



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:28 PM UTC

PDB ID : 3P9A / pdb_00003p9a
Title : An atomic view of the nonameric small terminase subunit of Bacteriophage P22
Authors : Bhardwaj, A.; Roy, A.; Cingolani, G.
Deposited on : 2010-10-17
Resolution : 1.75 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

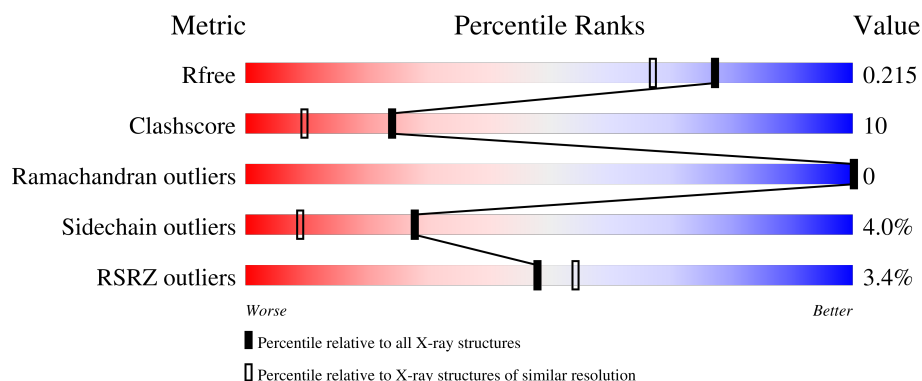
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	162	4% 70% 13% 14%
1	B	162	4% 60% 19% 19%
1	C	162	2% 67% 14% 18%
1	D	162	5% 67% 15% 17%
1	E	162	0% 68% 12% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	162	5% 65% 16% • 17%
1	G	162	2% 65% 16% • 18%
1	H	162	% 72% 9% • 19%
1	I	162	% 60% 19% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11158 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 DNA-packaging protein gp3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1120	711	190	213	6			
1	B	132	Total	C	N	O	S	0	0	0
			1074	683	181	205	5			
1	C	133	Total	C	N	O	S	0	0	0
			1082	687	183	207	5			
1	D	135	Total	C	N	O	S	0	0	0
			1095	695	186	209	5			
1	E	132	Total	C	N	O	S	0	0	0
			1074	683	181	205	5			
1	F	134	Total	C	N	O	S	0	0	0
			1086	689	184	208	5			
1	G	133	Total	C	N	O	S	0	0	0
			1082	687	183	207	5			
1	H	132	Total	C	N	O	S	0	0	0
			1074	683	181	205	5			
1	I	132	Total	C	N	O	S	0	0	0
			1074	683	181	205	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	147	Total	O	0	0
			147	147		
2	B	128	Total	O	0	0
			128	128		
2	C	200	Total	O	0	0
			200	200		
2	D	131	Total	O	0	0
			131	131		
2	E	160	Total	O	0	0
			160	160		

Continued on next page...

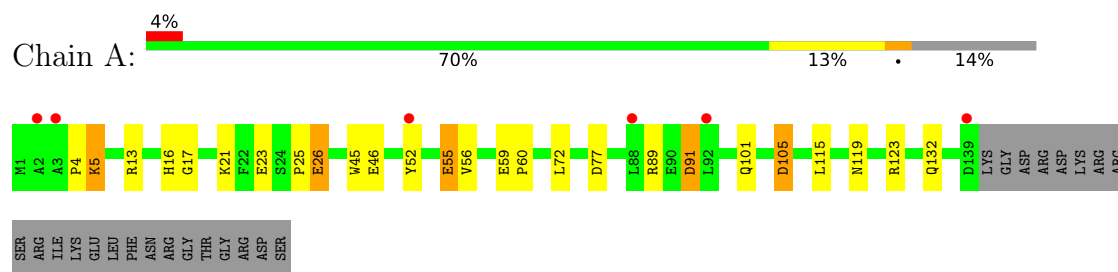
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	130	Total 130	O 130	0	0
2	G	160	Total 160	O 160	0	0
2	H	178	Total 178	O 178	0	0
2	I	163	Total 163	O 163	0	0

