



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:54 PM EDT

PDB ID : 1N0L / pdb_00001n0l
Title : Crystal structure of the PapD chaperone (C-terminally 6x histidine-tagged) bound to the PapE pilus subunit (N-terminal-deleted) from uropathogenic E. coli
Authors : Sauer, F.G.; Pinkner, J.S.; Waksman, G.; Hultgren, S.J.
Deposited on : 2002-10-14
Resolution : 2.30 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

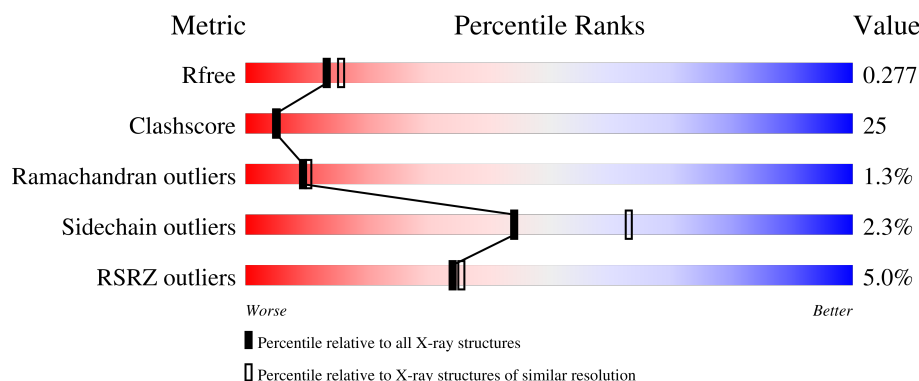
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	224	
1	C	224	
2	B	138	
2	D	138	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5226 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 Chaperone protein PapD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	Se	0	0	0
			1702	1076	293	328	2	3			
1	C	215	Total	C	N	O	S	Se	0	0	0
			1696	1073	290	328	2	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MSE	MET	modified residue	UNP P15319
A	66	MSE	MET	modified residue	UNP P15319
A	172	MSE	MET	modified residue	UNP P15319
A	219	HIS	-	expression tag	UNP P15319
A	220	HIS	-	expression tag	UNP P15319
A	221	HIS	-	expression tag	UNP P15319
A	222	HIS	-	expression tag	UNP P15319
A	223	HIS	-	expression tag	UNP P15319
A	224	HIS	-	expression tag	UNP P15319
C	18	MSE	MET	modified residue	UNP P15319
C	66	MSE	MET	modified residue	UNP P15319
C	172	MSE	MET	modified residue	UNP P15319
C	219	HIS	-	expression tag	UNP P15319
C	220	HIS	-	expression tag	UNP P15319
C	221	HIS	-	expression tag	UNP P15319
C	222	HIS	-	expression tag	UNP P15319
C	223	HIS	-	expression tag	UNP P15319
C	224	HIS	-	expression tag	UNP P15319

- Molecule 2 is a protein called mature Fimbrial protein PapE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	118	Total	C	N	O	S	Se	0	0	0
			877	550	146	177	2	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	107	Total	C	N	O	S	Se	0	0	0
			787	499	129	155	2	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP P08407
B	?	-	ASN	deletion	UNP P08407
B	?	-	LEU	deletion	UNP P08407
B	?	-	THR	deletion	UNP P08407
B	?	-	PHE	deletion	UNP P08407
B	?	-	ARG	deletion	UNP P08407
B	?	-	GLY	deletion	UNP P08407
B	?	-	LYS	deletion	UNP P08407
B	?	-	LEU	deletion	UNP P08407
B	?	-	ILE	deletion	UNP P08407
B	?	-	ILE	deletion	UNP P08407
B	46	MSE	MET	modified residue	UNP P08407
B	55	MSE	MET	modified residue	UNP P08407
B	130	MSE	MET	modified residue	UNP P08407
D	?	-	ASP	deletion	UNP P08407
D	?	-	ASN	deletion	UNP P08407
D	?	-	LEU	deletion	UNP P08407
D	?	-	THR	deletion	UNP P08407
D	?	-	PHE	deletion	UNP P08407
D	?	-	ARG	deletion	UNP P08407
D	?	-	GLY	deletion	UNP P08407
D	?	-	LYS	deletion	UNP P08407
D	?	-	LEU	deletion	UNP P08407
D	?	-	ILE	deletion	UNP P08407
D	?	-	ILE	deletion	UNP P08407
D	46	MSE	MET	modified residue	UNP P08407
D	55	MSE	MET	modified residue	UNP P08407
D	130	MSE	MET	modified residue	UNP P08407

