



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:33 PM GMT

PDB ID : 2UY6
Title : CRYSTAL STRUCTURE OF THE P PILUS ROD SUBUNIT PAPA
Authors : Verger, D.; Bullitt, E.; Hultgren, S.J.; Waksman, G.
Deposited on : 2007-04-02
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

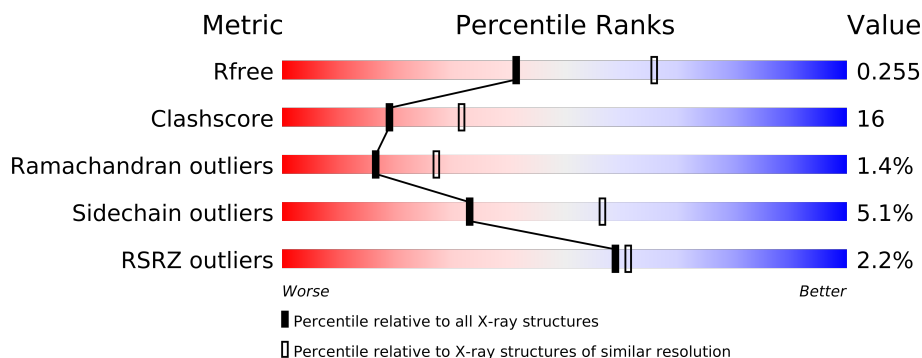
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	218	
2	B	163	
2	C	163	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3895 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PERIPLASMID CHAPERONE PAPD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	1
			1681	1062	289	325	5			

- Molecule 2 is a protein called PAP FIMBRIAL MAJOR PILIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	150	Total	C	N	O	S	0	0	0
			1043	649	173	218	3			
2	C	144	Total	C	N	O	S	0	0	0
			1016	630	170	213	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ASN	GLY	ENGINEERED MUTATION	UNP P04127
B	101	LEU	THR	ENGINEERED MUTATION	UNP P04127
C	15	ASN	GLY	ENGINEERED MUTATION	UNP P04127
C	101	LEU	THR	ENGINEERED MUTATION	UNP P04127

- Molecule 3 is water.

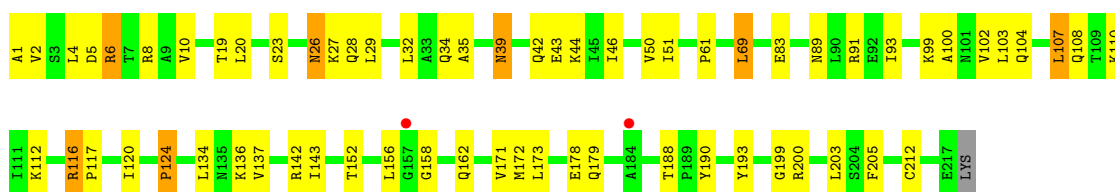
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	39	Total	O	0	0
			39	39		
3	C	35	Total	O	0	0
			35	35		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

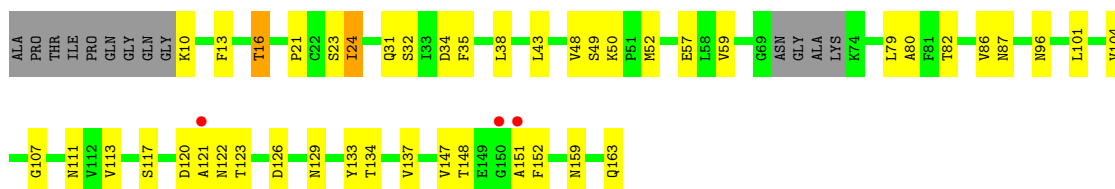
- Molecule 1: PERIPLASMID CHAPERONE PAPD PROTEIN

Chain A: 



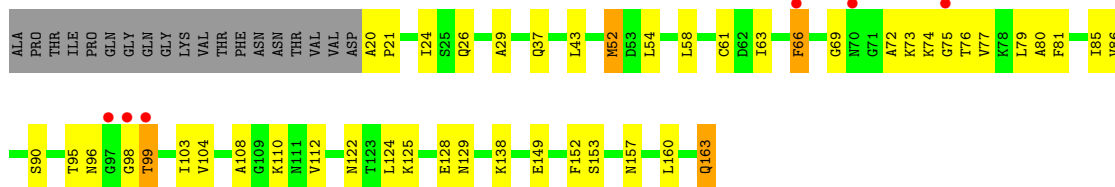
- Molecule 2: PAP FIMBRIAL MAJOR PILIN PROTEIN

Chain B: 