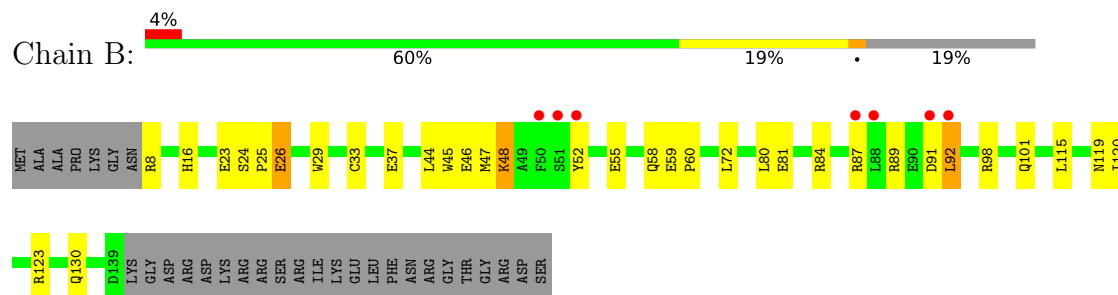
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

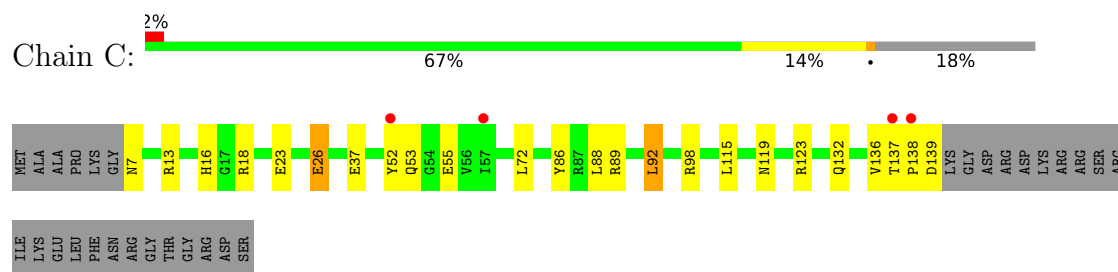
• Molecule 1: DNA-packaging protein gp3



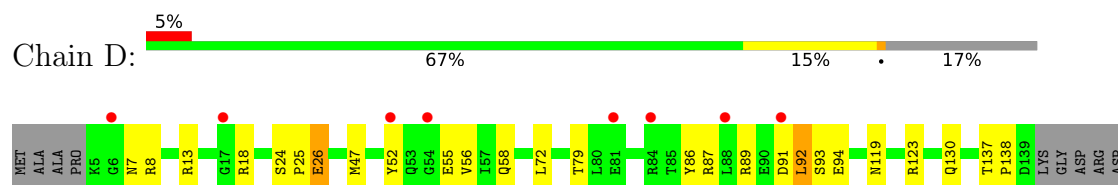
• Molecule 1: DNA-packaging protein gp3



• Molecule 1: DNA-packaging protein gp3



• Molecule 1: DNA-packaging protein gp3



LYS
ARG
ARG
SER
PRO
ARG
ARG
ILE
LYS
GLU
LEU
PHE
ASN
ARG
GLY
THR
GLY
ARG
ASP
SER

• Molecule 1: DNA-packaging protein gp3



MET ALA ALA PRO LYS LYS ASN R8 R9 W10 E26 E40 L44 W45 E46 Q53 Q54 E55 E59 E65 L72 L73 L74 E81 T85 L88 R89 E90 D91 L92 Q101 N119 R123 Q132 D139 LYS GLY ASP ARG LYS ARG ARG ARG

ILE
LYS
GLU
LEU
PHE
ASN
ARG
GLY
THR
GLY
ARG
ASP
SER

• Molecule 1: DNA-packaging protein gp3



MET ALA ALA PRO LYS LYS G6 G7 R8 R9 W10 N19 F22 E23 S24 P25 E26 F50 S51 Y52 E59 E60 M64 L72 L73 R84 T85 Y86 R87 L88 R89 E90 D91 L92 S93 V96 A113 D114 L115 N119 R123 K128 D139 LYS GLY ASP ARG LYS

ARG
ARG
SER
ARG
ILE
LYS
GLU
LEU
PHE
ASN
ARG
GLY
THR
GLY
ASP
SER

• Molecule 1: DNA-packaging protein gp3



MET ALA ALA PRO LYS LYS G7 R8 R9 W10 H16 P25 E26 E37 L44 W45 E46 M47 S51 Y52 Q53 Q54 E55 V56 I57 K63 R64 R65 L72 L73 L74 L80 E81 T82 T85 Y86 R87 L88 D91 L92 R98 M119 I120 R123 D139 LYS

