



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:26 am BST

PDB ID : 2R90
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

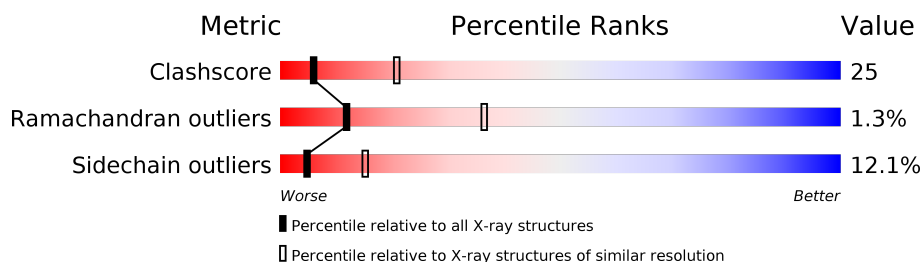
1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 on 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	<div> <div>61%</div> <div>31%</div> <div>6%</div> <div>•</div> </div>
1	B	171	<div> <div>64%</div> <div>27%</div> <div>7%</div> <div>•</div> </div>
1	C	171	<div> <div>56%</div> <div>37%</div> <div>6%</div> <div>•</div> </div>
1	D	171	<div> <div>49%</div> <div>42%</div> <div>7%</div> <div>•</div> </div>

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.

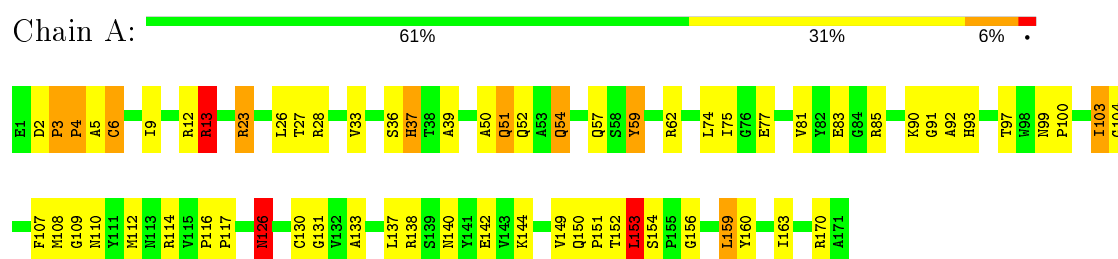
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total	O	0	0
			32	32		
2	B	40	Total	O	0	0
			40	40		
2	C	44	Total	O	0	0
			44	44		
2	D	50	Total	O	0	0
			50	50		

3 Residue-property plots [i](#)

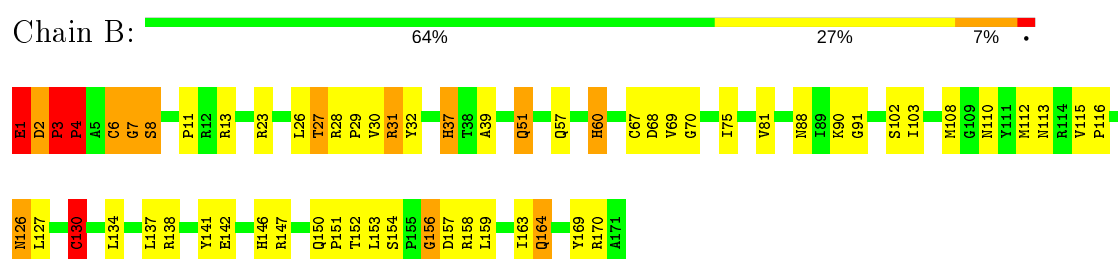
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

