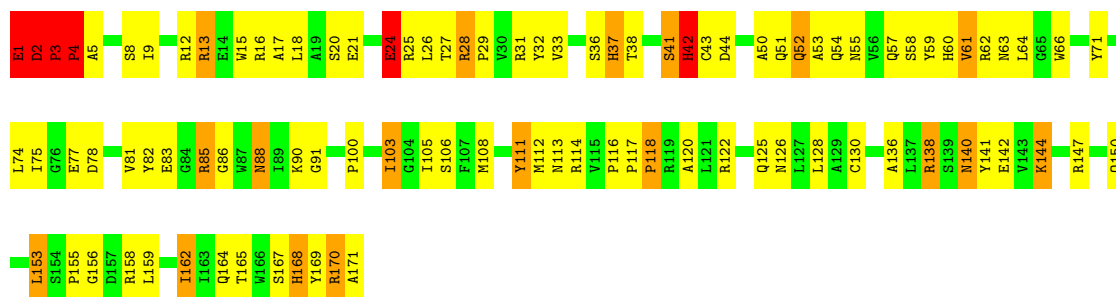


• Molecule 1: Peptidoglycan recognition protein



• Molecule 1: Peptidoglycan recognition protein





4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	89.85Å 102.37Å 164.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.73 – 2.80	Depositor
% Data completeness (in resolution range)	95.1 (46.73-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.205 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5513	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.10	15/1374 (1.1%)	1.77	31/1871 (1.7%)
1	B	0.78	6/1374 (0.4%)	1.55	35/1871 (1.9%)
1	C	0.93	7/1374 (0.5%)	1.56	30/1871 (1.6%)
1	D	0.82	6/1373 (0.4%)	1.44	32/1871 (1.7%)
All	All	0.92	34/5495 (0.6%)	1.59	128/7484 (1.7%)

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	1
1	B	0	1
1	C	0	2
All	All	0	4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	PRO	CA-C	18.14	1.69	1.52
1	C	4	PRO	N-CD	8.97	1.60	1.47
1	A	59	TYR	N-CA	8.52	1.56	1.46
1	A	23	ARG	CG-CD	8.27	1.77	1.52
1	A	23	ARG	CB-CG	8.26	1.77	1.52
1	B	50	ALA	C-N	-8.04	1.23	1.34
1	D	42	HIS	CA-CB	-7.88	1.41	1.53
1	C	154	SER	CA-CB	7.37	1.64	1.53
1	A	37	HIS	CB-CG	7.34	1.60	1.50
1	A	23	ARG	CA-CB	7.00	1.63	1.54
1	A	23	ARG	CA-C	6.78	1.61	1.52
1	A	59	TYR	CA-CB	6.71	1.63	1.53
1	D	41	SER	C-N	-6.69	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	GLY	C-N	-6.62	1.25	1.33
1	C	3	PRO	CA-CB	6.55	1.62	1.54
1	A	3	PRO	CA-C	6.49	1.58	1.52
1	B	2	ASP	CA-C	-6.15	1.45	1.52
1	A	126	ASN	CA-CB	6.00	1.62	1.53
1	B	2	ASP	CA-CB	5.71	1.60	1.53
1	A	4	PRO	N-CA	5.67	1.54	1.47
1	D	42	HIS	N-CA	-5.62	1.38	1.45
1	A	13	ARG	CG-CD	5.61	1.69	1.52
1	B	30	VAL	CA-C	-5.53	1.47	1.53
1	A	153	LEU	C-N	-5.45	1.25	1.33
1	B	1	GLU	C-N	-5.38	1.25	1.33
1	D	3	PRO	N-CA	5.38	1.57	1.46
1	B	51	GLN	C-N	5.31	1.41	1.34
1	A	59	TYR	CB-CG	5.26	1.63	1.51
1	A	23	ARG	CD-NE	5.23	1.53	1.46
1	C	4	PRO	CA-CB	-5.15	1.46	1.53
1	D	24	GLU	CA-CB	5.11	1.61	1.53
1	C	4	PRO	N-CA	5.10	1.53	1.47
1	C	3	PRO	C-N	5.07	1.45	1.33
1	D	2	ASP	N-CA	-5.01	1.41	1.46

