WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2024 – 09:26 AM EST

PDB ID	:	4EO2
Title	:	Structure of the bacteriophage C1 tail knob protein, gp12
Authors	:	Aksyuk, A.A.; Rossmann, M.G.
Deposited on	:	2012-04-13
Resolution	:	3.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

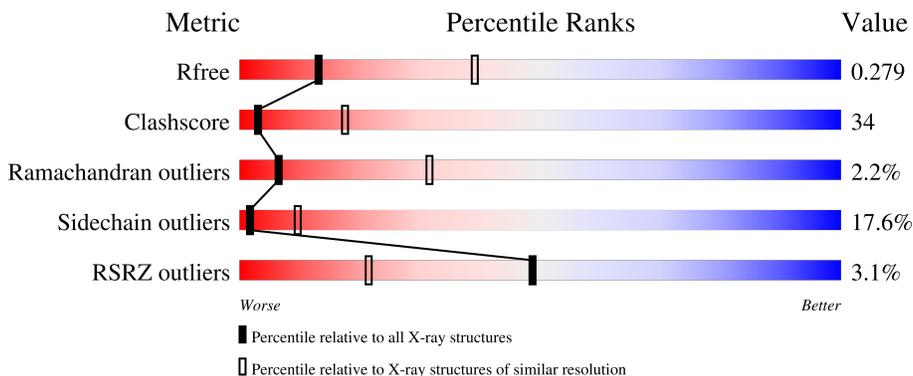|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.01 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.
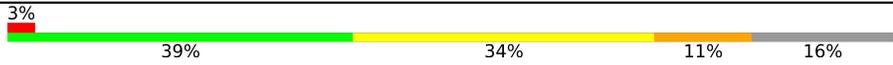
Metric	Percentile Ranks	Value
Rfree		0.279
Clashscore		34
Ramachandran outliers		2.2%
Sidechain outliers		17.6%
RSRZ outliers		3.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	583	2% 42% 30% 11% · 16%
1	B	583	.% 42% 31% 10% · 16%
1	C	583	3% 42% 30% 11% · 16%
1	D	583	4% 39% 34% 11% 16%
1	E	583	3% 39% 33% 11% · 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	583	3% ▮ 39% 34% 11% 16%

2　Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 23688 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 Major tail protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	B	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	C	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	D	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	E	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			
1	F	488	Total	C	N	O	S	0	0	0
			3948	2504	665	761	18			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	expression tag	UNP Q7Y3F0
A	576	LEU	-	expression tag	UNP Q7Y3F0
A	577	GLU	-	expression tag	UNP Q7Y3F0
A	578	HIS	-	expression tag	UNP Q7Y3F0
A	579	HIS	-	expression tag	UNP Q7Y3F0
A	580	HIS	-	expression tag	UNP Q7Y3F0
A	581	HIS	-	expression tag	UNP Q7Y3F0
A	582	HIS	-	expression tag	UNP Q7Y3F0
A	583	HIS	-	expression tag	UNP Q7Y3F0
B	575	SER	-	expression tag	UNP Q7Y3F0
B	576	LEU	-	expression tag	UNP Q7Y3F0
B	577	GLU	-	expression tag	UNP Q7Y3F0
B	578	HIS	-	expression tag	UNP Q7Y3F0
B	579	HIS	-	expression tag	UNP Q7Y3F0
B	580	HIS	-	expression tag	UNP Q7Y3F0
B	581	HIS	-	expression tag	UNP Q7Y3F0
B	582	HIS	-	expression tag	UNP Q7Y3F0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	583	HIS	-	expression tag	UNP Q7Y3F0
C	575	SER	-	expression tag	UNP Q7Y3F0
C	576	LEU	-	expression tag	UNP Q7Y3F0
C	577	GLU	-	expression tag	UNP Q7Y3F0
C	578	HIS	-	expression tag	UNP Q7Y3F0
C	579	HIS	-	expression tag	UNP Q7Y3F0
C	580	HIS	-	expression tag	UNP Q7Y3F0
C	581	HIS	-	expression tag	UNP Q7Y3F0
C	582	HIS	-	expression tag	UNP Q7Y3F0
C	583	HIS	-	expression tag	UNP Q7Y3F0
D	575	SER	-	expression tag	UNP Q7Y3F0
D	576	LEU	-	expression tag	UNP Q7Y3F0
D	577	GLU	-	expression tag	UNP Q7Y3F0
D	578	HIS	-	expression tag	UNP Q7Y3F0
D	579	HIS	-	expression tag	UNP Q7Y3F0
D	580	HIS	-	expression tag	UNP Q7Y3F0
D	581	HIS	-	expression tag	UNP Q7Y3F0
D	582	HIS	-	expression tag	UNP Q7Y3F0
D	583	HIS	-	expression tag	UNP Q7Y3F0
E	575	SER	-	expression tag	UNP Q7Y3F0
E	576	LEU	-	expression tag	UNP Q7Y3F0
E	577	GLU	-	expression tag	UNP Q7Y3F0
E	578	HIS	-	expression tag	UNP Q7Y3F0
E	579	HIS	-	expression tag	UNP Q7Y3F0
E	580	HIS	-	expression tag	UNP Q7Y3F0
E	581	HIS	-	expression tag	UNP Q7Y3F0
E	582	HIS	-	expression tag	UNP Q7Y3F0
E	583	HIS	-	expression tag	UNP Q7Y3F0
F	575	SER	-	expression tag	UNP Q7Y3F0
F	576	LEU	-	expression tag	UNP Q7Y3F0
F	577	GLU	-	expression tag	UNP Q7Y3F0
F	578	HIS	-	expression tag	UNP Q7Y3F0
F	579	HIS	-	expression tag	UNP Q7Y3F0
F	580	HIS	-	expression tag	UNP Q7Y3F0
F	581	HIS	-	expression tag	UNP Q7Y3F0
F	582	HIS	-	expression tag	UNP Q7Y3F0
F	583	HIS	-	expression tag	UNP Q7Y3F0

