W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:37 AM GMT

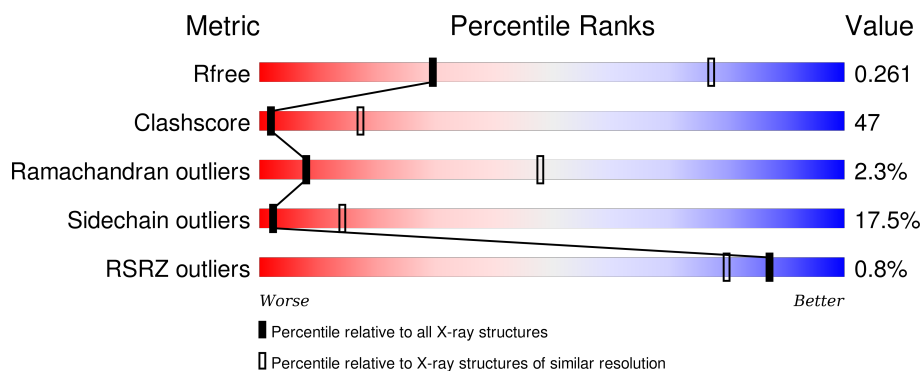|		
PDB ID	:	2XQ5
Title	:	PENTAMERIC LIGAND GATED ION CHANNEL GLIC IN COMPLEX WITH TETRAETHYLARSONIUM (TEAS)
Authors	:	Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on	:	2010-09-01
Resolution	:	3.50 Å(reported)

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 3.50 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		47
Ramachandran outliers		2.3%
Sidechain outliers		17.5%
RSRZ outliers		0.8%

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$_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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. 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	317	31% 54% 12% •
1	B	317	32% 53% 12% • •
1	C	317	35% 51% 12% •
1	D	317	32% 53% 13% •
1	E	317	34% 52% 11% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12606 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 GLR4197 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total 2521	C 1662	N 403	O 452	S 4	0	0	0
1	B	310	Total 2521	C 1662	N 403	O 452	S 4	0	0	0
1	C	310	Total 2521	C 1662	N 403	O 452	S 4	0	0	0
1	D	310	Total 2521	C 1662	N 403	O 452	S 4	0	0	0
1	E	310	Total 2521	C 1662	N 403	O 452	S 4	0	0	0

- Molecule 2 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	As 1	0	0

3 Residue-property plots (i)

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: GLR4197 PROTEIN
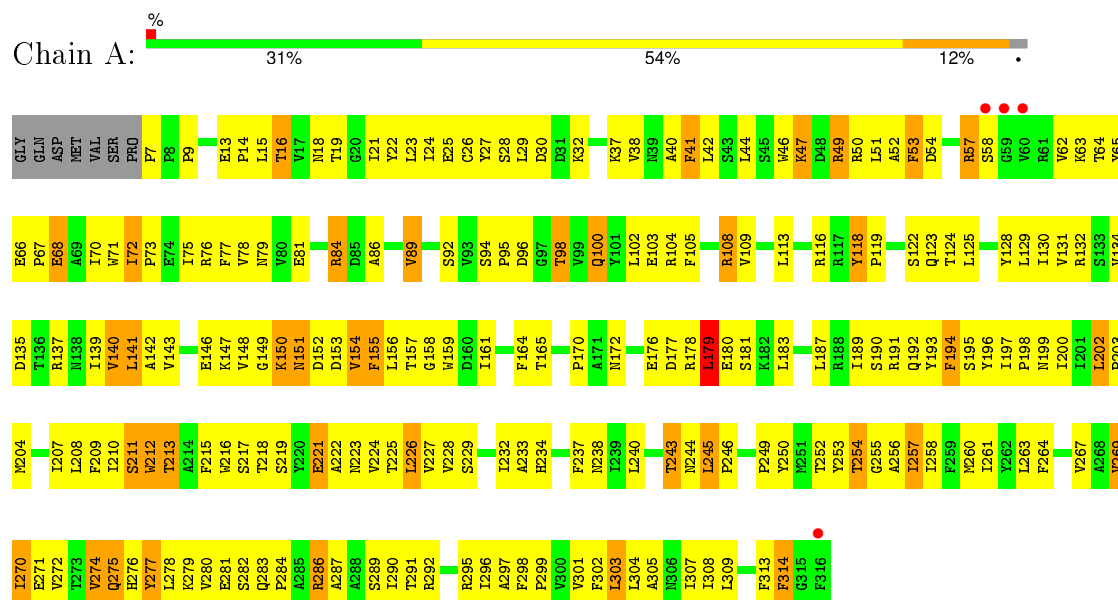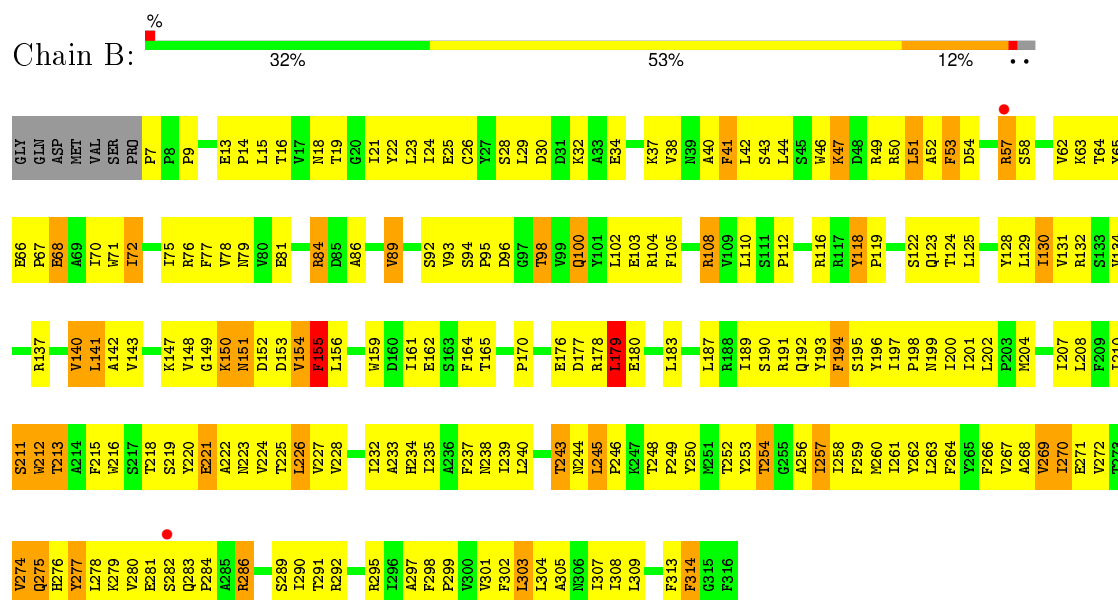
- Molecule 1: GLR4197 PROTEIN