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	21	Total	O	0	0
			21	21		

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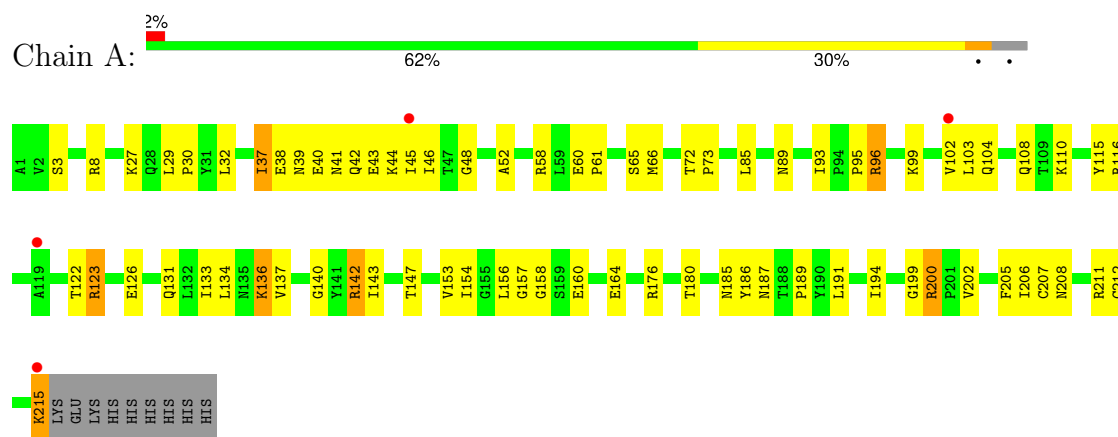
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	73	Total 73	O 73	0	0
3	D	16	Total 16	O 16	0	0

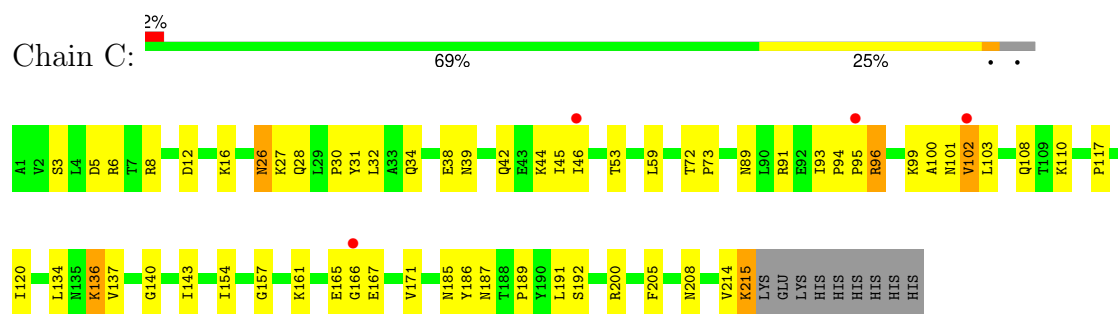
3 Residue-property plots [i](#)