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	PRO	N-CA-C	21.96	137.49	110.70
1	A	153	LEU	O-C-N	-21.16	91.53	122.43
1	B	3	PRO	N-CA-C	15.53	129.64	110.70
1	C	4	PRO	CA-N-CD	-14.59	91.58	112.00
1	A	153	LEU	CA-C-N	14.05	139.92	120.39
1	A	153	LEU	C-N-CA	14.05	139.92	120.39
1	A	126	ASN	CA-CB-CG	13.35	125.95	112.60
1	C	3	PRO	CA-C-N	12.70	135.71	119.84
1	C	3	PRO	C-N-CA	12.70	135.71	119.84
1	C	4	PRO	N-CA-CB	12.45	116.32	103.25
1	D	3	PRO	CA-N-CD	-12.16	94.98	112.00
1	B	2	ASP	CA-CB-CG	11.73	124.33	112.60
1	A	37	HIS	CA-CB-CG	11.43	125.23	113.80
1	B	2	ASP	N-CA-C	-11.43	84.40	108.39
1	A	55	ASN	CA-CB-CG	10.16	122.76	112.60
1	B	51	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	A	2	ASP	N-CA-C	9.52	129.69	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	PRO	C-N-CD	-9.45	86.25	125.00
1	C	156	GLY	N-CA-C	-9.31	99.70	112.18
1	B	95	GLY	CA-C-N	9.30	129.51	119.28
1	B	95	GLY	C-N-CA	9.30	129.51	119.28
1	A	150	GLN	OE1-CD-NE2	-9.29	113.31	122.60
1	A	3	PRO	N-CA-C	8.80	121.44	110.70
1	B	156	GLY	N-CA-C	-8.62	100.43	111.72
1	C	3	PRO	CA-C-O	-8.58	108.12	120.56
1	C	25	ARG	N-CA-C	8.52	123.28	109.40
1	B	1	GLU	N-CA-C	-8.41	87.45	111.00
1	A	59	TYR	N-CA-C	-8.30	102.23	111.28
1	D	42	HIS	CA-CB-CG	-8.22	105.58	113.80
1	D	61	VAL	N-CA-C	8.10	118.78	111.81
1	C	154	SER	CB-CA-C	-7.97	96.39	109.46
1	A	2	ASP	CB-CA-C	-7.96	98.39	110.97
1	A	146	HIS	CA-CB-CG	7.90	121.70	113.80
1	A	3	PRO	CA-N-CD	-7.82	101.05	112.00
1	B	4	PRO	N-CA-C	7.78	128.49	112.47
1	A	2	ASP	CA-CB-CG	7.74	120.34	112.60
1	A	59	TYR	N-CA-CB	7.63	121.34	110.12
1	D	88	ASN	N-CA-C	7.60	123.59	113.72
1	B	162	ILE	N-CA-C	7.49	118.25	110.62
1	A	6	CYS	N-CA-C	7.46	126.69	110.80
1	A	59	TYR	CB-CA-C	-7.40	98.50	110.79
1	A	153	LEU	N-CA-C	-7.37	104.27	113.18
1	A	13	ARG	CB-CG-CD	7.23	127.94	111.30
1	B	14	GLU	N-CA-C	7.23	119.24	111.36
1	D	1	GLU	CA-C-N	-7.18	115.13	122.74
1	D	1	GLU	C-N-CA	-7.18	115.13	122.74
1	C	13	ARG	N-CA-C	7.11	121.95	113.28
1	C	18	LEU	N-CA-C	-7.10	101.16	110.53
1	D	42	HIS	CB-CG-CD2	7.02	140.32	131.20
1	B	63	ASN	N-CA-C	6.99	119.93	111.40
1	B	170	ARG	N-CA-C	6.99	120.54	109.50
1	A	4	PRO	CA-N-CD	-6.89	102.36	112.00
1	B	1	GLU	CB-CA-C	6.87	123.15	110.10
1	C	157	ASP	N-CA-C	6.84	118.43	110.97
1	B	78	ASP	N-CA-C	-6.81	105.04	113.15
1	D	2	ASP	CA-CB-CG	6.78	119.38	112.60
1	D	32	TYR	N-CA-C	6.76	120.54	109.72
1	C	70	GLY	N-CA-C	6.72	122.37	113.37
1	A	51	GLN	N-CA-C	-6.70	103.67	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	ARG	N-CA-C	6.69	120.89	111.92
1	B	3	PRO	CB-CA-C	6.63	119.00	110.92
1	A	160	TYR	N-CA-C	-6.59	104.02	111.14
1	B	50	ALA	N-CA-C	-6.57	103.74	111.03