GLY
ASP
ASP
ARG
LYS
LYS
ARG
SER
ILE
LYS
LEU
PHE
ASN
ARG
GLY
THR
GLY
ASP
SER

• Molecule 1: DNA-packaging protein gp3



MET ALA ALA PRO LYS LYS ASN R8 R9 S24 P25 E26 E37 T70 L72 L73 L74 T82 T85 L88 D91 L92 L115 M119 R123 Q130 D139 LYS GLY ASP ARG ASP LYS ARG ARG SER ARG ILE LYS GLU LEU PHE ASN ARG GLY THR ARG

ASP
SER

• Molecule 1: DNA-packaging protein gp3



MET ALA ALA PRO LYS LYS ASN R8 R9 W10 H16 P25 E26 E46 Y52 Q53 V56 T70 G71 L72 L73 L74 T82 T85 L88 D91 L92 L115 M119 R123 Q130 D139 LYS GLY ASP ARG ASP LYS ARG ARG SER ARG ILE LYS GLU LEU PHE ASN ARG GLY THR ARG

P138

D139

LYS

GLY

ASP

ARG

ARG

ASP

LYS

ARG

ARG

SER

ARG

ILE

LYS

GLU

LEU

PHE

ASN

ARG

GLY

THR

GLY

ARG

ASP

SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.48Å 100.90Å 89.85Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	15.00 – 1.75 15.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	84.8 (15.00-1.75) 84.9 (15.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
R, R_{free}	0.177 , 0.216 0.175 , 0.215	Depositor DCC
R_{free} test set	1996 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11158	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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	0.40	0/1146	0.74	2/1555 (0.1%)
1	B	0.40	0/1099	0.66	0/1492
1	C	0.43	0/1107	0.69	0/1503
1	D	0.41	0/1120	0.75	0/1519
1	E	0.45	0/1099	0.71	0/1492
1	F	0.43	1/1111 (0.1%)	0.83	4/1508 (0.3%)
1	G	0.42	0/1107	0.67	0/1503
1	H	0.44	0/1099	0.73	0/1492
1	I	0.44	0/1099	0.72	0/1492
All	All	0.42	1/9987 (0.0%)	0.73	6/13556 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	19	ASN	C-O	5.31	1.26	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	24	SER	CB-CA-C	7.42	120.01	109.92
1	F	22	PHE	N-CA-C	7.07	119.98	109.59
1	F	23	GLU	N-CA-CB	-7.05	101.07	111.51
1	F	88	LEU	N-CA-C	6.88	118.44	111.07
1	A	77	ASP	N-CA-C	6.69	120.75	112.58
1	A	91	ASP	N-CA-C	5.13	116.56	111.07

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	1120	0	1087	32	0
1	B	1074	0	1036	29	0
1	C	1082	0	1042	21	0
1	D	1095	0	1058	24	0
1	E	1074	0	1036	18	0
1	F	1086	0	1045	21	0
1	G	1082	0	1042	26	0
1	H	1074	0	1036	12	0
1	I	1074	0	1036	40	0
2	A	147	0	0	2	0
2	B	128	0	0	2	0
2	C	200	0	0	6	0
2	D	131	0	0	2	0
2	E	160	0	0	3	0
2	F	130	0	0	7	0
2	G	160	0	0	6	0
2	H	178	0	0	4	0
2	I	163	0	0	5	0
All	All	11158	0	9418	191	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 10.