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

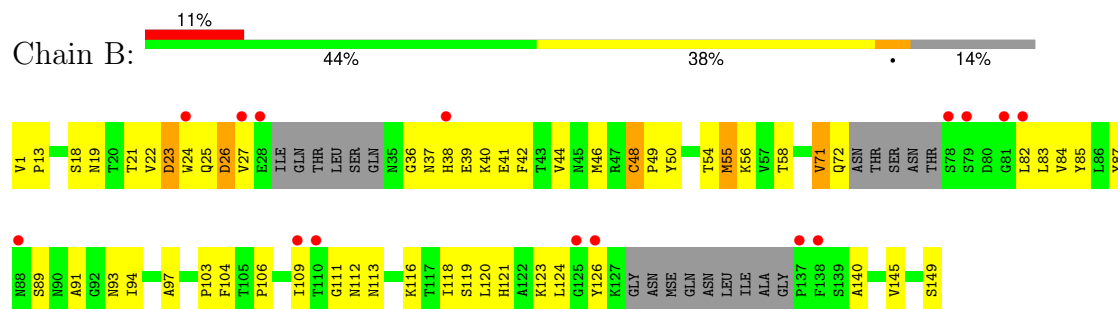
• Molecule 1: Chaperone protein PapD



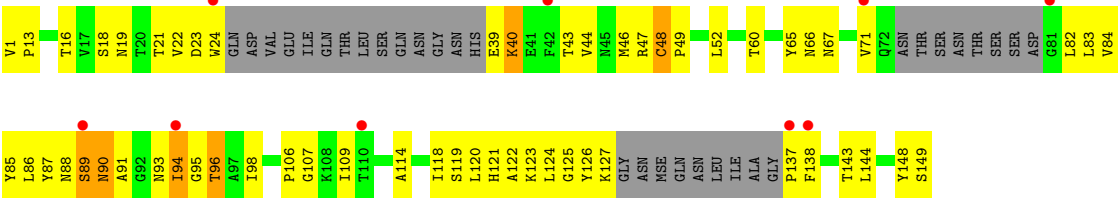
• Molecule 1: Chaperone protein PapD



• Molecule 2: mature Fimbrial protein PapE



• Molecule 2: mature Fimbrial protein PapE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.07Å 56.86Å 60.93Å 108.57° 89.26° 104.14°	Depositor
Resolution (Å)	24.73 – 2.30 24.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.9 (24.73-2.30) 90.9 (24.73-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.279 0.224 , 0.277	Depositor DCC
R_{free} test set	2107 reflections (7.24%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5226	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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	0.42	0/1734	0.91	5/2349 (0.2%)
1	C	0.42	0/1728	0.88	2/2342 (0.1%)
2	B	0.37	0/889	0.82	3/1208 (0.2%)
2	D	0.35	0/797	0.83	3/1083 (0.3%)
All	All	0.40	0/5148	0.87	13/6982 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	48	CYS	N-CA-C	6.19	120.23	110.58
1	C	102	VAL	N-CA-C	6.01	118.55	108.81
2	B	23	ASP	N-CA-C	5.82	119.15	110.14
2	D	89	SER	N-CA-C	-5.68	106.95	112.97
1	A	199	GLY	N-CA-C	-5.47	105.54	112.54
1	A	142	ARG	N-CA-C	-5.30	100.09	108.73
1	A	200	ARG	CA-C-N	5.18	125.08	119.85
1	A	200	ARG	C-N-CA	5.18	125.08	119.85
1	C	5	ASP	N-CA-C	5.14	119.31	113.19
2	B	48	CYS	CA-C-N	5.09	125.08	119.89
2	B	48	CYS	C-N-CA	5.09	125.08	119.89
2	D	148	TYR	N-CA-C	5.04	117.82	109.46
1	A	115	TYR	N-CA-C	-5.03	100.96	108.96

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	1702	0	1711	64	0
1	C	1696	0	1700	72	0
2	B	877	0	852	65	0
2	D	787	0	780	63	0
3	A	54	0	0	3	0
3	B	21	0	0	3	0
3	C	73	0	0	3	0
3	D	16	0	0	1	0
All	All	5226	0	5043	252	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 25.