- Molecule 2: PAP FIMBRIAL MAJOR PILIN PROTEIN

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.10Å 73.56Å 80.48Å 90.00° 108.84° 90.00°	Depositor
Resolution (Å)	76.30 – 2.50 63.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (76.30-2.50) 99.5 (63.52-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.262 0.218 , 0.255	Depositor DCC
R_{free} test set	1300 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25531 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3895	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 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0/1716	0.64	0/2337
2	B	0.35	0/1056	0.61	0/1436
2	C	0.34	0/1029	0.64	0/1393
All	All	0.36	0/3801	0.63	0/5166

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	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	206	ILE	CB

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1681	0	1656	63	0
2	B	1043	0	971	42	0
2	C	1016	0	969	35	0
3	A	81	0	0	1	0
3	B	39	0	0	4	0
3	C	35	0	0	1	0
All	All	3895	0	3596	121	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (121) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:VAL:HG21	1:A:179:GLN:NE2	1.88	0.87
2:C:125:LYS:H	2:C:129:ASN:HD21	1.23	0.84
1:A:39:ASN:ND2	1:A:43:GLU:H	1.73	0.84
1:A:171:VAL:HG21	1:A:179:GLN:HE22	1.45	0.80
2:B:16:THR:HG22	2:C:37:GLN:HA	1.67	0.77
1:A:39:ASN:HD21	1:A:43:GLU:H	1.31	0.76
1:A:107:LEU:HB2	2:B:24:ILE:HD12	1.68	0.75
1:A:44:LYS:HE2	1:A:46:ILE:HD11	1.68	0.74
1:A:112:LYS:HD3	1:A:172:MET:HE1	1.69	0.72
1:A:104:GLN:HG2	2:B:32:SER:HB3	1.72	0.71
1:A:171:VAL:CG2	1:A:179:GLN:HE22	2.05	0.69
2:C:20:ALA:HB3	2:C:21:PRO:HD3	1.75	0.68
1:A:10:VAL:HG13	1:A:116:ARG:NH2	2.08	0.67
2:C:98:GLY:HA3	2:C:152:PHE:HE2	1.59	0.67
1:A:107:LEU:HD22	1:A:108:GLN:N	2.10	0.66
2:B:50:LYS:HB3	2:B:52:MET:HE2	1.77	0.66
1:A:42:GLN:OE1	1:A:110:LYS:HE2	1.96	0.66
1:A:34:GLN:HE21	1:A:91:ARG:HD2	1.59	0.66
1:A:6:ARG:HG3	1:A:8:ARG:O	1.96	0.65
1:A:102:VAL:HG22	2:B:32:SER:HB2	1.78	0.65
2:B:159:ASN:HB3	3:B:2037:HOH:O	1.95	0.65
2:C:85:ILE:HG21	2:C:90:SER:HA	1.79	0.64
1:A:34:GLN:NE2	1:A:91:ARG:HD2	2.13	0.64
2:C:76:THR:HA	2:C:122:ASN:O	1.97	0.64
1:A:102:VAL:CG2	2:B:32:SER:HB2	2.28	0.63
1:A:26:ASN:ND2	1:A:29:LEU:H	1.95	0.63
1:A:32:LEU:HB2	1:A:93:ILE:HB	1.81	0.62
2:B:57:GLU:HG2	2:B:59:VAL:HG13	1.83	0.58
1:A:1:ALA:H1	2:B:31:GLN:HE22	1.52	0.57
1:A:1:ALA:N	2:B:31:GLN:HE22	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:81:PHE:CD1	2:C:112:VAL:HG11	2.39	0.57
1:A:34:GLN:HE22	1:A:91:ARG:HH21	1.53	0.57
1:A:143:ILE:HB	1:A:173:LEU:HD21	1.86	0.57
1:A:107:LEU:HB2	2:B:24:ILE:CD1	2.36	0.56
2:C:98:GLY:O	2:C:99:THR:HG23	2.06	0.56
2:C:69:GLY:HA3	3:C:2018:HOH:O	2.04	0.56
1:A:26:ASN:ND2	1:A:28:GLN:H	2.03	0.56
1:A:100:ALA:HB1	2:B:151:ALA:HB1	1.88	0.55
2:C:104:VAL:HG21	2:C:138:LYS:HE3	1.89	0.54
1:A:8:ARG:NH2	2:B:163:GLN:O	2.35	0.54
1:A:136:LYS:HD3	1:A:137:VAL:N	2.23	0.54
2:C:95:THR:HG21	2:C:152:PHE:HB3	1.91	0.53
2:C:85:ILE:CG2	2:C:90:SER:HA	2.38	0.53
1:A:117:PRO:HD2	1:A:120:ILE:HD11	1.91	0.53
2:B:48:VAL:HG12	2:B:49:SER:O	2.09	0.52
2:B:120:ASP:OD1	2:B:123:THR:HG23	2.09	0.52
1:A:173:LEU:HD12	1:A:173:LEU:N	2.24	0.52
2:C:76:THR:OG1	2:C:163:GLN:HB2	2.10	0.52
1:A:193:TYR:O	1:A:200:ARG:HA	2.11	0.51
2:B:79:LEU:C	2:B:79:LEU:HD23	2.31	0.51
2:C:77:VAL:HB	2:C:124:LEU:HD11	1.92	0.50
