Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:19 PM EDT

PDB ID	:	1N0L
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 (i) 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 (i)) were used in the production of this report:

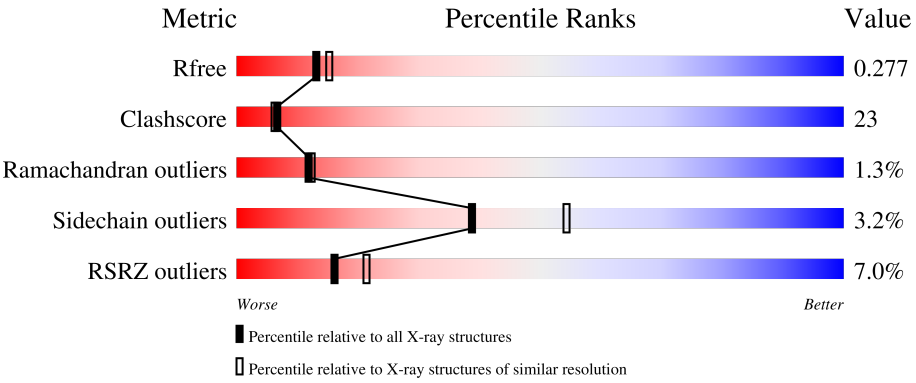
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	2% 63% 31%
1	C	224	% 70% 24%
2	B	138	15% 49% 35% 14%
2	D	138	12% 36% 37% 22%

2 Entry composition (i)

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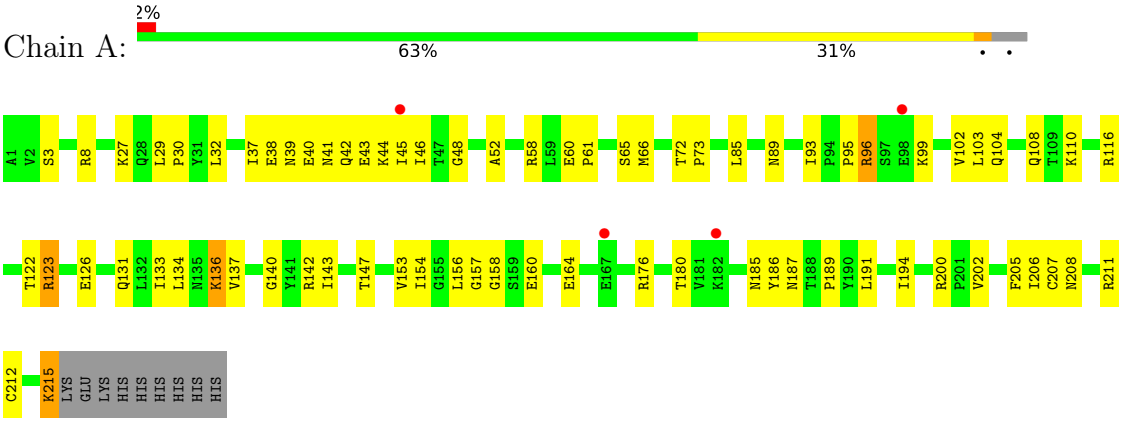
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	73	Total O 73 73	0	0
3	D	16	Total O 16 16	0	0

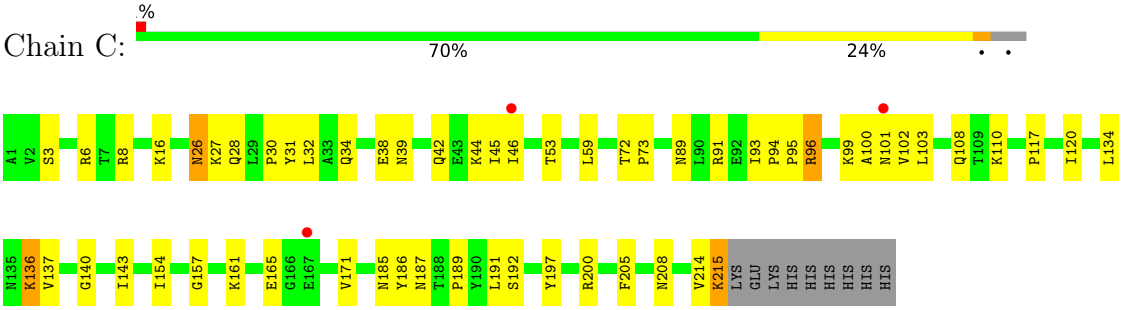
3 Residue-property plots (i)

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.