All (252) 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:215:LYS:H	1:A:215:LYS:HD2	1.17	1.04
1:A:32:LEU:HB2	1:A:93:ILE:HB	1.38	1.00
1:A:89:ASN:HD21	1:A:110:LYS:HE2	1.27	0.99
1:C:44:LYS:HE2	1:C:46:ILE:HD11	1.44	0.97
2:B:71:VAL:HG12	2:B:72:GLN:H	1.31	0.95
1:A:206:ILE:HG12	1:A:215:LYS:HE2	1.49	0.94
1:C:214:VAL:HG12	1:C:215:LYS:HG3	1.48	0.94
1:A:39:ASN:HB3	1:A:45:ILE:HD11	1.49	0.93
2:D:21:THR:HG22	2:D:22:VAL:H	1.34	0.91
2:D:39:GLU:HG2	2:D:123:LYS:HG2	1.54	0.89
2:D:1:VAL:HG11	2:D:49:PRO:HB3	1.52	0.89
1:C:136:LYS:HZ3	1:C:185:ASN:HD22	1.22	0.88
2:D:13:PRO:O	2:D:49:PRO:HG3	1.76	0.85
1:A:96:ARG:HB2	1:A:96:ARG:NH1	1.94	0.83
1:A:136:LYS:HE3	1:A:140:GLY:O	1.78	0.82
1:A:215:LYS:H	1:A:215:LYS:CD	1.92	0.81
1:C:89:ASN:HD21	1:C:110:LYS:HE2	1.45	0.81
1:C:32:LEU:HB2	1:C:93:ILE:HB	1.63	0.80
1:A:96:ARG:HB2	1:A:96:ARG:HH11	1.44	0.79
1:A:215:LYS:HD2	1:A:215:LYS:N	1.96	0.79
1:A:44:LYS:HE2	1:A:46:ILE:HD11	1.64	0.78
2:D:43:THR:HG22	2:D:119:SER:HA	1.66	0.78
2:B:71:VAL:HG13	2:B:140:ALA:HB2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:ASN:HD21	2:D:95:GLY:HA3	1.48	0.76
1:A:30:PRO:O	1:A:95:PRO:HG3	1.85	0.76
1:C:161:LYS:O	1:C:165:GLU:HG2	1.86	0.75
1:A:40:GLU:OE1	1:A:85:LEU:HB3	1.87	0.75
1:A:160:GLU:HG3	1:A:202:VAL:HG11	1.69	0.75
1:A:136:LYS:HZ3	1:A:185:ASN:HB2	1.52	0.74
1:A:29:LEU:HB3	1:A:95:PRO:HG2	1.70	0.74
2:B:27:VAL:HG11	2:B:37:ASN:HD21	1.53	0.73
2:D:21:THR:HG22	2:D:22:VAL:N	2.03	0.73
2:B:56:LYS:HG2	3:B:158:HOH:O	1.87	0.73
1:C:34:GLN:HE21	1:C:91:ARG:HB3	1.52	0.72
1:C:34:GLN:HE22	1:C:91:ARG:HH21	1.38	0.71
2:D:83:LEU:HG	2:D:126:TYR:HA	1.71	0.71
1:C:136:LYS:NZ	1:C:185:ASN:HD22	1.89	0.71
2:B:1:VAL:HG12	2:B:13:PRO:HD2	1.74	0.70
2:B:94:ILE:HA	2:B:121:HIS:CD2	2.26	0.70
2:B:41:GLU:HG2	2:B:121:HIS:CE1	2.26	0.70
1:C:136:LYS:HD3	1:C:137:VAL:N	2.07	0.69
2:B:56:LYS:HE2	2:B:103:PRO:HB2	1.74	0.69
2:B:36:GLY:HA3	2:B:123:LYS:HD3	1.73	0.69
1:C:26:ASN:HD22	1:C:26:ASN:C	1.99	0.69
2:D:47:ARG:HD2	2:D:114:ALA:O	1.92	0.69
2:B:46:MSE:HE2	2:B:118:ILE:HD11	1.73	0.69
2:B:87:TYR:HB2	2:B:121:HIS:HB2	1.75	0.68
1:C:34:GLN:OE1	1:C:93:ILE:HD11	1.92	0.68
2:D:1:VAL:CG1	2:D:49:PRO:HB3	2.23	0.68
2:B:71:VAL:HG12	2:B:72:GLN:N	2.08	0.68
1:A:96:ARG:HH11	1:A:96:ARG:CB	2.06	0.68
2:B:44:VAL:CG1	2:B:118:ILE:HB	2.24	0.68
2:B:1:VAL:CG1	2:B:13:PRO:HD2	2.24	0.67
1:C:89:ASN:HD21	1:C:110:LYS:CE	2.06	0.67
1:A:89:ASN:HD21	1:A:110:LYS:CE	2.06	0.67
2:B:40:LYS:O	2:B:121:HIS:HA	1.96	0.65
1:C:8:ARG:NH2	2:D:149:SER:O	2.29	0.64
2:B:27:VAL:CG1	2:B:37:ASN:HD21	2.11	0.64
2:B:89:SER:HA	2:B:121:HIS:CD2	2.33	0.64
1:A:40:GLU:OE1	1:A:85:LEU:HD23	1.99	0.63
1:C:34:GLN:HE22	1:C:91:ARG:HD3	1.64	0.63
2:B:48:CYS:HB3	2:B:49:PRO:HD2	1.79	0.63
1:C:134:LEU:HD22	1:C:143:ILE:HG12	1.79	0.62
1:A:160:GLU:O	1:A:164:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ASN:HD22	1:C:108:GLN:HE21	1.46	0.62
2:D:44:VAL:HG13	2:D:118:ILE:HB	1.81	0.62