All (191) 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:89:ARG:HD3	1:B:92:LEU:HD22	1.48	0.95
1:A:59:GLU:HG2	1:I:56:VAL:HG11	1.50	0.92
1:B:33:CYS:O	1:B:37:GLU:HG3	1.69	0.92
1:A:101:GLN:HG2	1:I:74:LEU:HD21	1.57	0.86
1:A:56:VAL:HG11	1:B:59:GLU:HG2	1.57	0.85
1:F:91:ASP:HB2	2:F:318:HOH:O	1.75	0.84
1:H:82:THR:O	1:H:85:THR:HG22	1.81	0.81
1:D:56:VAL:HG11	1:E:59:GLU:HG2	1.64	0.79
1:G:87:ARG:HG2	1:G:88:LEU:HD12	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:ARG:HB2	2:F:318:HOH:O	1.84	0.77
1:H:119:ASN:HB2	2:H:376:HOH:O	1.87	0.73
1:G:8:ARG:HD3	1:G:10:TRP:CZ2	2.23	0.73
1:D:119:ASN:HD21	1:D:123:ARG:HE	1.36	0.73
1:B:119:ASN:HD21	1:B:123:ARG:HE	1.35	0.72
1:E:101:GLN:HG2	2:E:348:HOH:O	1.91	0.71
1:F:26:GLU:H	1:F:26:GLU:CD	1.97	0.71
1:A:119:ASN:HD21	1:A:123:ARG:HE	1.39	0.71
1:C:53:GLN:HA	1:D:52:TYR:CZ	2.25	0.71
1:G:52:TYR:O	1:G:55:GLU:HG2	1.90	0.70
1:B:47:MET:HE3	1:B:58:GLN:HG2	1.74	0.70
1:D:24:SER:OG	1:D:26:GLU:HG2	1.92	0.69
1:B:72:LEU:C	1:B:72:LEU:HD23	2.18	0.69
1:C:7:ASN:N	2:C:387:HOH:O	2.26	0.67
1:I:70:THR:O	1:I:74:LEU:HD23	1.94	0.67
1:D:79:THR:HG22	2:D:302:HOH:O	1.94	0.66
1:D:87:ARG:HA	1:D:93:SER:HB3	1.77	0.66
1:G:119:ASN:HD21	1:G:123:ARG:HE	1.41	0.65
1:A:105:ASP:OD2	1:I:70:THR:CG2	2.45	0.65
1:G:25:PRO:HD2	1:G:26:GLU:OE2	1.97	0.65
1:E:119:ASN:HD21	1:E:123:ARG:HE	1.42	0.64
1:I:8:ARG:HD3	1:I:10:TRP:CZ2	2.32	0.64
1:C:13:ARG:NH1	1:C:18:ARG:HG2	2.12	0.64
1:D:13:ARG:NH1	1:D:18:ARG:HG3	2.13	0.64
1:C:136:VAL:C	1:C:138:PRO:HD3	2.22	0.63
1:F:89:ARG:HA	2:F:323:HOH:O	1.96	0.63
1:B:26:GLU:H	1:B:26:GLU:CD	2.06	0.63
1:E:8:ARG:HB3	1:E:10:TRP:CZ2	2.34	0.63
1:I:138:PRO:O	1:I:139:ASP:HB2	1.99	0.62
1:G:7:ASN:HB2	2:H:349:HOH:O	1.98	0.61
1:F:119:ASN:HD21	1:F:123:ARG:HE	1.46	0.61
1:A:52:TYR:O	1:A:55:GLU:HG3	2.01	0.60
1:A:101:GLN:CG	1:I:74:LEU:HD21	2.31	0.60
1:F:90:GLU:HA	1:F:93:SER:HB3	1.83	0.60
1:A:105:ASP:OD2	1:I:70:THR:HG22	2.01	0.60
1:H:24:SER:OG	1:H:26:GLU:HG2	2.02	0.60
1:G:16:HIS:HE1	2:G:224:HOH:O	1.84	0.59
1:B:45:TRP:CE3	1:B:60:PRO:HB2	2.37	0.59
1:C:16:HIS:HE1	2:C:230:HOH:O	1.85	0.59
1:I:87:ARG:HH12	1:I:100:GLU:CD	2.10	0.59
1:G:25:PRO:HG3	1:G:91:ASP:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:ASN:HD21	1:I:123:ARG:HE	1.50	0.59
1:C:139:ASP:N	2:C:396:HOH:O	2.20	0.59
1:B:89:ARG:HG3	1:B:92:LEU:HB2	1.84	0.58
1:G:8:ARG:CZ	1:H:37:GLU:HG2	2.33	0.58
1:H:72:LEU:C	1:H:72:LEU:HD23	2.29	0.58
1:A:26:GLU:CD	1:A:26:GLU:H	2.11	0.58
1:C:72:LEU:HD23	1:C:72:LEU:C	2.28	0.58
1:A:59:GLU:CB	1:I:56:VAL:HG21	2.35	0.57
1:B:24:SER:OG	1:B:26:GLU:HG2	2.05	0.57
1:F:8:ARG:HD3	1:F:10:TRP:CH2	2.41	0.56
1:I:95:VAL:HG23	2:I:267:HOH:O	2.05	0.56
1:B:72:LEU:HD23	1:B:72:LEU:O	2.06	0.56
1:H:70:THR:HG21	2:I:237:HOH:O	2.06	0.56
1:A:101:GLN:CG	1:I:70:THR:HG23	2.35	0.55
1:B:16:HIS:HE1	2:B:299:HOH:O	1.89	0.55
1:I:25:PRO:HD2	1:I:26:GLU:OE2	2.06	0.55
1:A:101:GLN:HG3	1:I:70:THR:CG2	2.37	0.55
1:A:101:GLN:HE22	1:I:80:LEU:HD11	1.72	0.55
1:E:72:LEU:C	1:E:72:LEU:HD23	2.32	0.54
1:D:8:ARG:HH11	1:D:8:ARG:HG3	1.73	0.54