1	D	111	TYR	N-CA-C	6.56	121.91	111.81
1	A	159	LEU	N-CA-C	-6.52	105.48	113.50
1	B	51	GLN	CG-CD-NE2	6.43	126.04	116.40
1	B	51	GLN	CB-CA-C	6.40	122.47	110.63
1	B	103	ILE	N-CA-C	-6.39	99.07	108.97
1	D	2	ASP	C-N-CD	-6.36	98.91	125.00
1	B	135	GLY	N-CA-C	-6.35	106.47	115.43
1	A	50	ALA	N-CA-C	-6.33	104.61	112.90
1	A	88	ASN	N-CA-C	6.29	121.14	112.90
1	C	87	TRP	N-CA-C	6.21	119.02	111.82
1	D	138	ARG	N-CA-C	-6.18	101.14	110.28
1	C	45	THR	N-CA-C	-6.16	101.60	110.40
1	B	26	LEU	CA-C-N	-6.16	112.80	121.72
1	B	26	LEU	C-N-CA	-6.16	112.80	121.72
1	D	20	SER	N-CA-C	-6.13	101.85	110.50
1	D	2	ASP	CB-CA-C	-6.11	101.07	111.15
1	D	170	ARG	CA-C-N	6.06	132.60	121.70
1	D	170	ARG	C-N-CA	6.06	132.60	121.70
1	C	154	SER	O-C-N	-6.04	114.66	121.43
1	D	25	ARG	N-CA-C	6.04	118.75	108.90
1	B	164	GLN	N-CA-C	-6.02	104.83	111.82
1	A	150	GLN	CG-CD-NE2	6.01	125.42	116.40
1	D	86	GLY	N-CA-C	5.89	124.83	112.45
1	B	1	GLU	CA-C-N	5.82	130.32	123.16
1	B	1	GLU	C-N-CA	5.82	130.32	123.16
1	C	32	TYR	N-CA-C	5.82	119.03	109.72
1	D	42	HIS	CB-CG-ND1	-5.79	114.01	122.70
1	B	7	GLY	N-CA-C	5.79	126.90	113.18
1	A	23	ARG	CB-CG-CD	5.76	124.55	111.30
1	C	2	ASP	CA-C-N	-5.75	114.46	120.38
1	C	2	ASP	C-N-CA	-5.75	114.46	120.38
1	B	21	GLU	N-CA-C	-5.68	104.11	111.71
1	C	14	GLU	N-CA-C	-5.67	106.36	113.28
1	B	154	SER	CA-C-N	5.63	140.51	127.00
1	B	154	SER	C-N-CA	5.63	140.51	127.00
1	A	152	THR	CA-C-N	-5.57	110.72	121.58
1	A	152	THR	C-N-CA	-5.57	110.72	121.58
1	B	145	GLY	N-CA-C	-5.54	104.21	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	ILE	CB-CA-C	-5.54	104.76	112.02
1	D	168	HIS	N-CA-C	-5.54	105.87	113.30
1	A	70	GLY	N-CA-C	5.53	119.37	112.73
1	D	2	ASP	O-C-N	-5.53	116.47	121.17
1	C	154	SER	C-N-CD	-5.49	108.53	120.60
1	D	2	ASP	CA-C-O	-5.49	114.86	121.22
1	C	88	ASN	N-CA-C	5.47	120.23	113.50
1	D	3	PRO	N-CD-CG	5.46	111.40	103.20
1	C	51	GLN	N-CA-C	-5.45	104.98	111.03
1	D	8	SER	N-CA-C	5.43	117.52	108.02
1	C	77	GLU	N-CA-C	-5.40	106.53	113.01
1	B	91	GLY	N-CA-C	5.36	121.68	112.51
1	C	115	VAL	CA-C-N	-5.32	114.90	120.38
1	C	115	VAL	C-N-CA	-5.32	114.90	120.38
1	D	170	ARG	O-C-N	5.26	129.59	122.59
1	C	5	ALA	N-CA-C	5.25	121.99	110.80
1	D	150	GLN	CA-C-N	5.25	126.40	119.84
1	D	150	GLN	C-N-CA	5.25	126.40	119.84
1	D	21	GLU	N-CA-C	-5.22	105.64	113.89
1	D	37	HIS	N-CA-C	-5.15	101.25	109.23
1	B	20	SER	N-CA-C	-5.14	103.75	110.53
1	C	6	CYS	N-CA-C	-5.13	107.70	114.31
1	A	58	SER	CA-C-O	-5.11	115.01	120.42
1	D	18	LEU	N-CA-C	-5.11	104.13	110.41
1	D	136	ALA	N-CA-C	-5.10	105.36	112.45
1	B	152	THR	N-CA-C	5.06	116.93	108.99
1	B	70	GLY	N-CA-C	5.01	120.41	113.99