2:D:44:VAL:CG1	2:D:118:ILE:HB	2.30	0.62
1:C:187:ASN:HB2	3:C:230:HOH:O	2.00	0.61
2:B:27:VAL:HG11	2:B:37:ASN:ND2	2.15	0.61
1:A:89:ASN:HD22	1:A:108:GLN:HE21	1.48	0.61
2:D:90:ASN:ND2	2:D:95:GLY:HA3	2.16	0.61
1:A:154:ILE:CD1	1:A:200:ARG:HD3	2.30	0.60
2:B:56:LYS:HE2	2:B:103:PRO:CG	2.32	0.60
2:B:56:LYS:HG3	2:B:103:PRO:HB2	1.83	0.60
2:B:97:ALA:HB1	3:B:155:HOH:O	2.02	0.60
1:A:44:LYS:HE2	1:A:46:ILE:CD1	2.32	0.60
2:D:21:THR:CG2	2:D:22:VAL:H	2.13	0.60
1:C:189:PRO:HG2	1:C:205:PHE:HB2	1.83	0.59
2:B:13:PRO:O	2:B:49:PRO:HG3	2.03	0.59
2:D:98:ILE:HD11	2:D:120:LEU:HD22	1.83	0.59
1:A:206:ILE:HG12	1:A:215:LYS:CE	2.28	0.59
2:D:60:THR:HG23	2:D:143:THR:HB	1.84	0.59
1:C:154:ILE:CD1	1:C:200:ARG:HD3	2.32	0.58
1:A:37:ILE:CD1	1:A:52:ALA:HB2	2.34	0.58
1:C:117:PRO:HG2	1:C:120:ILE:HG12	1.86	0.57
2:D:49:PRO:HD2	2:D:52:LEU:HD22	1.86	0.56
1:A:153:VAL:HG11	1:A:191:LEU:HD11	1.87	0.56
2:B:56:LYS:HE2	2:B:103:PRO:CB	2.34	0.56
1:C:191:LEU:C	1:C:191:LEU:HD23	2.31	0.56
1:A:102:VAL:HG12	2:B:23:ASP:OD1	2.06	0.56
1:A:123:ARG:HG3	1:A:126:GLU:OE2	2.06	0.56
2:D:65:TYR:CE2	2:D:127:LYS:HG2	2.42	0.55
1:C:136:LYS:HD3	1:C:136:LYS:C	2.32	0.55
1:C:30:PRO:O	1:C:95:PRO:HD3	2.07	0.54
1:C:96:ARG:HG3	1:C:96:ARG:HH11	1.71	0.54
1:A:103:LEU:HB3	2:B:22:VAL:HG12	1.90	0.54
1:C:34:GLN:CD	1:C:93:ILE:HD11	2.33	0.54
2:B:48:CYS:HB3	2:B:49:PRO:CD	2.38	0.54
1:A:8:ARG:NH2	2:B:149:SER:O	2.35	0.53
2:B:44:VAL:HG13	2:B:118:ILE:HB	1.88	0.53
1:A:189:PRO:HG2	1:A:205:PHE:HB2	1.89	0.53
1:C:136:LYS:NZ	1:C:185:ASN:HB2	2.23	0.53
1:A:187:ASN:HB2	3:A:277:HOH:O	2.08	0.53
2:D:90:ASN:HA	2:D:107:GLY:HA3	1.90	0.53
2:B:112:ASN:N	2:B:112:ASN:HD22	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:NH2	1:A:122:THR:HG21	2.23	0.53
1:C:46:ILE:O	1:C:46:ILE:HG22	2.09	0.53
2:D:90:ASN:HD21	2:D:96:THR:N	2.07	0.53
2:B:25:GLN:O	2:B:26:ASP:HB3	2.09	0.52
2:D:90:ASN:HD21	2:D:96:THR:H	1.57	0.52
2:D:85:TYR:O	2:D:122:ALA:HA	2.10	0.52
1:C:96:ARG:HG3	1:C:96:ARG:NH1	2.25	0.52
2:D:39:GLU:O	2:D:40:LYS:HB2	2.10	0.52
2:D:126:TYR:O	2:D:127:LYS:HB3	2.09	0.52
2:B:89:SER:HB3	2:B:119:SER:O	2.10	0.52
2:B:37:ASN:O	2:B:38:HIS:HB2	2.10	0.52
1:C:26:ASN:HD22	1:C:27:LYS:N	2.06	0.52
2:D:46:MSE:HE2	2:D:118:ILE:HD11	1.92	0.52
1:A:131:GLN:NE2	1:A:147:THR:HG22	2.25	0.51
2:B:89:SER:HA	2:B:121:HIS:HD2	1.75	0.51
1:C:99:LYS:HD3	2:D:23:ASP:OD1	2.10	0.51
2:D:85:TYR:HB3	2:D:87:TYR:CE1	2.45	0.51
1:C:34:GLN:NE2	1:C:91:ARG:HH21	2.06	0.51
2:D:93:ASN:CG	2:D:94:ILE:H	2.17	0.51
1:A:157:GLY:HA2	1:A:186:TYR:CE1	2.46	0.51
1:C:136:LYS:HZ3	1:C:185:ASN:ND2	1.99	0.51
2:D:82:LEU:HD12	2:D:125:GLY:O	2.11	0.51
2:B:54:THR:O	2:B:55:MSE:C	2.53	0.51
1:A:72:THR:HB	1:A:73:PRO:HD2	1.92	0.51
1:A:72:THR:HB	1:A:73:PRO:CD	2.40	0.51
1:C:101:ASN:HB3	2:D:24:TRP:HB2	1.92	0.51
1:A:60:GLU:HB3	1:A:61:PRO:HD2	1.92	0.51
2:D:89:SER:HB2	2:D:121:HIS:NE2	2.26	0.51
1:C:31:TYR:CE1	1:C:94:PRO:HB3	2.46	0.50