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: Major tail protein

Chain A:

• Molecule 1: Major tail protein

Chain B:

• Molecule 1: Major tail protein

• Molecule 1: Major tail protein

V553 R554 L555 E559 S560 I563 N564 N565 T566 V567 V568 N569 N570 V571 I572 I573 LYS SER LEU HIS HIS HIS HIS HIS

• Molecule 1: Major tail protein

Chain D:

4%

39%   34%   11%   16%

MET THR L3 S4 K5 I6 K7 L8 F9 Y10 N11 T12 P13 F14 N15 N16 M17 Q18 F23 N24 S25 N26 E27 E28 R29 D30 F37 D38 V39 H40 E41 F42 T43 S44 T45 F46 N47 Y48 R49 ASN MET LYS G53 V54 L55 R56 V57 T58 I59 D60 L61 V62 R65 S66 C67 F68 E69

Q70 L71 M72 G73 V74 N75 Y76 C77 Q78 V79 Q80 Y81 I82 Q83 R86 V87 E88 Y89 L90 F91 V92 T93 D94 I95 L98 C103 E104 L105 S106 L107 V108 P109 D110 V111 V112 M113 T114 Y115 T116 Q117 V120 L121 N122 T123 L124 V127 N128 V129 I130 H133 Y134 T135 Q136

I146 R147 S148 V152 L153 A154 T155 S156 T157 M158 R159 I163 K164 S165 E172 Y173 I174 L175 T176 I177 N180 L181 R182 K183 S184 F185 E189 K190 P191 S199 T200 H201 D202 G203 I204 N206 M210 Y211 W212 F213 N214 D215 Y216 E217 K220 E221 D224 Y225 L226 T227

G228 Y229 Q233 I236 V239 S244 G245 F246 I247 K248 Q249 E250 E256 P257 V258 N259 G260 L263 S264 K267 S274 N275 Q276 K277 D278 F279 I282 D285 Y286 Q287 S288 L289 M290 F291 T292 L293 G294 L295 N299 D300 K301 H302 L303 L304 R305 P306 N307 I308 V309

T310 A311 E312 L313 T314 D315 Y316 R320 L321 P322 I323 D324 L325 S326 T330 N331 V338 T339 K347 Y348 Y349 V350 K351 N352 Y353 R356 G357 N358 N359 V360 Y363 I364 D365 L368 T369 I370 N371 D374 T375 I376 V380 D381 SER GLY GLU LEU GLY LYS ALA ASN SER