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	LEU	Mainchain
1	B	1	GLU	Mainchain
1	C	154	SER	Mainchain
1	C	3	PRO	Mainchain

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	1337	0	1288	62	2
1	B	1337	0	1288	57	0
1	C	1337	0	1288	68	0
1	D	1336	0	1288	91	5
2	A	32	0	0	4	0
2	B	40	0	0	4	0
2	C	44	0	0	4	0
2	D	50	0	0	5	0
All	All	5513	0	5152	270	5

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 26.

All (270) 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:23:ARG:CD	1:A:23:ARG:CG	1.77	1.57
1:A:23:ARG:CG	1:A:23:ARG:CB	1.77	1.55
1:D:74:LEU:HD22	1:D:108:MET:HE3	1.31	1.11
1:D:1:GLU:HG3	1:D:2:ASP:H	1.21	1.04
1:B:112:MET:HE3	1:B:153:LEU:HG	1.40	1.03
1:A:112:MET:HE3	1:A:153:LEU:HD23	1.39	1.03
1:A:6:CYS:O	1:A:130:CYS:HB2	1.58	1.02
1:B:112:MET:HE2	1:B:156:GLY:HA2	1.42	1.01
1:C:151:PRO:HD3	1:D:64:LEU:CD1	1.91	1.00
1:A:112:MET:CE	1:A:153:LEU:HD23	1.98	0.94
1:B:37:HIS:CD2	1:B:154:SER:HB2	2.05	0.92
1:D:42:HIS:H	1:D:42:HIS:CD2	1.60	0.92
1:B:60:HIS:HD2	1:B:70:GLY:H	1.06	0.91
1:C:35:VAL:HG22	1:C:105:ILE:HD11	1.52	0.91
1:C:52:GLN:HB3	1:C:108:MET:CE	2.02	0.90
1:C:151:PRO:HD3	1:D:64:LEU:HD11	1.53	0.90
1:D:42:HIS:H	1:D:42:HIS:HD2	1.20	0.89
1:B:1:GLU:HB3	2:B:207:HOH:O	1.71	0.89
1:C:112:MET:HE3	1:C:153:LEU:HB3	1.53	0.89
1:A:52:GLN:HB3	1:A:108:MET:HE1	1.54	0.88
1:C:146:HIS:HB3	1:C:154:SER:HB3	1.57	0.85
1:D:114:ARG:HG3	1:D:114:ARG:HH11	1.42	0.85
1:A:52:GLN:HB3	1:A:108:MET:CE	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:HB2	2:A:194:HOH:O	1.77	0.85
1:D:112:MET:HE2	1:D:156:GLY:HA2	1.60	0.84
1:B:8:SER:HA	2:B:200:HOH:O	1.79	0.81
1:D:112:MET:CE	1:D:153:LEU:HB3	2.11	0.80
1:D:42:HIS:CD2	1:D:42:HIS:N	2.43	0.80
1:B:37:HIS:HD2	1:B:154:SER:HB2	1.43	0.80
1:B:31:ARG:HG2	1:B:32:TYR:CD1	2.17	0.79
1:B:2:ASP:HB2	1:B:6:CYS:HB2	1.65	0.79
1:C:12:ARG:HG3	1:C:83:GLU:OE1	1.84	0.78
1:D:53:ALA:HA	1:D:108:MET:HE1	1.65	0.78
1:B:11:PRO:HB2	1:B:13:ARG:HG2	1.65	0.78
1:B:3:PRO:HG3	1:D:138:ARG:NH2	1.99	0.77
1:D:57:GLN:O	1:D:61:VAL:HG12	1.83	0.77
1:D:33:VAL:HG13	1:D:103:ILE:HG22	1.65	0.77
1:A:112:MET:HE1	1:A:153:LEU:HB3	1.67	0.75
1:B:6:CYS:HA	1:B:130:CYS:HB2	1.69	0.75
1:D:71:TYR:CD2	1:D:106:SER:HB2	2.22	0.74
1:B:60:HIS:CD2	1:B:70:GLY:H	1.98	0.74
1:A:9:ILE:HG21	1:A:83:GLU:HB2	1.71	0.72
1:C:42:HIS:CD2	1:C:42:HIS:H	2.06	0.71
1:D:59:TYR:O	1:D:63:ASN:HB2	1.91	0.70
1:B:4:PRO:HD2	1:B:134:LEU:CD2	2.22	0.69
1:D:53:ALA:CA	1:D:108:MET:HE1	2.22	0.69
1:D:85:ARG:NH1	1:D:91:GLY:HA2	2.08	0.68
1:D:53:ALA:HA	1:D:108:MET:CE	2.24	0.68
1:B:112:MET:CE	1:B:153:LEU:HG	2.20	0.68
1:C:146:HIS:CB	1:C:154:SER:HB3	2.23	0.68
1:D:50:ALA:O	1:D:54:GLN:HG3	1.93	0.68
1:D:112:MET:HE1	1:D:153:LEU:HB3	1.73	0.68
1:D:138:ARG:HG2	1:D:140:ASN:ND2	2.08	0.68
1:C:9:ILE:HG23	1:C:81:VAL:HG12	1.75	0.68
1:D:1:GLU:HG3	1:D:2:ASP:N	1.99	0.68
1:B:30:VAL:O	1:B:137:LEU:HD23	1.94	0.67
1:C:151:PRO:HD3	1:D:64:LEU:HD13	1.73	0.67
1:C:162:ILE:O	1:C:165:THR:HB	1.94	0.67
1:D:43:CYS:O	1:D:77:GLU:HB2	1.94	0.67