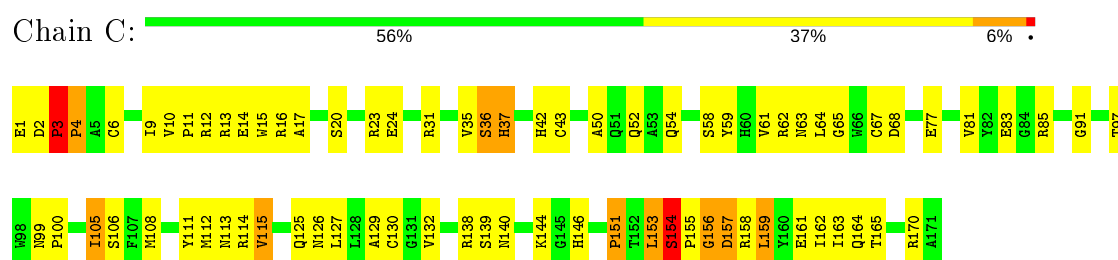
• Molecule 1: Peptidoglycan recognition protein



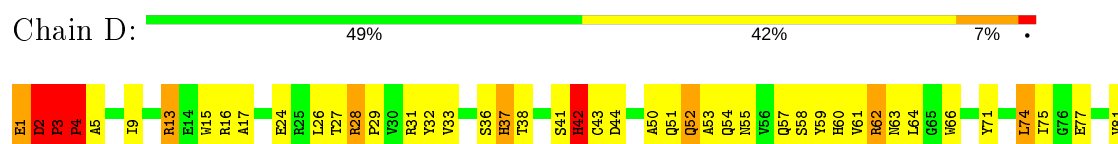
• Molecule 1: Peptidoglycan recognition protein

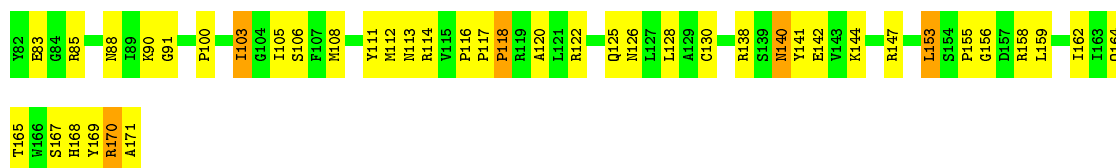


• Molecule 1: Peptidoglycan recognition protein



• 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	0.88	8/1374 (0.6%)	1.31	18/1871 (1.0%)
1	B	0.58	1/1374 (0.1%)	1.03	9/1871 (0.5%)
1	C	0.69	4/1374 (0.3%)	1.09	8/1871 (0.4%)
1	D	0.61	2/1373 (0.1%)	1.01	4/1871 (0.2%)
All	All	0.70	15/5495 (0.3%)	1.12	39/7484 (0.5%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	ARG	CG-CD	10.12	1.77	1.51
1	A	23	ARG	CB-CG	9.14	1.77	1.52
1	C	4	PRO	N-CD	8.89	1.60	1.47
1	C	3	PRO	CA-C	8.09	1.69	1.52
1	A	59	TYR	CB-CG	7.71	1.63	1.51
1	C	154	SER	CA-CB	7.62	1.64	1.52
1	B	1	GLU	CB-CG	7.20	1.65	1.52
1	A	13	ARG	CG-CD	6.93	1.69	1.51
1	D	3	PRO	N-CA	6.24	1.57	1.47
1	C	3	PRO	C-N	6.03	1.45	1.34
1	A	37	HIS	CB-CG	5.77	1.60	1.50
1	D	42	HIS	CA-CB	-5.56	1.41	1.53
1	A	59	TYR	CG-CD2	5.45	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	TYR	N-CA	5.16	1.56	1.46
1	A	13	ARG	CB-CG	5.05	1.66	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	LEU	O-C-N	-19.48	91.53	122.70
1	C	3	PRO	C-N-CD	-15.62	86.25	120.60
1	C	4	PRO	CA-N-CD	-14.23	91.58	111.50
1	D	3	PRO	CA-N-CD	-11.80	94.98	111.50
1	C	4	PRO	N-CA-CB	10.85	116.32	103.30
1	D	2	ASP	C-N-CD	-9.86	98.91	120.60
1	A	153	LEU	CA-C-N	9.85	138.88	117.20
1	B	2	ASP	N-CA-C	-9.85	84.40	111.00
1	C	3	PRO	N-CA-C	9.76	137.49	112.10
1	B	1	GLU	N-CA-C	-8.72	87.45	111.00
1	A	59	TYR	CB-CG-CD2	8.64	126.19	121.00
1	A	13	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	3	PRO	CA-N-CD	-7.46	101.05	111.50
1	A	153	LEU	C-N-CA	7.29	139.92	121.70
1	C	154	SER	CB-CA-C	-7.22	96.39	110.10
1	A	2	ASP	N-CA-C	6.92	129.69	111.00
1	A	37	HIS	CA-CB-CG	6.84	125.23	113.60
1	B	3	PRO	N-CA-C	6.75	129.64	112.10
1	A	4	PRO	CA-N-CD	-6.53	102.36	111.50
1	A	2	ASP	C-N-CD	-6.42	106.48	120.60
1	B	1	GLU	CB-CA-C	6.37	123.15	110.40
1	B	4	PRO	N-CA-C	6.30	128.49	112.10
1	A	13	ARG	CB-CG-CD	6.28	127.94	111.60
1	B	130	CYS	CA-CB-SG	6.27	125.29	114.00
1	B	51	GLN	CB-CA-C	6.04	122.47	110.40
1	A	2	ASP	CB-CA-C	-6.00	98.39	110.40
1	A	59	TYR	N-CA-CB	5.97	121.34	110.60
1	A	59	TYR	CB-CA-C	-5.95	98.50	110.40
1	A	6	CYS	N-CA-C	5.81	126.69	111.00
1	A	126	ASN	CA-CB-CG	5.70	125.95	113.40
1	D	170	ARG	CA-C-N	-5.70	104.67	117.20
1	A	59	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	B	7	GLY	N-CA-C	5.52	126.90	113.10
1	C	154	SER	C-N-CD	-5.49	108.53	120.60
1	D	3	PRO	N-CD-CG	5.46	111.40	103.20
1	C	156	GLY	N-CA-C	-5.36	99.70	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	156	GLY	N-CA-C	-5.07	100.43	113.10
1	C	3	PRO	CA-C-O	-5.04	108.12	120.20