ALA TYR SER GLU LEU SER ASN SER ARG GLN MET SER SER ARG ASN THR VAL LEU ASP ASP ALA SER VAL LYS ASP ARG LEU PHE ASN ALA ILE SER LEU GLY LEU SER ILE LYS SER ALA LEU GLU SER GLY PHE ASN GLU TYR GLU HIS TYR ARG ASP GLN LYS

ALA GLN PHE LYS GLN MET ASP ALA LEU PRO ASN A462 I463 Y470 A471 P472 K475 Q476 D477 K478 F479 L483 R484 L485 G486 R487 I488 S489 Q490 D491 E492 L493 N494 N495 V496 K497 K498 Y499 M502 D509 Y510 S511 T512 K513 L514 S515 D516 I517 T518 S519 M520 N524 W525 V526

Q527 F528 K529 G530 I531 W532 T533 L534 V537 D538 T539 G540 H541 M542 N543 M544 L545 R546 A547 L548 F549 E550 A551 G552 V553 R554 L555 E559 S560 D561 M562 I563 N564 N565 T566 V567 V568 N569 N570 V571 I572 I573 LYS SER LEU HIS HIS HIS HIS HIS

• Molecule 1: Major tail protein

Chain E:

3%

39%   33%   11%   •   16%

MET THR L3 S4 K5 I6 K7 L8 F9 Y10 N11 T12 P13 F14 N15 N16 M17 Q18 L21 H22 F23 N26 R29 D30 F37 D38 V39 H40 E41 F42 T43 S44 T45 F46 N47 Y48 R49 ASN MET LYS G53 V54 L55 R56 V57 T58 I59 D60 L61 V62 R65 S66 C67 F68 E69

Q70 L71 M72 G73 V74 N75 Y76 C77 Q78 V79 Q80 Y81 Y89 L90 F91 V92 T93 D94 I95 Q96 Q97 L98 V102 C103 E104 L105 S106 L107 V108 P109 D110 V111 Y115 T116 Q117 V120 L121 N122 T123 L124 V127 N128 V129 I130 H133 Y134 T135 Q136 T137 E138 I146 R147 S148

V152 L153 A154 T155 S156 T157 M158 R159 I163 K164 S165 T169 Q170 L171 E172 Y173 I174 L175 T176 I177 N180 L181 R182 K183 S184 F185 E189 K190 P191 S199 T200 H201 D202 G203 I204 Y205 N206 P207 Y208 D209 M210 Y211 W212 F213 N214 D215 Y216 E217 S218 L219 K220 E221 D224

Y225 L226 T227 G228 Y229 Q233 I236 V239 S244 G245 F246 I247 K248 Q249 E256 P257 V258 N259 L263 S264 K267 S274 N275 Q276 K277 D278 I282 D285 Y286 Q287 S288 L289 M290 F291 T292 L293 G294 L295 N296 N299 D300 K301 H302 L303 L304 R305 P306 N307 I308

• Molecule 1: Major tail protein

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	205.61Å　209.64Å　102.97Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	50.00　–　3.01 50.00　–　3.01	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-3.01) 98.1 (50.00-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.21 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238　,　0.282 0.235　,　0.279	Depositor DCC
R_{free} test set	4390 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	75.3	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 98.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23688	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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 (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	0.90	0/4030	0.97	4/5464 (0.1%)
1	B	0.89	3/4030 (0.1%)	0.94	3/5464 (0.1%)
1	C	0.80	1/4030 (0.0%)	0.89	2/5464 (0.0%)
1	D	0.77	0/4030	0.88	1/5464 (0.0%)
1	E	0.81	2/4030 (0.0%)	0.90	1/5464 (0.0%)
1	F	0.87	1/4030 (0.0%)	0.94	1/5464 (0.0%)
All	All	0.84	7/24180 (0.0%)	0.92	12/32784 (0.0%)

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	0	2
1	B	0	3
1	C	0	2
1	D	0	3
1	E	0	3
1	F	0	2
All	All	0	15

