WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2024 – 08:26 AM EST

PDB ID	:	4JDM
Title	:	Secreted Chlamydial Protein PGP3, full-length
Authors	:	Galaleldeen, A.; Taylor, A.B.; Chen, D.; Holloway, S.P.; Zhong, G.; Hart, P.J.
Deposited on	:	2013-02-25
Resolution	:	3.10 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.10 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.
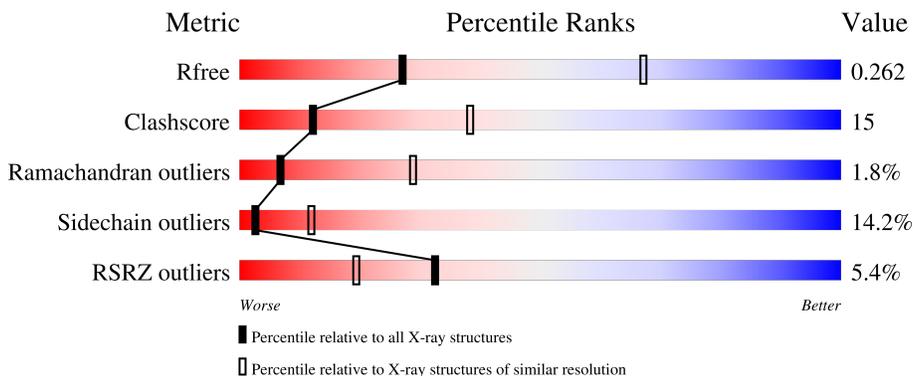
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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	269	5% / 63% / 31%
1	B	269	3% / 58% / 37%
1	C	269	3% / 64% / 31%
1	D	269	6% / 63% / 30%
1	E	269	5% / 58% / 33% / 6%

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Mol	Chain	Length	Quality of chain
1	F	269	

9%

62%

33%

6%

2 Entity composition (i)

There is only 1 type of molecule in this entry. The entry contains 11712 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 Virulence plasmid protein pGP3-D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	Se	0	0	0
			1939	1215	317	399	4	4			
1	B	263	Total	C	N	O	S	Se	0	0	0
			1941	1217	317	398	4	5			
1	C	269	Total	C	N	O	S	Se	0	0	0
			1976	1238	323	406	4	5			
1	D	263	Total	C	N	O	S	Se	0	0	0
			1939	1215	317	399	4	4			
1	E	263	Total	C	N	O	S	Se	0	0	0
			1941	1217	317	398	4	5			
1	F	269	Total	C	N	O	S	Se	0	0	0
			1976	1238	323	406	4	5			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP D7DHH5
A	-3	PRO	-	expression tag	UNP D7DHH5
A	-2	LEU	-	expression tag	UNP D7DHH5
A	-1	GLY	-	expression tag	UNP D7DHH5
A	0	SER	-	expression tag	UNP D7DHH5
B	-4	GLY	-	expression tag	UNP D7DHH5
B	-3	PRO	-	expression tag	UNP D7DHH5
B	-2	LEU	-	expression tag	UNP D7DHH5
B	-1	GLY	-	expression tag	UNP D7DHH5
B	0	SER	-	expression tag	UNP D7DHH5
C	-4	GLY	-	expression tag	UNP D7DHH5
C	-3	PRO	-	expression tag	UNP D7DHH5
C	-2	LEU	-	expression tag	UNP D7DHH5
C	-1	GLY	-	expression tag	UNP D7DHH5
C	0	SER	-	expression tag	UNP D7DHH5
D	-4	GLY	-	expression tag	UNP D7DHH5
D	-3	PRO	-	expression tag	UNP D7DHH5

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| Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	expression tag	UNP D7DHH5
D	-1	GLY	-	expression tag	UNP D7DHH5
D	0	SER	-	expression tag	UNP D7DHH5
E	-4	GLY	-	expression tag	UNP D7DHH5
E	-3	PRO	-	expression tag	UNP D7DHH5
E	-2	LEU	-	expression tag	UNP D7DHH5
E	-1	GLY	-	expression tag	UNP D7DHH5
E	0	SER	-	expression tag	UNP D7DHH5
F	-4	GLY	-	expression tag	UNP D7DHH5
F	-3	PRO	-	expression tag	UNP D7DHH5
F	-2	LEU	-	expression tag	UNP D7DHH5
F	-1	GLY	-	expression tag	UNP D7DHH5
F	0	SER	-	expression tag	UNP D7DHH5