1:A:154:ILE:HG21	1:A:194:ILE:HD11	1.93	0.50
1:C:136:LYS:HE3	1:C:140:GLY:O	2.12	0.50
1:A:136:LYS:NZ	1:A:185:ASN:HB2	2.23	0.50
2:B:1:VAL:HG12	2:B:13:PRO:CD	2.41	0.50
1:C:26:ASN:C	1:C:26:ASN:ND2	2.69	0.49
1:A:142:ARG:HA	1:A:180:THR:HA	1.94	0.49
2:D:106:PRO:HB2	2:D:109:ILE:CG1	2.41	0.49
1:C:26:ASN:ND2	1:C:28:GLN:H	2.11	0.49
2:B:56:LYS:HB2	2:B:104:PHE:O	2.12	0.49
1:C:39:ASN:HB3	1:C:45:ILE:HD12	1.95	0.49
1:C:44:LYS:CE	1:C:46:ILE:HD11	2.31	0.49
2:D:71:VAL:HG11	2:D:138:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:GLU:HG2	2:B:121:HIS:HE1	1.75	0.49
2:D:18:SER:O	2:D:19:ASN:C	2.55	0.48
1:C:73:PRO:HA	3:C:296:HOH:O	2.12	0.48
1:C:103:LEU:HB3	2:D:22:VAL:CG1	2.44	0.48
1:C:136:LYS:HZ3	1:C:185:ASN:HB2	1.79	0.48
1:A:104:GLN:HA	2:B:21:THR:HG22	1.96	0.47
1:A:134:LEU:HD22	1:A:143:ILE:HG12	1.95	0.47
1:A:136:LYS:HD3	1:A:137:VAL:N	2.29	0.47
2:D:46:MSE:CE	2:D:118:ILE:HD11	2.44	0.47
1:A:65:SER:OG	1:A:66:MSE:N	2.48	0.47
1:C:34:GLN:NE2	1:C:91:ARG:HD3	2.29	0.47
1:C:72:THR:HB	1:C:73:PRO:CD	2.45	0.47
1:A:45:ILE:HG21	1:A:48:GLY:O	2.13	0.47
2:B:113:ASN:OD1	2:B:116:LYS:HE3	2.15	0.47
2:D:84:VAL:HG22	2:D:124:LEU:CD2	2.45	0.47
2:B:106:PRO:HB2	2:B:109:ILE:HD11	1.97	0.47
1:C:16:LYS:HD2	1:C:16:LYS:N	2.30	0.47
1:A:39:ASN:ND2	1:A:43:GLU:HB2	2.30	0.47
2:B:56:LYS:HB2	2:B:104:PHE:C	2.40	0.47
1:C:99:LYS:CD	1:C:102:VAL:HG11	2.45	0.47
2:B:111:GLY:C	2:B:112:ASN:HD22	2.23	0.47
1:C:99:LYS:HB2	1:C:102:VAL:HG21	1.97	0.46
1:A:3:SER:HB2	3:A:256:HOH:O	2.15	0.46
2:B:44:VAL:HG13	2:B:44:VAL:O	2.15	0.46
2:D:60:THR:CG2	2:D:143:THR:HB	2.45	0.46
2:D:127:LYS:C	2:D:127:LYS:HD2	2.41	0.46
1:A:156:LEU:HD13	1:A:191:LEU:HD13	1.98	0.46
1:C:34:GLN:NE2	1:C:91:ARG:HB3	2.27	0.46
2:B:24:TRP:CD1	2:B:40:LYS:HZ2	2.34	0.46
2:D:90:ASN:HD21	2:D:95:GLY:CA	2.24	0.45
1:A:116:ARG:HH21	1:A:122:THR:CG2	2.29	0.45
2:B:89:SER:HB3	2:B:119:SER:C	2.41	0.45
2:B:112:ASN:N	2:B:112:ASN:ND2	2.62	0.45
1:A:156:LEU:HD13	1:A:191:LEU:CD1	2.46	0.45
1:C:154:ILE:HD12	1:C:200:ARG:HD3	1.97	0.45
2:D:71:VAL:HB	2:D:82:LEU:HB3	1.97	0.45
2:B:82:LEU:HA	2:B:126:TYR:HD1	1.81	0.45
1:C:27:LYS:O	1:C:28:GLN:HG3	2.17	0.45
1:C:30:PRO:O	1:C:95:PRO:CD	2.64	0.45
2:B:106:PRO:HB2	2:B:109:ILE:CG1	2.47	0.45
1:C:99:LYS:HD3	1:C:102:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:HB3	1:A:42:GLN:HA	1.98	0.45
1:C:46:ILE:HD13	3:C:256:HOH:O	2.15	0.45
1:A:27:LYS:HE2	3:A:275:HOH:O	2.17	0.45
1:C:27:LYS:C	1:C:28:GLN:HG3	2.41	0.45
2:B:42:PHE:CZ	2:B:120:LEU:HB2	2.53	0.44
2:D:39:GLU:CD	2:D:123:LYS:HE2	2.42	0.44
1:A:58:ARG:HD3	1:A:60:GLU:OE2	2.17	0.44
1:A:157:GLY:O	1:A:189:PRO:HA	2.17	0.44
2:D:82:LEU:O	2:D:83:LEU:HD23	2.17	0.44
2:D:85:TYR:HB2	2:D:123:LYS:HB2	1.99	0.44
2:D:66:ASN:O	2:D:66:ASN:CG	2.61	0.44
1:C:6:ARG:HA	2:D:1:VAL:O	2.18	0.44
1:C:30:PRO:HG2	1:C:95:PRO:HG2	2.00	0.44
2:D:94:ILE:HA	2:D:121:HIS:CD2	2.52	0.44
1:A:133:ILE:HD13	1:A:211:ARG:NH2	2.33	0.43