1:D:1:GLU:CG	1:D:2:ASP:H	2.02	0.67
1:A:6:CYS:C	1:A:130:CYS:HB2	2.20	0.67
1:A:77:GLU:CD	1:A:114:ARG:HH21	2.03	0.67
1:A:37:HIS:HD2	1:A:39:ALA:CA	2.08	0.67
1:D:74:LEU:HD22	1:D:108:MET:CE	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:VAL:HG12	1:C:162:ILE:HD11	1.78	0.66
1:B:29:PRO:HB2	1:B:138:ARG:HG3	1.78	0.66
1:D:112:MET:HE3	1:D:153:LEU:HB3	1.77	0.65
1:D:142:GLU:CD	1:D:170:ARG:HD3	2.22	0.65
1:C:43:CYS:O	1:C:77:GLU:HB2	1.97	0.65
1:D:75:ILE:HD12	1:D:81:VAL:HG22	1.78	0.65
1:C:112:MET:HE2	1:C:156:GLY:HA2	1.79	0.64
1:C:146:HIS:HB3	1:C:154:SER:CB	2.27	0.63
1:D:38:THR:OG1	1:D:108:MET:HA	1.99	0.62
1:A:112:MET:HE1	1:A:153:LEU:CB	2.29	0.62
1:A:142:GLU:HG2	1:A:170:ARG:CG	2.29	0.62
1:A:149:VAL:O	1:A:150:GLN:HB3	1.98	0.62
1:C:59:TYR:HA	1:C:63:ASN:HD22	1.63	0.62
1:C:132:VAL:HG13	1:C:139:SER:HA	1.81	0.62
1:D:75:ILE:CD1	1:D:81:VAL:HG22	2.29	0.62
1:A:39:ALA:HA	1:A:110:ASN:HB2	1.81	0.61
1:C:157:ASP:CG	2:C:209:HOH:O	2.43	0.61
1:B:31:ARG:NH2	2:B:183:HOH:O	2.33	0.61
1:B:2:ASP:HB2	1:B:6:CYS:CB	2.30	0.61
1:A:142:GLU:HG2	1:A:170:ARG:HG3	1.83	0.61
1:D:155:PRO:HB3	1:D:159:LEU:HD23	1.83	0.60
1:A:9:ILE:CG2	1:A:83:GLU:HB2	2.30	0.60
1:D:140:ASN:C	1:D:140:ASN:HD22	2.09	0.59
1:C:127:LEU:O	1:C:130:CYS:HB3	2.02	0.59
1:D:155:PRO:CB	1:D:159:LEU:HD23	2.33	0.59
1:C:12:ARG:HA	1:C:15:TRP:NE1	2.17	0.59
1:D:114:ARG:HH11	1:D:114:ARG:CG	2.16	0.58
1:B:4:PRO:HD2	1:B:134:LEU:HD23	1.85	0.58
1:C:85:ARG:HD2	1:C:91:GLY:HA2	1.84	0.58
1:D:60:HIS:O	1:D:66:TRP:HB2	2.03	0.58
1:B:37:HIS:ND1	1:B:110:ASN:HA	2.19	0.58
1:C:112:MET:HE3	1:C:153:LEU:CB	2.31	0.58
1:A:51:GLN:HG2	2:A:183:HOH:O	2.04	0.58
1:D:29:PRO:HG2	1:D:138:ARG:NH2	2.18	0.58
1:D:122:ARG:HD3	2:D:187:HOH:O	2.04	0.58
1:A:77:GLU:CD	1:A:114:ARG:NH2	2.62	0.57
1:B:146:HIS:CD2	1:B:152:THR:HG21	2.39	0.57
1:D:111:TYR:CE2	1:D:116:PRO:HG3	2.39	0.57
1:C:52:GLN:HB3	1:C:108:MET:HE2	1.86	0.57
1:B:3:PRO:CB	1:B:4:PRO:HD3	2.35	0.56
1:A:50:ALA:O	1:A:54:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ARG:NH1	1:B:88:ASN:OD1	2.38	0.56
1:B:31:ARG:HG2	1:B:32:TYR:CE1	2.41	0.56
1:B:116:PRO:HG2	1:B:159:LEU:HD13	1.88	0.56
1:C:144:LYS:HB3	2:C:195:HOH:O	2.04	0.56
1:C:159:LEU:HD12	1:C:159:LEU:O	2.06	0.56
1:B:3:PRO:HB3	1:D:31:ARG:NH2	2.19	0.56
1:A:4:PRO:O	1:A:5:ALA:HB3	2.05	0.56
1:A:126:ASN:OD1	1:B:8:SER:HB2	2.06	0.55
1:A:52:GLN:C	1:A:108:MET:HE1	2.31	0.55
1:B:26:LEU:HG	1:B:90:LYS:HA	1.88	0.55
1:C:157:ASP:HB3	1:C:158:ARG:HH11	1.72	0.55
1:D:28:ARG:NH1	1:D:88:ASN:OD1	2.40	0.55
1:C:112:MET:CE	1:C:153:LEU:HB3	2.31	0.55
1:A:37:HIS:HD2	1:A:39:ALA:N	2.05	0.55
1:B:30:VAL:HG13	1:B:102:SER:HA	1.89	0.55
1:B:3:PRO:CG	1:D:138:ARG:NH2	2.69	0.54
1:C:157:ASP:O	1:C:161:GLU:HG3	2.07	0.54
1:D:114:ARG:HG3	1:D:114:ARG:NH1	2.17	0.54
1:A:77:GLU:OE1	1:A:114:ARG:NH2	2.40	0.54
1:B:6:CYS:HA	1:B:130:CYS:CB	2.37	0.54
1:A:52:GLN:HB3	1:A:108:MET:HE2	1.88	0.54
1:A:37:HIS:HD2	1:A:39:ALA:HA	1.72	0.53
1:C:11:PRO:C	1:C:13:ARG:N	2.64	0.53
1:C:58:SER:O	1:C:62:ARG:HB2	2.09	0.53