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	1287	59	2
1	B	1337	0	1288	57	0
1	C	1337	0	1288	66	0
1	D	1336	0	1288	87	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	5151	261	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 25.

All (261) 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:CB	1:A:23:ARG:CG	1.77	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:HE3	1:A:153:LEU:HD23	1.24	1.12
1:D:1:GLU:HG3	1:D:2:ASP:H	1.21	1.04
1:A:6:CYS:O	1:A:130:CYS:HB2	1.58	1.02
1:C:151:PRO:HD3	1:D:64:LEU:CD1	1.91	1.00
1:D:74:LEU:HD22	1:D:108:MET:HE2	1.42	0.99
1:D:112:MET:HE3	1:D:153:LEU:HB3	1.47	0.95
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:A:52:GLN:HB3	1:A:108:MET:HE2	1.55	0.88
1:A:112:MET:HE3	1:A:153:LEU:CD2	2.05	0.86
1:C:146:HIS:HB3	1:C:154:SER:HB3	1.57	0.85
1:D:114:ARG:HH11	1:D:114:ARG:HG3	1.42	0.85
1:A:28:ARG:HB2	2:A:194:HOH:O	1.77	0.85
1:A:52:GLN:HB3	1:A:108:MET:CE	2.07	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:N	1:D:42:HIS:CD2	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: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: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:D:53:ALA:HA	1:D:108:MET:HE1	1.70	0.74
1:B:112:MET:HE1	1:B:153:LEU:HG	1.68	0.74
1:B:60:HIS:CD2	1:B:70:GLY:H	1.98	0.74
1:C:112:MET:HE1	1:C:153:LEU:HG	1.70	0.73
1:A:9:ILE:HG21	1:A:83:GLU:HB2	1.71	0.72
1:D:74:LEU:HD22	1:D:108:MET:CE	2.19	0.72
1:B:112:MET:CE	1:B:153:LEU:HG	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:HIS:H	1:C:42:HIS:CD2	2.06	0.71
1:D:1:GLU:HG3	1:D:2:ASP:N	1.99	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: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: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: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: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:37:HIS:HD2	1:A:39:ALA:CA	2.08	0.67
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: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:146:HIS:HB3	1:C:154:SER:CB	2.27	0.63
1:B:112:MET:HE2	1:B:156:GLY:HA2	1.81	0.62
1:D:38:THR:OG1	1:D:108:MET:HA	1.99	0.62
1:A:142:GLU:HG2	1:A:170:ARG:CG	2.29	0.62
1:A:6:CYS:C	1:A:130:CYS:HB2	2.20	0.62
1:A:149:VAL:O	1:A:150:GLN:HB3	1.98	0.62
1:C:132:VAL:HG13	1:C:139:SER:HA	1.81	0.62
1:C:59:TYR:HA	1:C:63:ASN:HD22	1.63	0.62
1:A:77:GLU:CD	1:A:114:ARG:HH21	2.03	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:112:MET:CE	1:C:153:LEU:HB3	2.31	0.61
1:C:112:MET:HE3	1:C:153:LEU:HB3	1.83	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:C:127:LEU:O	1:C:130:CYS:HB3	2.02	0.59
1:D:142:GLU:CD	1:D:170:ARG:HD3	2.22	0.59
1:D:155:PRO:CB	1:D:159:LEU:HD23	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:51:GLN:HG2	2:A:183:HOH:O	2.04	0.58
1:D:122:ARG:HD3	2:D:187:HOH:O	2.04	0.58
1:D:29:PRO:HG2	1:D:138:ARG:NH2	2.18	0.58
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	1.85	0.57
1:C:157:ASP:CG	2:C:209:HOH:O	2.43	0.56
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
1:B:116:PRO:HG2	1:B:159:LEU:HD13	1.88	0.56
1:B:31:ARG:HG2	1:B:32:TYR:CE1	2.41	0.56
1:B:28:ARG:NH1	1:B:88:ASN:OD1	2.38	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: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:D:140:ASN:HD22	1:D:140:ASN:C	2.09	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:NH1	1:D:114:ARG:HG3	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:37:HIS:HD2	1:A:39:ALA:HA	1.72	0.53