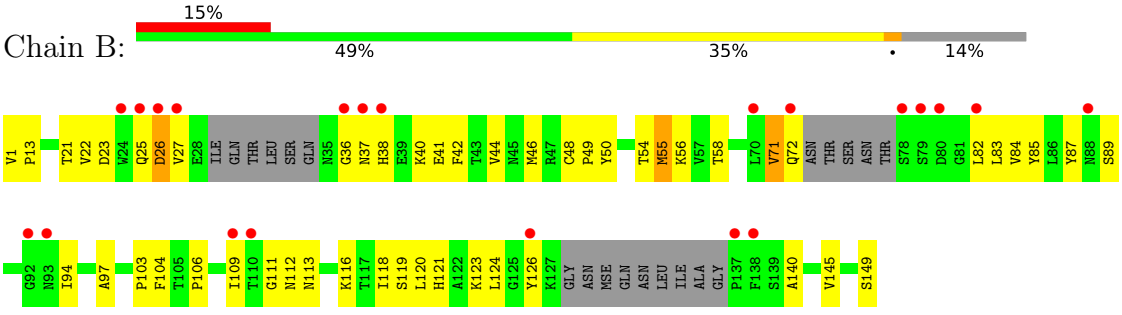
• Molecule 1: Chaperone protein PapD



• Molecule 1: Chaperone protein PapD

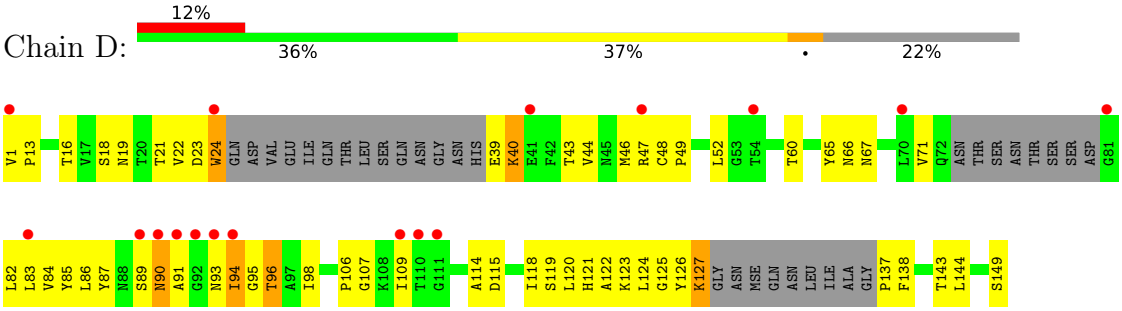


• Molecule 2: mature Fimbrial protein PapE



• Molecule 2: mature Fimbrial protein PapE

Chain D:


12%
36%
37%
22%
V1 P13 T16 V17 S18 N19 T20 T21 V22 D23 W24 GLN ASP VAL GLU ILE GLN THR LEU SER GLN ASN GLY ASN HIS E39 K40 E41 F42 T43 V44 N45 M46 R47 C48 P49 L52 G53 T54 T60 Y65 N66 N67 L70 V71 Q72 ASN THR SER ASN THR SER SER ASP G81
L82 L83 V84 Y85 L86 Y87 N88 S89 N90 A91 G92 N93 I94 G95 T96 A97 I98 P106 G107 K108 T109 T110 G111 A114 D115 I118 S119 L120 H121 A122 K123 L124 G125 Y126 K127 GLY ASN MSE GLN ASN LEU ILE ALA GLY P137 F138 T143 L144 S149

4 Data and refinement statistics (i)

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 28.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.9 (24.73-2.30) 91.0 (28.81-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [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)	0.31 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.37	0/1734	0.64	0/2349
1	C	0.37	0/1728	0.64	0/2342
2	B	0.34	0/889	0.61	0/1208
2	D	0.31	0/797	0.60	0/1083
All	All	0.35	0/5148	0.63	0/6982

There are no bond length outliers.

There are no bond angle outliers.

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	63	0
1	C	1696	0	1700	67	0
2	B	877	0	852	61	0
2	D	787	0	780	57	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	237	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 23.