1:C:3:SER:HB2	3:D:164:HOH:O	2.17	0.43
2:D:88:ASN:C	2:D:90:ASN:H	2.25	0.43
2:B:85:TYR:HB2	2:B:123:LYS:HB2	2.01	0.43
2:D:89:SER:O	2:D:90:ASN:C	2.62	0.43
2:D:85:TYR:O	2:D:86:LEU:HD23	2.19	0.43
2:B:58:THR:HB	2:B:145:VAL:HB	2.01	0.43
2:B:106:PRO:HB2	2:B:109:ILE:HG13	2.00	0.43
2:B:18:SER:O	2:B:19:ASN:C	2.61	0.43
1:C:191:LEU:HD23	1:C:192:SER:N	2.34	0.43
1:A:103:LEU:HD22	2:B:84:VAL:HG11	2.01	0.43
2:B:56:LYS:CE	2:B:103:PRO:HB2	2.45	0.42
2:B:36:GLY:HA2	2:B:123:LYS:HB3	2.01	0.42
1:C:72:THR:HB	1:C:73:PRO:HD2	2.00	0.42
1:A:39:ASN:HD21	1:A:43:GLU:HB2	1.85	0.42
1:A:207:CYS:HA	1:A:212:CYS:HA	2.00	0.42
2:D:66:ASN:O	2:D:67:ASN:HB3	2.19	0.42
1:C:12:ASP:C	1:C:12:ASP:OD2	2.61	0.42
1:C:208:ASN:C	1:C:208:ASN:HD22	2.27	0.42
1:C:215:LYS:HD2	1:C:215:LYS:C	2.44	0.42
2:D:46:MSE:HE2	2:D:118:ILE:CD1	2.48	0.42
2:D:94:ILE:HG12	2:D:95:GLY:N	2.34	0.42
2:B:91:ALA:C	2:B:93:ASN:H	2.28	0.42
1:C:26:ASN:HD21	1:C:28:GLN:HB2	1.83	0.42
1:C:136:LYS:NZ	1:C:185:ASN:CB	2.82	0.42
1:C:157:GLY:HA2	1:C:186:TYR:CE1	2.53	0.42
1:A:208:ASN:C	1:A:208:ASN:HD22	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:THR:O	2:B:55:MSE:O	2.38	0.41
2:D:1:VAL:HG13	2:D:13:PRO:HD2	2.02	0.41
1:A:41:ASN:O	1:A:42:GLN:HB2	2.20	0.41
1:C:166:GLY:O	1:C:167:GLU:C	2.63	0.41
1:C:8:ARG:HH22	2:D:149:SER:C	2.27	0.41
2:B:50:TYR:HD2	3:B:151:HOH:O	2.04	0.41
1:A:158:GLY:HA2	1:A:186:TYR:HB3	2.02	0.41
2:B:38:HIS:O	2:B:39:GLU:C	2.62	0.41
1:C:100:ALA:HB1	2:D:137:PRO:HA	2.03	0.41
1:A:44:LYS:HG2	1:A:46:ILE:HD11	2.03	0.41
2:B:82:LEU:HD12	2:B:126:TYR:HD1	1.85	0.41
2:B:83:LEU:O	2:B:124:LEU:HD12	2.21	0.41
2:D:16:THR:OG1	2:D:47:ARG:HB2	2.21	0.41
2:D:67:ASN:O	2:D:67:ASN:CG	2.63	0.41
1:C:31:TYR:O	1:C:59:LEU:N	2.37	0.41
2:B:46:MSE:CE	2:B:118:ILE:HD11	2.49	0.40
1:C:136:LYS:NZ	1:C:185:ASN:ND2	2.62	0.40
2:D:48:CYS:HB3	2:D:49:PRO:HD2	2.03	0.40
2:D:48:CYS:HB3	2:D:49:PRO:CD	2.50	0.40
2:D:86:LEU:HA	2:D:121:HIS:O	2.21	0.40
1:A:99:LYS:HB2	1:A:102:VAL:HG11	2.03	0.40
2:B:71:VAL:CG1	2:B:140:ALA:HB2	2.42	0.40
1:C:38:GLU:HB3	1:C:42:GLN:HA	2.03	0.40
2:D:65:TYR:CG	2:D:127:LYS:HE2	2.57	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	213/224 (95%)	203 (95%)	10 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	213/224 (95%)	201 (94%)	12 (6%)	0	100	100
2	B	110/138 (80%)	95 (86%)	12 (11%)	3 (3%)	4	3
2	D	99/138 (72%)	89 (90%)	5 (5%)	5 (5%)	1	1
All	All	635/724 (88%)	588 (93%)	39 (6%)	8 (1%)	9	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	55	MSE
2	D	94	ILE
2	D	40	LYS
2	D	90	ASN
2	D	91	ALA
2	B	26	ASP
2	D	96	THR
2	B	71	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/197 (97%)	185 (97%)	6 (3%)	35	52
1	C	190/197 (96%)	184 (97%)	6 (3%)	34	51
2	B	97/113 (86%)	97 (100%)	0	100	100
2	D	86/113 (76%)	85 (99%)	1 (1%)	63	79
All	All	564/620 (91%)	551 (98%)	13 (2%)	44	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	96	ARG
1	A	123	ARG