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: Virulence plasmid protein pGP3-D
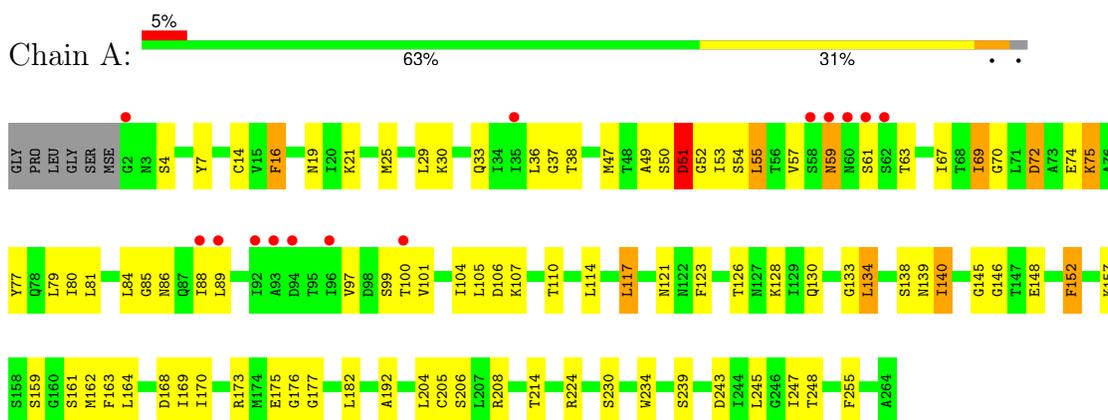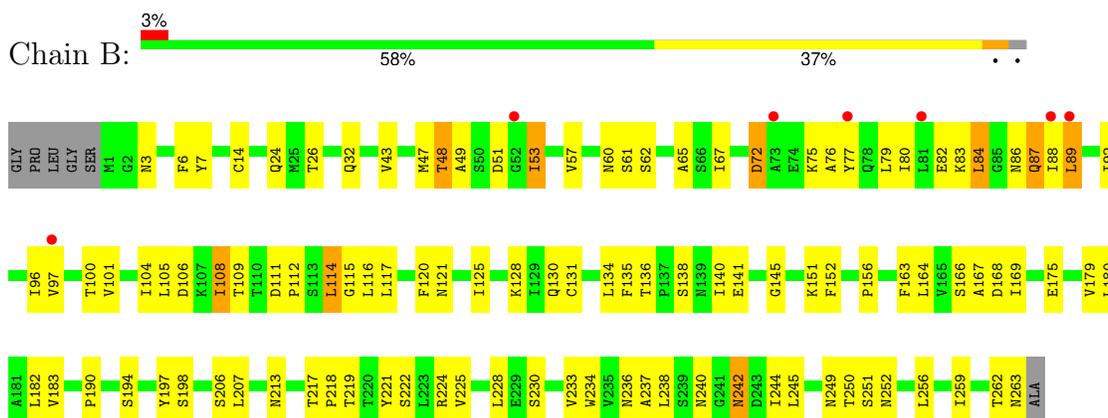
Chain A:

- Molecule 1: Virulence plasmid protein pGP3-D

Chain B:

- Molecule 1: Virulence plasmid protein pGP3-D

Chain C:
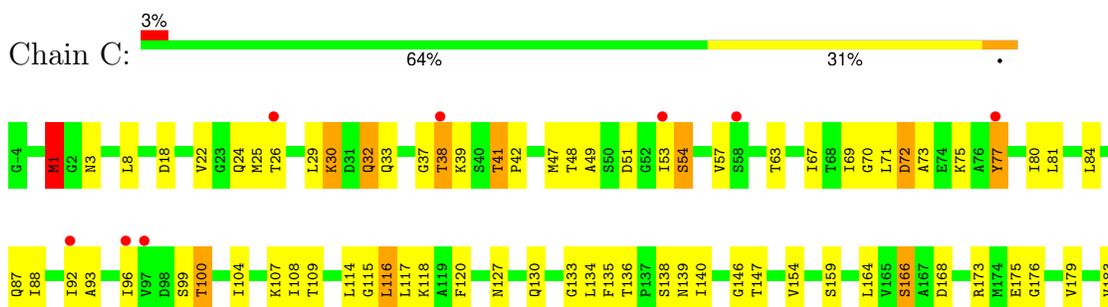
• Molecule 1: Virulence plasmid protein pGP3-D

Chain D:

• Molecule 1: Virulence plasmid protein pGP3-D

Chain E:

• Molecule 1: Virulence plasmid protein pGP3-D

Chain F:
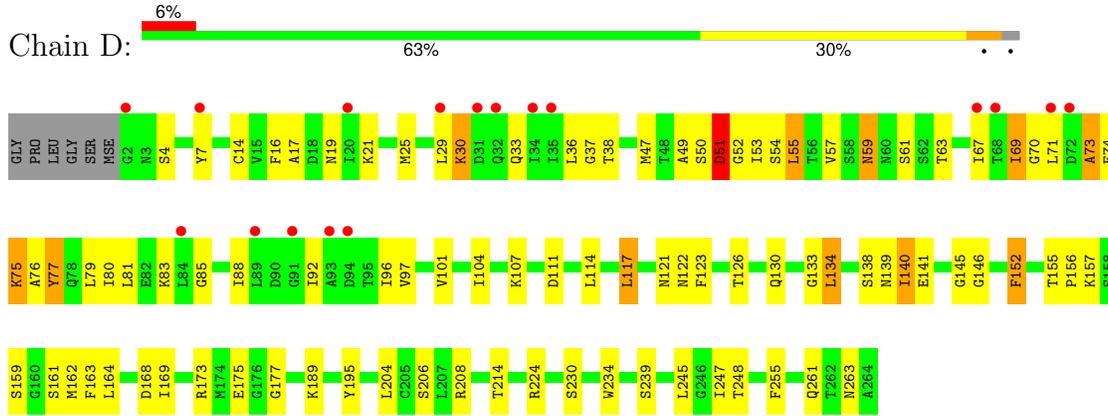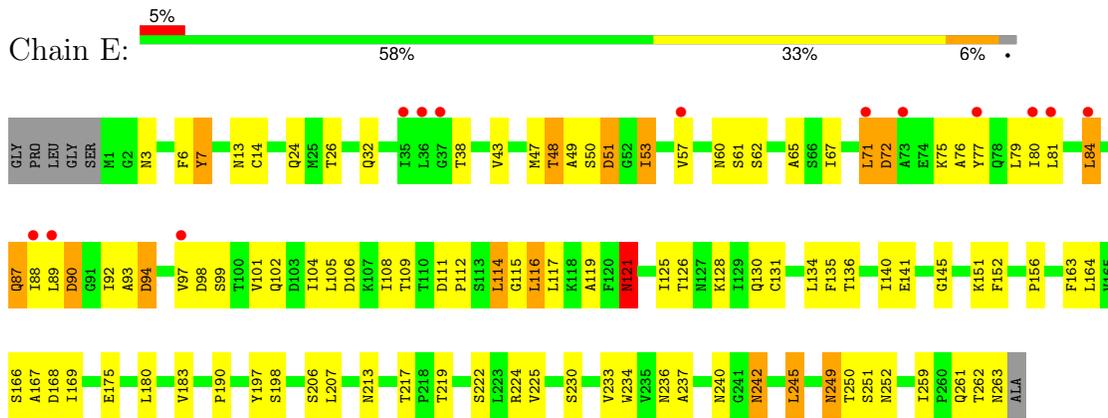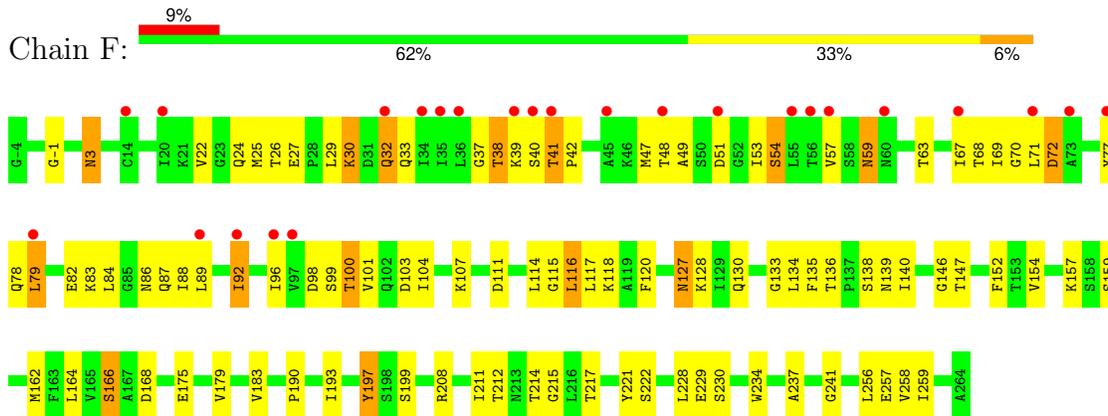
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	188.70Å 223.79Å 79.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.12 – 3.10 48.12 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.4 (48.12-3.10) 90.7 (48.12-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.231 , 0.264 0.234 , 0.262	Depositor DCC
R_{free} test set	2828 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 41.9	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11712	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5988e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1   Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.59	1/1960 (0.1%)	0.73	0/2660
1	B	0.58	2/1962 (0.1%)	0.73	0/2663
1	C	0.57	0/1997	0.73	0/2708
1	D	0.56	0/1960	0.72	0/2660
1	E	0.55	1/1962 (0.1%)	0.72	1/2663 (0.0%)
1	F	0.56	0/1997	0.72	0/2708
All	All	0.57	4/11838 (0.0%)	0.73	1/16062 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	ASN	CG-OD1	-5.96	1.10	1.24
1	B	121	ASN	CG-ND2	-5.76	1.18	1.32
1	A	205	CYS	CB-SG	-5.49	1.72	1.81
1	E	121	ASN	CG-ND2	-5.22	1.19	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	71	LEU	CB-CG-CD2	5.44	120.25	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1939	0	1957	76	0
1	B	1941	0	1964	64	0
1	C	1976	0	1998	57	0
1	D	1939	0	1957	73	0
1	E	1941	0	1964	79	0
1	F	1976	0	1998	61	0
All	All	11712	0	11838	361	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 15.