1:A:59:GLU:HB2	1:I:56:VAL:HG21	1.89	0.54
1:F:72:LEU:C	1:F:72:LEU:HD23	2.33	0.54
1:D:89:ARG:HD3	1:D:92:LEU:HD22	1.90	0.54
1:C:52:TYR:CZ	1:C:53:GLN:HG3	2.43	0.54
1:H:119:ASN:CB	2:H:376:HOH:O	2.48	0.54
1:I:16:HIS:HE1	2:I:242:HOH:O	1.91	0.54
1:I:118:ALA:HB2	2:I:351:HOH:O	2.08	0.54
1:A:25:PRO:HD2	1:A:26:GLU:OE2	2.07	0.54
1:G:82:THR:O	1:G:85:THR:HB	2.08	0.53
1:A:5:LYS:NZ	1:A:45:TRP:HE1	2.05	0.53
1:F:59:GLU:HG3	1:F:60:PRO:HD2	1.90	0.53
1:A:46:GLU:HB2	1:B:115:LEU:HD21	1.90	0.53
1:F:8:ARG:HD2	1:G:37:GLU:OE2	2.09	0.53
1:C:137:THR:N	1:C:138:PRO:HD3	2.24	0.52
1:F:25:PRO:C	2:F:321:HOH:O	2.53	0.52
1:I:26:GLU:H	1:I:26:GLU:CD	2.16	0.52
1:G:26:GLU:H	1:G:26:GLU:CD	2.17	0.52
1:A:59:GLU:HG2	1:I:56:VAL:CG1	2.32	0.52
1:D:86:TYR:HB3	1:D:92:LEU:HB3	1.92	0.52
1:D:47:MET:HE3	1:D:58:GLN:HB3	1.90	0.52
1:D:72:LEU:C	1:D:72:LEU:HD23	2.34	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:LEU:C	1:I:72:LEU:HD23	2.35	0.52
1:G:88:LEU:HD12	1:G:88:LEU:N	2.25	0.51
1:A:72:LEU:C	1:A:72:LEU:HD23	2.34	0.51
1:H:119:ASN:HD21	1:H:123:ARG:HE	1.56	0.51
1:C:119:ASN:HD21	1:C:123:ARG:HE	1.57	0.51
1:G:87:ARG:NH1	1:G:88:LEU:HD11	2.26	0.51
1:F:25:PRO:HD2	1:F:26:GLU:OE2	2.11	0.51
1:B:52:TYR:O	1:B:55:GLU:HG2	2.11	0.51
1:E:53:GLN:HA	1:F:52:TYR:CE1	2.47	0.50
1:H:26:GLU:H	1:H:26:GLU:CD	2.18	0.50
1:I:81:GLU:H	1:I:81:GLU:CD	2.18	0.50
1:I:82:THR:O	1:I:85:THR:HG22	2.12	0.50
1:E:46:GLU:HB2	1:F:115:LEU:HD21	1.93	0.50
1:G:63:LYS:NZ	2:G:346:HOH:O	2.38	0.50
1:D:52:TYR:O	1:D:55:GLU:HG2	2.11	0.50
1:B:72:LEU:C	1:B:72:LEU:CD2	2.84	0.49
1:G:98:ARG:NH1	2:G:310:HOH:O	2.43	0.49
1:D:25:PRO:HD2	1:D:26:GLU:OE2	2.12	0.49
1:I:84:ARG:O	1:I:88:LEU:HD13	2.11	0.49
1:E:44:LEU:HD12	1:E:44:LEU:N	2.27	0.49
1:F:89:ARG:NE	2:F:318:HOH:O	2.43	0.49
1:E:8:ARG:HB3	1:E:10:TRP:CE2	2.48	0.48
1:A:45:TRP:CE3	1:A:60:PRO:HB2	2.48	0.48
1:B:8:ARG:NH1	1:C:37:GLU:HG2	2.28	0.48
1:G:119:ASN:ND2	1:G:123:ARG:HE	2.11	0.48
1:B:119:ASN:ND2	1:B:123:ARG:HE	2.09	0.48
1:C:53:GLN:HG2	1:D:52:TYR:OH	2.14	0.48
1:G:72:LEU:C	1:G:72:LEU:HD23	2.39	0.47
1:B:81:GLU:HG2	2:B:303:HOH:O	2.14	0.47
1:F:84:ARG:O	1:F:87:ARG:HB2	2.15	0.47
1:D:26:GLU:CD	1:D:26:GLU:H	2.23	0.47
1:F:86:TYR:CD1	1:F:92:LEU:HD23	2.49	0.47
1:B:25:PRO:HD2	1:B:26:GLU:OE2	2.16	0.46
1:A:5:LYS:HZ1	1:A:45:TRP:HE1	1.63	0.46
1:E:44:LEU:CD1	1:E:65:ARG:HB2	2.46	0.46
1:G:7:ASN:ND2	2:G:332:HOH:O	2.49	0.46
1:A:132:GLN:HE21	1:I:130:GLN:HG2	1.81	0.46
1:C:26:GLU:H	1:C:26:GLU:CD	2.22	0.46
1:G:8:ARG:HD3	1:G:10:TRP:CH2	2.51	0.46
1:G:51:SER:HA	1:G:55:GLU:O	2.16	0.46
1:I:52:TYR:CE1	1:I:53:GLN:HG3	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASP:CA	2:C:396:HOH:O	2.63	0.45
1:A:89:ARG:C	1:A:91:ASP:N	2.74	0.45
1:C:139:ASP:HA	2:C:396:HOH:O	2.16	0.45
1:I:25:PRO:HG3	1:I:91:ASP:O	2.15	0.45
1:I:89:ARG:CZ	1:I:92:LEU:HD22	2.47	0.45
1:A:101:GLN:HG2	1:I:74:LEU:CD2	2.40	0.45
1:D:25:PRO:HG3	1:D:91:ASP:OD1	2.17	0.45
1:A:101:GLN:CG	1:I:70:THR:CG2	2.96	0.44
1:F:87:ARG:HD3	1:F:96:VAL:HG11	1.99	0.44
1:I:8:ARG:N	2:I:271:HOH:O	2.51	0.44
1:I:87:ARG:NH1	1:I:100:GLU:OE2	2.47	0.44