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Mol	Chain	Res	Type
1	A	136	LYS
1	A	176	ARG
1	A	215	LYS
1	C	26	ASN
1	C	53	THR
1	C	96	ARG
1	C	136	LYS
1	C	171	VAL
1	C	215	LYS
2	D	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	89	ASN
1	A	104	GLN
1	A	131	GLN
1	A	135	ASN
1	A	179	GLN
1	A	185	ASN
1	A	208	ASN
2	B	35	ASN
2	B	63	ASN
2	B	66	ASN
2	B	112	ASN
2	B	121	HIS
1	C	26	ASN
1	C	34	GLN
1	C	80	GLN
1	C	89	ASN
1	C	101	ASN
1	C	108	GLN
1	C	125	ASN
1	C	131	GLN
1	C	179	GLN
1	C	185	ASN
1	C	208	ASN
2	D	88	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 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 ⓘ

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	212/224 (94%)	0.19	4 (1%) 66 68	13, 34, 54, 74	0
1	C	212/224 (94%)	0.15	4 (1%) 66 68	12, 34, 53, 65	0
2	B	116/138 (84%)	0.97	15 (12%) 7 8	17, 53, 74, 80	0
2	D	105/138 (76%)	0.96	9 (8%) 16 17	18, 54, 75, 83	0
All	All	645/724 (89%)	0.44	32 (4%) 34 35	12, 38, 69, 83	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	110	THR	4.6
2	B	78	SER	3.4
2	D	81	GLY	3.3
2	B	137	PRO	3.2
2	B	27	VAL	3.2
2	B	88	ASN	3.1
2	B	126	TYR	3.1
2	D	94	ILE	3.0
2	B	109	ILE	3.0
1	A	45	ILE	3.0
2	D	110	THR	2.8
2	B	82	LEU	2.7
2	B	24	TRP	2.7
2	B	38	HIS	2.6
2	B	28	GLU	2.5
1	A	215	LYS	2.4
2	D	89	SER	2.4
2	D	24	TRP	2.4
1	A	102	VAL	2.4
1	C	166	GLY	2.3
2	B	125	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	46	ILE	2.3
2	B	79	SER	2.3
2	D	42	PHE	2.3
2	D	138	PHE	2.3
2	B	81	GLY	2.3
1	A	119	ALA	2.2
1	C	102	VAL	2.2
1	C	95	PRO	2.2
2	D	71	VAL	2.1
2	B	138	PHE	2.1
2	D	137	PRO	2.0

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.