1:C:155:PRO:HB2	1:C:159:LEU:HG	1.90	0.53
1:D:1:GLU:CG	1:D:2:ASP:N	2.67	0.53
1:B:3:PRO:CB	1:B:4:PRO:CD	2.87	0.53
1:B:67:CYS:O	1:B:68:ASP:HB2	2.09	0.53
1:D:52:GLN:HA	1:D:52:GLN:NE2	2.24	0.53
1:B:11:PRO:HB2	1:B:13:ARG:CG	2.38	0.53
1:B:150:GLN:HG2	1:B:151:PRO:HD2	1.89	0.52
1:A:12:ARG:HG3	1:A:83:GLU:OE1	2.08	0.52
1:C:59:TYR:HA	1:C:63:ASN:ND2	2.25	0.52
1:D:24:GLU:OE1	1:D:90:LYS:HE2	2.08	0.52
1:A:112:MET:HE1	1:A:153:LEU:HD23	1.89	0.52
1:D:3:PRO:HB3	1:D:4:PRO:HD2	1.92	0.52
1:A:77:GLU:HG2	1:A:117:PRO:CD	2.39	0.52
1:A:37:HIS:HB2	1:A:109:GLY:O	2.10	0.52
1:A:99:ASN:N	1:A:100:PRO:HD3	2.24	0.51
1:C:99:ASN:HB2	1:C:100:PRO:HD3	1.91	0.51
1:A:28:ARG:CB	2:A:194:HOH:O	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:PRO:O	1:D:5:ALA:HB3	2.09	0.51
1:B:29:PRO:CB	1:B:138:ARG:HG3	2.41	0.51
1:C:6:CYS:CB	1:C:130:CYS:HA	2.41	0.51
1:A:93:HIS:CE1	1:A:104:GLY:HA3	2.46	0.51
1:B:3:PRO:HB2	1:B:4:PRO:CD	2.41	0.51
1:C:42:HIS:H	1:C:42:HIS:HD2	1.59	0.50
1:A:93:HIS:CE1	1:A:104:GLY:N	2.79	0.50
1:C:158:ARG:N	1:C:158:ARG:HD2	2.27	0.50
1:B:75:ILE:HD13	1:B:81:VAL:HG13	1.93	0.50
1:D:105:ILE:O	1:D:105:ILE:HG13	2.11	0.50
1:D:140:ASN:ND2	1:D:140:ASN:C	2.66	0.49
1:A:3:PRO:HB2	2:A:197:HOH:O	2.12	0.49
1:D:71:TYR:CE2	1:D:106:SER:HB2	2.47	0.49
1:C:13:ARG:HB2	2:C:205:HOH:O	2.12	0.49
1:D:85:ARG:HD2	1:D:91:GLY:CA	2.43	0.49
1:C:59:TYR:HD1	1:C:63:ASN:HD22	1.60	0.49
1:A:99:ASN:N	1:A:100:PRO:CD	2.75	0.48
1:C:31:ARG:HA	1:C:138:ARG:HG3	1.94	0.48
1:A:75:ILE:HD13	1:A:81:VAL:HG22	1.94	0.48
1:D:15:TRP:CH2	1:D:17:ALA:HB2	2.48	0.48
1:D:116:PRO:HG2	1:D:159:LEU:HD13	1.93	0.48
1:B:3:PRO:HB2	1:B:4:PRO:HD3	1.95	0.48
1:C:52:GLN:CB	1:C:108:MET:CE	2.85	0.48
1:B:138:ARG:O	1:B:141:TYR:HB3	2.13	0.48
1:D:26:LEU:CD1	1:D:103:ILE:HD12	2.44	0.48
1:C:146:HIS:ND1	1:C:154:SER:CB	2.77	0.48
1:D:141:TYR:CE2	1:D:168:HIS:CE1	3.01	0.48
1:D:16:ARG:HD2	2:D:189:HOH:O	2.14	0.47
1:B:90:LYS:HG2	1:B:91:GLY:N	2.29	0.47
1:C:10:VAL:CG1	1:C:14:GLU:HB3	2.43	0.47
1:C:50:ALA:O	1:C:54:GLN:HG3	2.14	0.47
1:D:58:SER:O	1:D:62:ARG:HG2	2.14	0.47
1:B:75:ILE:HD12	1:B:81:VAL:HG22	1.94	0.47
1:D:122:ARG:O	1:D:126:ASN:HB2	2.15	0.47
1:C:67:CYS:O	1:C:68:ASP:HB2	2.14	0.47
1:D:28:ARG:HB2	1:D:29:PRO:HA	1.95	0.47
1:A:26:LEU:HG	1:A:90:LYS:HA	1.96	0.47
1:B:126:ASN:ND2	1:B:126:ASN:C	2.73	0.47
1:C:77:GLU:OE1	1:C:111:TYR:OH	2.28	0.47
1:D:85:ARG:HH11	1:D:91:GLY:HA2	1.80	0.47
1:A:57:GLN:O	1:A:57:GLN:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:O	1:C:65:GLY:HA2	2.16	0.46
1:D:117:PRO:O	1:D:118:PRO:C	2.59	0.46
1:D:158:ARG:O	1:D:162:ILE:HG12	2.16	0.46
1:A:150:GLN:O	1:A:152:THR:HG22	2.14	0.46
1:C:52:GLN:HB3	1:C:108:MET:HE1	1.94	0.46
1:D:114:ARG:CG	1:D:114:ARG:NH1	2.74	0.46
1:D:85:ARG:HD2	1:D:91:GLY:HA3	1.98	0.46
1:C:23:ARG:HG2	1:C:23:ARG:HH11	1.80	0.46
1:A:37:HIS:HD2	1:A:39:ALA:H	1.65	0.45
1:A:131:GLY:HA3	1:A:137:LEU:HD12	1.98	0.45
1:C:36:SER:OG	1:C:106:SER:HB2	2.16	0.45
1:D:9:ILE:CG2	1:D:83:GLU:HB2	2.47	0.45
1:A:74:LEU:C	1:A:75:ILE:HG12	2.40	0.45