2:E:207:HOH:O	1:F:113:ALA:HA	2.18	0.44
2:H:303:HOH:O	1:I:113:ALA:HA	2.16	0.44
1:D:7:ASN:O	1:E:40:GLU:OE2	2.36	0.43
1:G:46:GLU:HB2	1:H:115:LEU:HD21	2.00	0.43
1:G:63:LYS:HB3	1:G:63:LYS:HE3	1.76	0.43
1:A:13:ARG:HD3	1:A:17:GLY:O	2.19	0.43
1:A:4:PRO:HG3	1:A:45:TRP:CD2	2.53	0.43
1:A:16:HIS:HE1	2:A:246:HOH:O	2.01	0.43
1:B:130:GLN:HG2	1:C:132:GLN:HE21	1.84	0.43
1:A:56:VAL:CG1	1:B:59:GLU:HG2	2.38	0.43
1:C:86:TYR:HB3	1:C:92:LEU:HB3	2.01	0.42
1:G:44:LEU:HD13	1:G:65:ARG:HB2	2.00	0.42
1:B:46:GLU:OE2	1:B:48:LYS:HE2	2.19	0.42
1:E:74:LEU:HD12	2:E:284:HOH:O	2.19	0.42
1:B:89:ARG:NH2	1:B:91:ASP:OD2	2.53	0.42
1:D:89:ARG:C	1:D:91:ASP:N	2.78	0.42
1:A:13:ARG:HD2	2:A:205:HOH:O	2.20	0.42
1:B:25:PRO:HG3	1:B:91:ASP:CG	2.45	0.42
1:A:21:LYS:HE3	1:A:23:GLU:OE1	2.20	0.42
1:D:13:ARG:CZ	1:D:18:ARG:HG3	2.49	0.42
1:E:81:GLU:O	1:E:85:THR:HG23	2.20	0.42
1:E:89:ARG:HB2	1:E:92:LEU:HB2	2.01	0.42
1:I:8:ARG:HD3	1:I:10:TRP:CH2	2.54	0.42
1:C:52:TYR:CE2	1:C:53:GLN:HG3	2.55	0.41
1:I:84:ARG:O	1:I:87:ARG:HB2	2.20	0.41
1:F:64:MET:HE1	2:F:283:HOH:O	2.19	0.41
1:G:16:HIS:CE1	2:G:224:HOH:O	2.67	0.41
1:H:130:GLN:HG2	1:I:132:GLN:HE21	1.85	0.41
1:B:44:LEU:HD23	1:C:115:LEU:HD12	2.02	0.41
1:G:47:MET:HG2	2:G:335:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:TYR:CD1	1:D:92:LEU:HD23	2.55	0.41
1:E:119:ASN:HD21	1:E:123:ARG:NE	2.14	0.41
1:A:115:LEU:HD21	1:I:46:GLU:HB2	2.03	0.41
1:E:85:THR:O	1:E:88:LEU:HB2	2.21	0.41
1:H:25:PRO:HD2	1:H:26:GLU:OE2	2.21	0.41
1:F:128:LYS:NZ	2:F:302:HOH:O	2.53	0.41
1:B:80:LEU:HD23	1:B:80:LEU:HA	1.95	0.41
1:C:89:ARG:NE	1:C:92:LEU:HD22	2.36	0.41
1:D:137:THR:HA	1:D:138:PRO:HD3	1.94	0.41
1:I:137:THR:HA	1:I:138:PRO:HD3	1.94	0.41
1:B:59:GLU:HG3	1:B:60:PRO:HD2	2.02	0.41
1:D:94:GLU:HG3	2:D:262:HOH:O	2.19	0.41
1:I:72:LEU:HD23	1:I:72:LEU:O	2.21	0.41
1:B:29:TRP:CH2	1:B:98:ARG:HG2	2.56	0.40
1:E:26:GLU:H	1:E:26:GLU:CD	2.29	0.40
1:B:84:ARG:O	1:B:87:ARG:HB2	2.21	0.40
1:D:130:GLN:HG2	1:E:132:GLN:HE21	1.86	0.40
1:C:98:ARG:NH2	2:C:245:HOH:O	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	137/162 (85%)	136 (99%)	1 (1%)	0	100	100
1	B	130/162 (80%)	128 (98%)	2 (2%)	0	100	100
1	C	131/162 (81%)	131 (100%)	0	0	100	100
1	D	133/162 (82%)	130 (98%)	3 (2%)	0	100	100
1	E	130/162 (80%)	129 (99%)	1 (1%)	0	100	100
1	F	132/162 (82%)	131 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	131/162 (81%)	130 (99%)	1 (1%)	0	100	100
1	H	130/162 (80%)	129 (99%)	1 (1%)	0	100	100
1	I	130/162 (80%)	128 (98%)	2 (2%)	0	100	100
All	All	1184/1458 (81%)	1172 (99%)	12 (1%)	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	117/137 (85%)	113 (97%)	4 (3%)	32	13
1	B	113/137 (82%)	107 (95%)	6 (5%)	20	5
1	C	114/137 (83%)	109 (96%)	5 (4%)	25	7
1	D	115/137 (84%)	113 (98%)	2 (2%)	53	36
1	E	113/137 (82%)	108 (96%)	5 (4%)	25	7
1	F	114/137 (83%)	112 (98%)	2 (2%)	51	33
1	G	114/137 (83%)	108 (95%)	6 (5%)	20	5
1	H	113/137 (82%)	107 (95%)	6 (5%)	20	5
1	I	113/137 (82%)	108 (96%)	5 (4%)	25	7
All	All	1026/1233 (83%)	985 (96%)	41 (4%)	28	9