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	ASN	CG-ND2	-9.03	1.10	1.32
1	B	299	ASN	CG-OD1	-7.23	1.08	1.24
1	C	299	ASN	CG-ND2	-6.63	1.16	1.32
1	F	492	GLU	CG-CD	5.74	1.60	1.51
1	E	551	ALA	CA-CB	-5.69	1.40	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	304	LEU	CB-CG-CD1	-8.30	96.89	111.00
1	B	374	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	C	304	LEU	CB-CG-CD1	-5.99	100.81	111.00
1	B	304	LEU	CB-CG-CD1	-5.98	100.83	111.00
1	D	365	ASP	CB-CG-OD2	5.83	123.55	118.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	ARG	Peptide
1	A	71	LEU	Peptide
1	B	183	LYS	Peptide
1	B	356	ARG	Peptide
1	B	71	LEU	Peptide

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	3948	0	3832	264	3
1	B	3948	0	3832	264	3
1	C	3948	0	3832	282	1
1	D	3948	0	3832	284	0
1	E	3948	0	3832	271	0
1	F	3948	0	3832	279	1
All	All	23688	0	22992	1585	4

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 34.

The worst 5 of 1585 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:573:ILE:O	1:A:573:ILE:HG22	1.66	0.93
1:F:573:ILE:O	1:F:573:ILE:HG22	1.70	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:MET:O	1:D:159:ARG:HD3	1.70	0.91
1:E:573:ILE:HG22	1:E:573:ILE:O	1.71	0.91
1:C:299:ASN:N	1:C:299:ASN:HD22	1.63	0.89

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:HIS:O	1:B:291:PHE:CZ[2_665]	1.96	0.24
1:C:295:LEU:O	1:F:65:ARG:NH2[1_556]	2.07	0.13
1:A:255:HIS:O	1:B:291:PHE:CE2[2_665]	2.09	0.11
1:A:255:HIS:C	1:B:291:PHE:CZ[2_665]	2.19	0.01

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	482/583 (83%)	386 (80%)	82 (17%)	14 (3%)	4	24
1	B	482/583 (83%)	390 (81%)	82 (17%)	10 (2%)	7	33
1	C	482/583 (83%)	387 (80%)	86 (18%)	9 (2%)	8	36
1	D	482/583 (83%)	388 (80%)	81 (17%)	13 (3%)	5	26
1	E	482/583 (83%)	390 (81%)	85 (18%)	7 (2%)	10	42
1	F	482/583 (83%)	387 (80%)	85 (18%)	10 (2%)	7	33
All	All	2892/3498 (83%)	2328 (80%)	501 (17%)	63 (2%)	6	31

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	VAL
1	A	530	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	539	THR
1	B	258	VAL
1	B	530	GLY

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	446/529 (84%)	368 (82%)	78 (18%)	2	10
1	B	446/529 (84%)	369 (83%)	77 (17%)	2	10
1	C	446/529 (84%)	369 (83%)	77 (17%)	2	10
1	D	446/529 (84%)	367 (82%)	79 (18%)	2	9
1	E	446/529 (84%)	365 (82%)	81 (18%)	1	9
1	F	446/529 (84%)	367 (82%)	79 (18%)	2	9
All	All	2676/3174 (84%)	2205 (82%)	471 (18%)	2	10

5 of 471 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	573	ILE
1	F	303	LEU
1	D	330	THR
1	F	274	SER
1	F	55	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	299	ASN
1	F	233	GLN
1	D	40	HIS
1	F	564	ASN
1	E	233	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 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, 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	488/583 (83%)	-0.12	11 (2%)	60	31	48, 91, 189, 275	0
1	B	488/583 (83%)	-0.31	4 (0%)	86	65	50, 92, 180, 276	0
1	C	488/583 (83%)	-0.23	15 (3%)	49	21	58, 102, 192, 278	0
1	D	488/583 (83%)	-0.12	25 (5%)	28	10	65, 104, 205, 279	0
1	E	488/583 (83%)	-0.19	15 (3%)	49	21	58, 103, 198, 275	0
1	F	488/583 (83%)	-0.24	20 (4%)	37	14	52, 94, 194, 281	0
All	All	2928/3498 (83%)	-0.20	90 (3%)	49	21	48, 99, 194, 281	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	VAL	9.7
1	F	39	VAL	8.7
1	B	39	VAL	7.5
1	D	40	HIS	7.2
1	A	68	PHE	7.2

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.