1:D:58:SER:HA	1:D:61:VAL:HG12	1.97	0.45
1:C:12:ARG:HA	1:C:15:TRP:HE1	1.82	0.45
1:D:78:ASP:OD1	1:D:82:TYR:OH	2.27	0.45
1:C:6:CYS:HB2	1:C:130:CYS:HB2	1.88	0.45
1:A:156:GLY:O	1:A:160:TYR:HB2	2.16	0.45
1:A:36:SER:HB2	1:A:154:SER:OG	2.16	0.44
1:C:11:PRO:C	1:C:13:ARG:H	2.23	0.44
1:D:37:HIS:ND1	1:D:155:PRO:O	2.51	0.44
1:D:12:ARG:O	1:D:13:ARG:C	2.59	0.44
1:D:55:ASN:ND2	2:D:211:HOH:O	2.44	0.44
1:B:27:THR:HG21	2:B:191:HOH:O	2.17	0.44
1:D:138:ARG:HG2	1:D:140:ASN:HD21	1.80	0.44
1:D:147:ARG:NH2	1:D:153:LEU:O	2.43	0.44
1:B:57:GLN:HG3	1:B:69:VAL:HB	1.99	0.43
1:C:163:ILE:HG13	1:C:164:GLN:N	2.32	0.43
1:D:44:ASP:OD2	1:D:44:ASP:N	2.46	0.43
1:B:75:ILE:CD1	1:B:81:VAL:HG13	2.48	0.43
1:D:15:TRP:CZ3	1:D:17:ALA:HB2	2.54	0.43
1:C:126:ASN:O	1:C:129:ALA:HB3	2.18	0.43
1:A:37:HIS:CD2	1:A:39:ALA:H	2.37	0.43
1:B:3:PRO:HB3	1:D:31:ARG:HH22	1.84	0.43
1:D:37:HIS:C	1:D:37:HIS:CD2	2.95	0.43
1:B:164:GLN:HG3	1:B:169:TYR:CE2	2.54	0.43
1:D:164:GLN:HB2	2:D:215:HOH:O	2.18	0.43
1:D:164:GLN:HG2	1:D:169:TYR:CE2	2.53	0.43
1:B:147:ARG:NH2	1:B:157:ASP:OD2	2.44	0.43
1:D:4:PRO:HB2	1:D:5:ALA:H	1.58	0.43
1:A:75:ILE:HB	1:A:107:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:PRO:HD2	1:D:120:ALA:HB2	2.01	0.42
1:B:39:ALA:HA	1:B:110:ASN:HB2	2.01	0.42
1:C:10:VAL:HG13	1:C:14:GLU:HB3	2.01	0.42
1:B:32:TYR:HB2	1:B:102:SER:HB3	2.01	0.42
1:B:81:VAL:HG11	1:B:127:LEU:HD22	2.01	0.42
1:A:33:VAL:HG13	1:A:103:ILE:HG22	2.01	0.42
1:A:77:GLU:HG2	1:A:117:PRO:HD2	2.01	0.42
1:C:113:ASN:HA	1:C:158:ARG:HD3	2.02	0.42
1:D:13:ARG:HH11	1:D:13:ARG:HD3	1.74	0.42
1:D:90:LYS:HD2	1:D:100:PRO:HB3	2.00	0.42
1:D:144:LYS:HE3	1:D:171:ALA:HA	2.01	0.42
1:A:13:ARG:H	1:A:13:ARG:HG2	1.23	0.42
1:B:142:GLU:OE1	1:B:170:ARG:HG3	2.19	0.42
1:C:42:HIS:CE1	1:C:114:ARG:NH1	2.88	0.41
1:D:128:LEU:HB2	2:D:212:HOH:O	2.20	0.41
1:A:37:HIS:CD2	1:A:39:ALA:N	2.88	0.41
1:A:130:CYS:O	1:A:133:ALA:HB3	2.20	0.41
1:C:37:HIS:CD2	1:C:37:HIS:C	2.98	0.41
1:D:28:ARG:HA	1:D:29:PRO:C	2.45	0.41
1:A:85:ARG:NH1	1:A:91:GLY:HA2	2.36	0.41
1:C:112:MET:CE	1:C:153:LEU:HG	2.50	0.41
1:C:52:GLN:CB	1:C:108:MET:HE1	2.51	0.41
1:C:15:TRP:CZ2	1:C:17:ALA:HB2	2.56	0.41
1:B:30:VAL:HG11	1:B:103:ILE:N	2.36	0.41
1:B:68:ASP:O	1:B:69:VAL:C	2.63	0.41
1:C:42:HIS:HB2	1:C:77:GLU:HG3	2.02	0.41
1:C:68:ASP:O	1:C:69:VAL:C	2.63	0.41
1:D:77:GLU:OE1	1:D:111:TYR:OH	2.32	0.41
1:A:37:HIS:CD2	1:A:39:ALA:HB2	2.56	0.41
1:A:74:LEU:HD12	1:A:108:MET:HG2	2.02	0.41
1:A:140:ASN:O	1:A:141:TYR:C	2.63	0.41
1:A:159:LEU:O	1:A:163:ILE:HG23	2.21	0.41
1:D:111:TYR:CD2	1:D:116:PRO:HG3	2.56	0.41
1:A:116:PRO:HA	1:A:117:PRO:HD3	1.82	0.40
1:B:163:ILE:O	1:B:169:TYR:HB2	2.21	0.40
1:C:149:VAL:C	1:C:150:GLN:HG2	2.46	0.40
1:D:37:HIS:HD2	1:D:37:HIS:O	2.04	0.40
1:D:58:SER:HA	1:D:61:VAL:CG1	2.50	0.40
1:C:37:HIS:HD2	1:C:37:HIS:O	2.03	0.40
1:C:64:LEU:N	1:C:64:LEU:HD23	2.36	0.40
1:A:108:MET:HE2	1:A:108:MET:HB3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ARG:NH2	2:C:211:HOH:O	2.55	0.40