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	26	GLU
1	A	55	GLU
1	A	105	ASP
1	B	23	GLU
1	B	26	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	48	LYS
1	B	92	LEU
1	B	101	GLN
1	B	120	ILE
1	C	23	GLU
1	C	26	GLU
1	C	55	GLU
1	C	88	LEU
1	C	92	LEU
1	D	26	GLU
1	D	92	LEU
1	E	26	GLU
1	E	55	GLU
1	E	88	LEU
1	E	90	GLU
1	E	92	LEU
1	F	8	ARG
1	F	26	GLU
1	G	26	GLU
1	G	74	LEU
1	G	80	LEU
1	G	91	ASP
1	G	92	LEU
1	G	120	ILE
1	H	26	GLU
1	H	74	LEU
1	H	85	THR
1	H	88	LEU
1	H	91	ASP
1	H	92	LEU
1	I	26	GLU
1	I	81	GLU
1	I	85	THR
1	I	92	LEU
1	I	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	101	GLN
1	A	119	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	132	GLN
1	B	16	HIS
1	B	58	GLN
1	B	101	GLN
1	B	119	ASN
1	B	130	GLN
1	B	132	GLN
1	C	16	HIS
1	C	101	GLN
1	C	119	ASN
1	C	132	GLN
1	D	101	GLN
1	D	119	ASN
1	D	132	GLN
1	E	119	ASN
1	E	132	GLN
1	F	101	GLN
1	F	119	ASN
1	F	132	GLN
1	G	119	ASN
1	G	132	GLN
1	H	53	GLN
1	H	58	GLN
1	H	119	ASN
1	I	16	HIS
1	I	19	ASN
1	I	101	GLN
1	I	119	ASN
1	I	132	GLN