1:A:158:GLY:H	1:A:162:GLN:NE2	2.10	0.50
2:B:101:LEU:HD21	2:B:147:VAL:HG13	1.93	0.49
2:B:96:ASN:O	2:B:152:PHE:HA	2.12	0.49
1:A:99:LYS:HD3	2:B:34:ASP:HB2	1.95	0.49
2:B:10:LYS:N	2:C:29:ALA:O	2.45	0.48
2:B:10:LYS:HB3	2:C:157:ASN:ND2	2.28	0.48
1:A:6:ARG:O	2:B:21:PRO:HG3	2.14	0.48
2:C:103:ILE:N	2:C:103:ILE:HD12	2.29	0.48
2:B:113:VAL:HG21	2:B:117:SER:HB2	1.95	0.48
1:A:20:LEU:CD1	1:A:69:LEU:HD22	2.43	0.48
2:C:61:CYS:HB3	2:C:63:ILE:CD1	2.44	0.47
2:B:52:MET:O	2:B:134:THR:HA	2.15	0.47
2:C:24:ILE:HD11	2:C:160:LEU:HD11	1.97	0.47
1:A:107:LEU:CB	2:B:24:ILE:HD12	2.42	0.47
2:C:108:ALA:O	2:C:110:LYS:HG3	2.14	0.47
1:A:136:LYS:HD3	1:A:137:VAL:H	1.80	0.47
2:B:113:VAL:CG2	2:B:117:SER:HB2	2.45	0.47
1:A:142:ARG:HD2	1:A:178:GLU:OE2	2.15	0.47
2:C:24:ILE:HD13	2:C:58:LEU:CD2	2.46	0.46
2:C:98:GLY:HA3	2:C:152:PHE:CE2	2.45	0.46
1:A:112:LYS:HD3	1:A:172:MET:CE	2.41	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:75:GLY:O	2:C:124:LEU:HB2	2.15	0.46
1:A:1:ALA:HB1	1:A:26:ASN:HB2	1.97	0.46
2:C:63:ILE:N	2:C:63:ILE:HD12	2.31	0.46
2:C:96:ASN:N	2:C:96:ASN:HD22	2.14	0.46
2:B:38:LEU:HB3	2:B:43:LEU:HD21	1.98	0.45
1:A:50:VAL:O	1:A:51:ILE:HD12	2.16	0.45
2:B:35:PHE:CD2	2:B:137:VAL:HG23	2.51	0.45
1:A:134:LEU:HB2	1:A:212:CYS:HB2	1.98	0.45
1:A:83:GLU:OE1	1:A:116:ARG:NH2	2.50	0.44
2:B:79:LEU:HB3	2:B:121:ALA:HB2	1.98	0.44
2:C:125:LYS:H	2:C:129:ASN:ND2	2.03	0.44
1:A:107:LEU:HD13	3:A:2049:HOH:O	2.17	0.44
1:A:134:LEU:HD13	1:A:205:PHE:CE2	2.52	0.44
1:A:2:VAL:HA	1:A:23:SER:O	2.17	0.44
1:A:188:THR:O	1:A:190:TYR:CD1	2.70	0.44
1:A:91:ARG:HD3	3:B:2036:HOH:O	2.16	0.44
2:B:79:LEU:HD23	2:B:80:ALA:N	2.33	0.44
2:C:96:ASN:ND2	2:C:96:ASN:N	2.65	0.44
2:B:57:GLU:HG3	2:B:129:ASN:ND2	2.33	0.43
1:A:156:LEU:HA	1:A:190:TYR:O	2.18	0.43
1:A:10:VAL:HG13	1:A:116:ARG:HH21	1.81	0.43
1:A:152:THR:OG1	1:A:172:MET:HE3	2.19	0.43
1:A:26:ASN:HD22	1:A:28:GLN:H	1.66	0.43
2:C:52:MET:CE	2:C:52:MET:HA	2.49	0.42
1:A:34:GLN:NE2	1:A:91:ARG:HH21	2.16	0.42
1:A:35:ALA:HA	1:A:89:ASN:O	2.20	0.42
1:A:39:ASN:HD22	1:A:39:ASN:C	2.21	0.42
2:B:86:VAL:O	2:B:87:ASN:C	2.58	0.42
2:C:79:LEU:HD23	2:C:80:ALA:N	2.34	0.42
2:B:48:VAL:CG1	2:B:49:SER:N	2.81	0.42
1:A:19:THR:C	1:A:20:LEU:HD12	2.40	0.42
2:C:21:PRO:HG3	2:C:66:PHE:CE2	2.55	0.42
2:B:104:VAL:HG12	3:B:2021:HOH:O	2.20	0.41
1:A:112:LYS:NZ	1:A:172:MET:HE3	2.36	0.41
1:A:116:ARG:HB2	1:A:116:ARG:HH21	1.85	0.41
2:B:13:PHE:O	2:C:153:SER:HA	2.20	0.41
2:B:82:THR:HB	2:B:159:ASN:HD21	1.85	0.41
2:B:107:GLY:HA2	2:B:133:TYR:CD2	2.56	0.41
2:B:16:THR:CG2	2:C:37:GLN:HG3	2.51	0.41
1:A:5:ASP:OD1	1:A:6:ARG:CD	2.69	0.41
1:A:8:ARG:HH22	2:B:163:GLN:C	2.20	0.41
2:C:24:ILE:HD11	2:C:160:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:199:GLY:N	2:C:149:GLU:HG3	2.36	0.41
1:A:27:LYS:C	1:A:61:PRO:HB3	2.42	0.40
2:B:10:LYS:HE3	3:B:2002:HOH:O	2.21	0.40
2:B:111:ASN:HA	2:B:111:ASN:HD22	1.74	0.40
1:A:27:LYS:HB2	1:A:28:GLN:NE2	2.36	0.40
2:C:85:ILE:HG22	2:C:86:VAL:N	2.37	0.40
2:B:23:SER:HB3	2:B:59:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/218 (99%)	202 (94%)	12 (6%)	1 (0%)	38	60
2	B	146/163 (90%)	137 (94%)	7 (5%)	2 (1%)	16	27
2	C	142/163 (87%)	131 (92%)	7 (5%)	4 (3%)	8	10
All	All	503/544 (92%)	470 (93%)	26 (5%)	7 (1%)	16	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	122	ASN
2	C	73	LYS
2	B	126	ASP
2	C	72	ALA
1	A	124	PRO
2	C	74	LYS
2	C	99	THR