The worst 5 of 361 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:123:PHE:CE2	1:A:152:PHE:HB3	1.71	1.25
1:D:123:PHE:CE2	1:D:152:PHE:HB3	1.74	1.21
1:A:123:PHE:HE2	1:A:152:PHE:HB3	1.11	0.96
1:A:123:PHE:CD2	1:A:152:PHE:HB3	2.05	0.92
1:E:156:PRO:HG3	1:E:213:ASN:HD22	1.35	0.92

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	261/269 (97%)	244 (94%)	12 (5%)	5 (2%)	6	27
1	B	261/269 (97%)	245 (94%)	13 (5%)	3 (1%)	12	39
1	C	267/269 (99%)	243 (91%)	18 (7%)	6 (2%)	5	24
1	D	261/269 (97%)	243 (93%)	13 (5%)	5 (2%)	6	27
1	E	261/269 (97%)	241 (92%)	17 (6%)	3 (1%)	12	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	267/269 (99%)	240 (90%)	21 (8%)	6 (2%)	5	24
All	All	1578/1614 (98%)	1456 (92%)	94 (6%)	28 (2%)	7	29

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	LEU
1	C	175	GLU
1	D	114	LEU
1	F	175	GLU
1	A	85	GLY

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	223/222 (100%)	193 (86%)	30 (14%)	3	13
1	B	224/222 (101%)	189 (84%)	35 (16%)	2	9
1	C	227/222 (102%)	195 (86%)	32 (14%)	3	12
1	D	223/222 (100%)	197 (88%)	26 (12%)	4	18
1	E	224/222 (101%)	191 (85%)	33 (15%)	2	11
1	F	227/222 (102%)	192 (85%)	35 (15%)	2	9
All	All	1348/1332 (101%)	1157 (86%)	191 (14%)	2	12

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	140	ILE
1	E	166	SER
1	D	169	ILE
1	E	72	ASP
1	E	242	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	139	ASN
1	F	32	GLN
1	E	213	ASN
1	C	139	ASN
1	E	249	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 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(Å²)	Q<0.9
1	A	259/269 (96%)	-0.04	14 (5%)	32	19	22, 51, 133, 151	0
1	B	258/269 (95%)	-0.04	7 (2%)	56	36	26, 49, 141, 158	0
1	C	264/269 (98%)	0.04	9 (3%)	48	28	22, 53, 136, 146	0
1	D	259/269 (96%)	0.07	17 (6%)	26	15	23, 54, 145, 152	0
1	E	258/269 (95%)	0.11	13 (5%)	35	21	31, 55, 145, 159	0
1	F	264/269 (98%)	0.15	25 (9%)	15	9	25, 52, 143, 152	0
All	All	1562/1614 (96%)	0.05	85 (5%)	32	19	22, 53, 142, 159	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	THR	4.6
1	F	55	LEU	4.5
1	D	71	LEU	4.1
1	A	92	ILE	4.0
1	F	35	ILE	4.0

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.