All (237) 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
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:C:136:LYS:HZ3	1:C:185:ASN:HD22	1.29	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
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:29:LEU:HB3	1:A:95:PRO:HG2	1.70	0.74
1:A:136:LYS:HZ3	1:A:185:ASN:HB2	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:26:ASN:HD22	1:C:26:ASN:C	1.99	0.64
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HZ3	1:C:185:ASN:HB2	1.72	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
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
1:C:46:ILE:O	1:C:46:ILE:HG22	2.09	0.53
1:A:116:ARG:NH2	1:A:122:THR:HG21	2.23	0.53
2:D:90:ASN:HD21	2:D:96:THR:N	2.07	0.53
1:C:26:ASN:HD22	1:C:27:LYS:N	2.06	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
2:D:126:TYR:O	2:D:127:LYS:HB3	2.09	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: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
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
1:A:157:GLY:HA2	1:A:186:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:LEU:HD12	2:D:125:GLY:O	2.11	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
1:C:191:LEU:C	1:C:191:LEU:HD23	2.31	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:HD3	1:C:136:LYS:C	2.32	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: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
1:C:34:GLN:CD	1:C:93:ILE:HD11	2.33	0.49
2:B:41:GLU:HG2	2:B:121:HIS:HE1	1.75	0.49
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: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
1:C:99:LYS:CD	1:C:102:VAL:HG11	2.45	0.47
1:C:99:LYS:HB2	1:C:102:VAL:HG21	1.97	0.46
2:D:93:ASN:CG	2:D:94:ILE:H	2.17	0.46
1:A:3:SER:HB2	3:A:256:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:54:THR:O	2:B:55:MSE:C	2.53	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
1:C:136:LYS:NZ	1:C:185:ASN:ND2	2.62	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: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
1:A:38:GLU:HB3	1:A:42:GLN:HA	1.98	0.45
1:C:26:ASN:C	1:C:26:ASN:ND2	2.69	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:136:LYS:HZ3	1:C:185:ASN:ND2	2.05	0.45
2:B:42:PHE:CZ	2:B:120:LEU:HB2	2.53	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
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
2:D:18:SER:O	2:D:19:ASN:C	2.55	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:B:85:TYR:HB2	2:B:123:LYS:HB2	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:56:LYS:HB2	2:B:104:PHE:C	2.40	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
2:B:111:GLY:C	2:B:112:ASN:HD22	2.23	0.42
2:D:127:LYS:C	2:D:127:LYS:HD2	2.41	0.42
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
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
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:B:89:SER:HB3	2:B:119:SER:C	2.41	0.41
2:D:16:THR:OG1	2:D:47:ARG:HB2	2.21	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:27:LYS:C	1:C:28:GLN:HG3	2.41	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
1	C	213/224 (95%)	201 (94%)	12 (6%)	0	100 100
2	B	110/138 (80%)	95 (86%)	12 (11%)	3 (3%)	5 3
2	D	99/138 (72%)	89 (90%)	5 (5%)	5 (5%)	2 1
All	All	635/724 (88%)	588 (93%)	39 (6%)	8 (1%)	12 12

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 (i)

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%)	40 55
1	C	190/197 (96%)	182 (96%)	8 (4%)	30 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	97/113 (86%)	97 (100%)	0	100 100
2	D	86/113 (76%)	82 (95%)	4 (5%)	26 37
All	All	564/620 (91%)	546 (97%)	18 (3%)	39 54

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	123	ARG
1	A	136	LYS
1	A	176	ARG
1	A	208	ASN
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	197	TYR
1	C	208	ASN
1	C	215	LYS
2	D	24	TRP
2	D	115	ASP
2	D	127	LYS
2	D	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	80	GLN
1	A	89	ASN
1	A	131	GLN
1	A	179	GLN
1	A	185	ASN
1	A	208	ASN
2	B	45	ASN
2	B	63	ASN
2	B	112	ASN
2	B	121	HIS

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Mol	Chain	Res	Type
1	C	26	ASN
1	C	34	GLN
1	C	80	GLN
1	C	89	ASN
1	C	125	ASN
1	C	131	GLN
1	C	179	GLN
1	C	185	ASN
1	C	208	ASN
2	D	66	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides 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, 95^{th} 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%)	-0.02	4 (1%) 66 73	13, 34, 54, 74	0
1	C	212/224 (94%)	-0.01	3 (1%) 75 80	12, 34, 53, 65	0
2	B	116/138 (84%)	0.93	21 (18%) 1 1	17, 53, 74, 80	0
2	D	105/138 (76%)	0.88	17 (16%) 1 2	18, 54, 75, 83	0
All	All	645/724 (89%)	0.30	45 (6%) 16 21	12, 38, 69, 83	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	110	THR	6.7
2	B	79	SER	5.0
2	B	27	VAL	4.8
2	D	92	GLY	4.6
2	D	94	ILE	4.4
2	B	126	TYR	4.2
2	B	92	GLY	4.2
2	D	110	THR	4.0
2	B	138	PHE	3.9
2	D	89	SER	3.6
2	D	90	ASN	3.6
1	C	46	ILE	3.5
2	B	38	HIS	3.5
2	D	91	ALA	3.4
2	B	78	SER	3.4
2	B	37	ASN	3.2
2	B	82	LEU	3.2
2	B	26	ASP	3.1
2	D	109	ILE	3.1
1	A	167	GLU	3.1
2	B	109	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	72	GLN	3.0
2	B	25	GLN	2.9
2	B	93	ASN	2.9
1	A	98	GLU	2.7
1	C	167	GLU	2.5
2	B	80	ASP	2.5
2	D	24	TRP	2.4
2	B	24	TRP	2.4
1	A	45	ILE	2.3
2	D	111	GLY	2.3
2	D	47	ARG	2.2
2	D	41	GLU	2.2
2	B	137	PRO	2.2
2	D	93	ASN	2.2
2	D	1	VAL	2.2
2	D	70	LEU	2.1
1	C	101	ASN	2.1
2	B	36	GLY	2.1
1	A	182	LYS	2.1
2	D	81	GLY	2.1
2	B	70	LEU	2.1
2	B	88	ASN	2.0
2	D	83	LEU	2.0
2	D	54	THR	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 monosaccharides 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.