1:A:52:GLN:HB3	1:A:108:MET:HE1	1.87	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:B:112:MET:CE	1:B:156:GLY:HA2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:CYS:O	1:B:68:ASP:HB2	2.09	0.53
1:A:77:GLU:CD	1:A:114:ARG:NH2	2.62	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:D:112:MET:HE2	1:D:156:GLY:HA2	1.89	0.52
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:D:53:ALA:CA	1:D:108:MET:HE1	2.37	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:D:32:TYR:HE2	1:D:144:LYS:HZ3	1.57	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
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:52:GLN:C	1:A:108:MET:HE1	2.31	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:11:PRO:C	1:C:13:ARG:N	2.64	0.50
1:C:42:HIS:HD2	1:C:42:HIS:H	1.59	0.50
1:A:93:HIS:CE1	1:A:104:GLY:N	2.79	0.50
1:C:158:ARG:HD2	1:C:158:ARG:N	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: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:D:140:ASN:C	1:D:140:ASN:ND2	2.66	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:D:44:ASP:N	1:D:44:ASP:OD2	2.46	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:C:112:MET:HE1	1:C:153:LEU:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:112:MET:HE2	1:C:156:GLY:HA2	1.95	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: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
1:C:61:VAL:O	1:C:65:GLY:HA2	2.16	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:D:114:ARG:NH1	1:D:114:ARG:CG	2.74	0.46
1:D:85:ARG:HD2	1:D:91:GLY:HA3	1.98	0.46
1:A:112:MET:HE3	1:A:153:LEU:CG	2.45	0.46
1:C:23:ARG:HH11	1:C:23:ARG:HG2	1.80	0.46
1:C:52:GLN:HB3	1:C:108:MET:HE1	1.94	0.46
1:A:131:GLY:HA3	1:A:137:LEU:HD12	1.98	0.45
1:A:37:HIS:HD2	1:A:39:ALA:H	1.65	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: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:C:6:CYS:HB2	1:C:130:CYS:HB2	1.88	0.45
1:C:77:GLU:OE1	1:C:111:TYR:OH	2.28	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:D:37:HIS:ND1	1:D:155:PRO:O	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:126:ASN:ND2	1:B:126:ASN:C	2.73	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:90:LYS:HD2	1:D:100:PRO:HB3	2.00	0.42
1:D:13:ARG:HD3	1:D:13:ARG:HH11	1.74	0.42
1:D:144:LYS:HE3	1:D:171:ALA:HA	2.01	0.42
1:A:13:ARG:HG2	1:A:13:ARG:H	1.23	0.42
1:B:142:GLU:OE1	1:B:170:ARG:HG3	2.19	0.42
1:D:117:PRO:O	1:D:118:PRO:C	2.59	0.41
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:130:CYS:O	1:A:133:ALA:HB3	2.20	0.41
1:A:37:HIS:CD2	1:A:39:ALA:N	2.88	0.41
1:A:85:ARG:NH1	1:A:91:GLY:HA2	2.36	0.41
1:C:11:PRO:C	1:C:13:ARG:H	2.23	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:C:42:HIS:HB2	1:C:77:GLU:HG3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD12	1:A:108:MET:HG2	2.02	0.41
1:C:15:TRP:O	1:C:16:ARG:HB2	2.21	0.41
1:A:74:LEU:C	1:A:75:ILE:HG12	2.40	0.41
1:C:52:GLN:CB	1:C:108:MET:HE1	2.51	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: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:O	1:C:37:HIS:HD2	2.03	0.40
1:C:64:LEU:HD23	1:C:64:LEU:N	2.36	0.40
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 [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%)	12 (7%)	2 (1%)	13	39
1	B	169/171 (99%)	155 (92%)	11 (6%)	3 (2%)	8	28
1	C	169/171 (99%)	153 (90%)	14 (8%)	2 (1%)	13	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	169/171 (99%)	150 (89%)	17 (10%)	2 (1%)	13	39
All	All	676/684 (99%)	613 (91%)	54 (8%)	9 (1%)	12	36