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 oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	139/162 (85%)	0.05	6 (4%)	40	46	17, 31, 92, 122	0
1	B	132/162 (81%)	0.09	7 (5%)	32	36	18, 33, 87, 113	0
1	C	133/162 (82%)	-0.26	4 (3%)	52	59	15, 25, 56, 87	0
1	D	135/162 (83%)	0.36	8 (5%)	28	32	16, 38, 89, 103	0
1	E	132/162 (81%)	-0.35	2 (1%)	72	78	15, 24, 59, 102	0
1	F	134/162 (82%)	0.14	8 (5%)	27	31	16, 33, 89, 122	0
1	G	133/162 (82%)	-0.17	4 (3%)	52	59	15, 28, 70, 91	0
1	H	132/162 (81%)	-0.21	1 (0%)	82	86	15, 26, 56, 83	0
1	I	132/162 (81%)	-0.19	1 (0%)	82	86	17, 27, 56, 107	0
All	All	1202/1458 (82%)	-0.06	41 (3%)	48	54	15, 29, 78, 122	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	88	LEU	5.6
1	A	52	TYR	5.6
1	D	88	LEU	4.3
1	A	2	ALA	4.1
1	G	52	TYR	4.0
1	D	17	GLY	3.3
1	A	139	ASP	3.3
1	B	52	TYR	3.2
1	A	3	ALA	3.1
1	A	88	LEU	2.9
1	D	52	TYR	2.8
1	D	91	ASP	2.7
1	F	24	SER	2.6
1	D	54	GLY	2.6
1	I	139	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	23	GLU	2.5
1	B	50	PHE	2.5
1	F	139	ASP	2.5
1	B	88	LEU	2.5
1	C	138	PRO	2.4
1	B	51	SER	2.4
1	D	81	GLU	2.4
1	G	57	ILE	2.3
1	F	50	PHE	2.3
1	D	6	GLY	2.3
1	E	139	ASP	2.3
1	B	87	ARG	2.2
1	E	8	ARG	2.2
1	F	85	THR	2.2
1	G	53	GLN	2.2
1	C	137	THR	2.2
1	G	91	ASP	2.2
1	F	22	PHE	2.2
1	B	91	ASP	2.1
1	F	91	ASP	2.1
1	H	139	ASP	2.1
1	B	92	LEU	2.1
1	D	84	ARG	2.1
1	C	52	TYR	2.1
1	A	92	LEU	2.1
1	C	57	ILE	2.1

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.