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	184/194 (95%)	174 (95%)	10 (5%)	31	53
2	B	106/125 (85%)	103 (97%)	3 (3%)	56	82
2	C	105/125 (84%)	98 (93%)	7 (7%)	23	40
All	All	395/444 (89%)	375 (95%)	20 (5%)	33	57

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	ARG
1	A	26	ASN
1	A	39	ASN
1	A	69	LEU
1	A	103	LEU
1	A	107	LEU
1	A	116	ARG
1	A	124	PRO
1	A	203	LEU
2	B	16	THR
2	B	24	ILE
2	B	148	THR
2	C	26	GLN
2	C	43	LEU
2	C	52	MET
2	C	54	LEU
2	C	66	PHE
2	C	128	GLU
2	C	163	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	28	GLN
1	A	34	GLN
1	A	39	ASN
1	A	89	ASN
1	A	131	GLN

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Mol	Chain	Res	Type
1	A	162	GLN
1	A	179	GLN
1	A	208	ASN
2	B	31	GLN
2	B	111	ASN
2	C	37	GLN
2	C	96	ASN
2	C	129	ASN
2	C	132	HIS
2	C	163	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	217/218 (99%)	0.01	2 (0%) 81 82	16, 30, 61, 71	0
2	B	150/163 (92%)	0.06	3 (2%) 62 64	20, 36, 68, 77	0
2	C	144/163 (88%)	0.22	6 (4%) 35 36	22, 41, 71, 91	0
All	All	511/544 (93%)	0.09	11 (2%) 59 61	16, 35, 66, 91	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	75	GLY	4.4
2	C	70	ASN	3.8
1	A	184	ALA	2.8
2	C	98	GLY	2.5
2	B	121	ALA	2.5
1	A	157	GLY	2.4
2	B	150	GLY	2.3
2	C	99	THR	2.1
2	C	66	PHE	2.1
2	B	151	ALA	2.1
2	C	97	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.