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
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%)	126 (91%)	13 (9%)	8	26
1	B	139/139 (100%)	124 (89%)	15 (11%)	6	19
1	C	139/139 (100%)	123 (88%)	16 (12%)	5	17
1	D	139/139 (100%)	116 (84%)	23 (16%)	2	7
All	All	556/556 (100%)	489 (88%)	67 (12%)	5	15

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	27	THR
1	A	51	GLN
1	A	54	GLN
1	A	62	ARG

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Mol	Chain	Res	Type
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
1	B	23	ARG
1	B	27	THR
1	B	31	ARG
1	B	37	HIS
1	B	51	GLN
1	B	60	HIS
1	B	108	MET
1	B	113	ASN
1	B	115	VAL
1	B	126	ASN
1	B	130	CYS
1	B	158	ARG
1	B	164	GLN
1	C	1	GLU
1	C	2	ASP
1	C	20	SER
1	C	24	GLU
1	C	36	SER
1	C	37	HIS
1	C	97	THR
1	C	105	ILE
1	C	115	VAL
1	C	125	GLN
1	C	140	ASN
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

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Mol	Chain	Res	Type
1	D	13	ARG
1	D	27	THR
1	D	28	ARG
1	D	36	SER
1	D	37	HIS
1	D	41	SER
1	D	42	HIS
1	D	51	GLN
1	D	52	GLN
1	D	62	ARG
1	D	74	LEU
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	153	LEU
1	D	165	THR
1	D	167	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	54	GLN
1	A	125	GLN
1	A	150	GLN
1	B	55	ASN
1	B	60	HIS
1	B	125	GLN
1	C	37	HIS
1	C	42	HIS
1	C	52	GLN
1	C	55	ASN
1	C	63	ASN
1	C	140	ASN
1	D	52	GLN
1	D	55	ASN
1	D	63	ASN
1	D	113	ASN
1	D	125	GLN

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Mol	Chain	Res	Type
1	D	126	ASN
1	D	140	ASN

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 carbohydrates 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.