All (5) 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:D:2:ASP:CG	1:D:2:ASP:OD1[2_565]	1.21	0.99
1:D:2:ASP:CG	1:D:2:ASP:CG[2_565]	1.88	0.32
1:A:59:TYR:OH	1:D:4:PRO:CB[7_545]	2.09	0.11
1:A:59:TYR:OH	1:D:4:PRO:CG[7_545]	2.11	0.09
1:D:2:ASP:CB	1:D:2:ASP:OD1[2_565]	2.14	0.06

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%)	155 (92%)	12 (7%)	2 (1%)	10	34
1	B	169/171 (99%)	155 (92%)	11 (6%)	3 (2%)	6	23
1	C	169/171 (99%)	153 (90%)	14 (8%)	2 (1%)	10	34
1	D	169/171 (99%)	150 (89%)	17 (10%)	2 (1%)	10	34
All	All	676/684 (99%)	613 (91%)	54 (8%)	9 (1%)	9	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	PRO
1	B	4	PRO
1	B	7	GLY
1	C	3	PRO
1	C	4	PRO

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Mol	Chain	Res	Type
1	A	92	ALA
1	D	4	PRO
1	A	151	PRO
1	D	3	PRO

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	139/139 (100%)	124 (89%)	15 (11%)	6	21
1	B	139/139 (100%)	123 (88%)	16 (12%)	5	18
1	C	139/139 (100%)	121 (87%)	18 (13%)	4	14
1	D	139/139 (100%)	116 (84%)	23 (16%)	2	8
All	All	556/556 (100%)	484 (87%)	72 (13%)	4	14

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	27	THR
1	A	45	THR
1	A	51	GLN
1	A	54	GLN
1	A	62	ARG
1	A	75	ILE
1	A	97	THR
1	A	103	ILE
1	A	126	ASN
1	A	138	ARG
1	A	140	ASN
1	A	144	LYS
1	A	153	LEU
1	A	159	LEU
1	B	6	CYS
1	B	8	SER

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Mol	Chain	Res	Type
1	B	23	ARG
1	B	27	THR
1	B	31	ARG
1	B	51	GLN
1	B	54	GLN
1	B	103	ILE
1	B	108	MET
1	B	113	ASN
1	B	115	VAL
1	B	125	GLN
1	B	126	ASN
1	B	130	CYS
1	B	158	ARG
1	B	164	GLN
1	C	1	GLU
1	C	20	SER
1	C	24	GLU
1	C	36	SER
1	C	61	VAL
1	C	64	LEU
1	C	97	THR
1	C	103	ILE
1	C	105	ILE
1	C	115	VAL
1	C	125	GLN
1	C	140	ASN
1	C	150	GLN
1	C	151	PRO
1	C	153	LEU
1	C	154	SER
1	C	157	ASP
1	C	159	LEU
1	D	1	GLU
1	D	2	ASP
1	D	4	PRO
1	D	13	ARG
1	D	24	GLU
1	D	27	THR
1	D	28	ARG
1	D	36	SER
1	D	41	SER
1	D	42	HIS

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Mol	Chain	Res	Type
1	D	51	GLN
1	D	52	GLN
1	D	85	ARG
1	D	103	ILE
1	D	113	ASN
1	D	118	PRO
1	D	125	GLN
1	D	130	CYS
1	D	140	ASN
1	D	144	LYS
1	D	153	LEU
1	D	165	THR
1	D	167	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	51	GLN
1	A	54	GLN
1	A	55	ASN
1	A	125	GLN
1	B	55	ASN
1	B	60	HIS
1	B	93	HIS
1	B	126	ASN
1	C	37	HIS
1	C	42	HIS
1	C	51	GLN
1	C	52	GLN
1	C	55	ASN
1	C	63	ASN
1	C	93	HIS
1	C	140	ASN
1	D	52	GLN
1	D	55	ASN
1	D	113	ASN
1	D	125	GLN
1	D	140	ASN
1	D	164	GLN

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](#)

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.