• Molecule 1: GLR4197 PROTEIN

Chain C:

• Molecule 1: GLR4197 PROTEIN

Chain D:

• Molecule 1: GLR4197 PROTEIN

Chain E:

T213 A214 F215 W216 S217 T218 S219 Y220 E221 A222 N223 V224 T225 L226 V227 V228 A233 H234 F237 N238 I239 L240 T243 N244 L245 P246 K247 T248 P249 Y250 M251 T252 Y253 T254 G255 A256 I257 I258 F259 M260 I261 Y262 L263 F264 Y265 F266 V267 A268 V269 I270 E271 V272 T273 V274 Q275 H276 Y277

L278 K279 V280 E281 S282 Q283 P284 A285 R286 A287 A288 S289 I290 T291 R292 R295 I296 A297 F298 P299 V300 V301 F302 L303 L304 A305 N306 I307 I308 L309 F313 F314 G315 F316
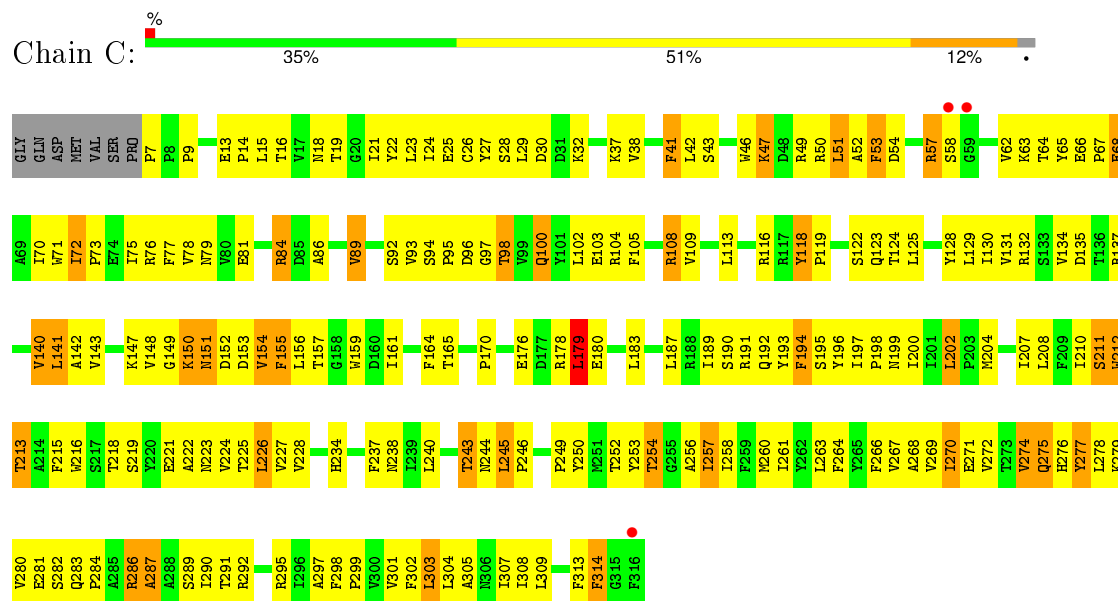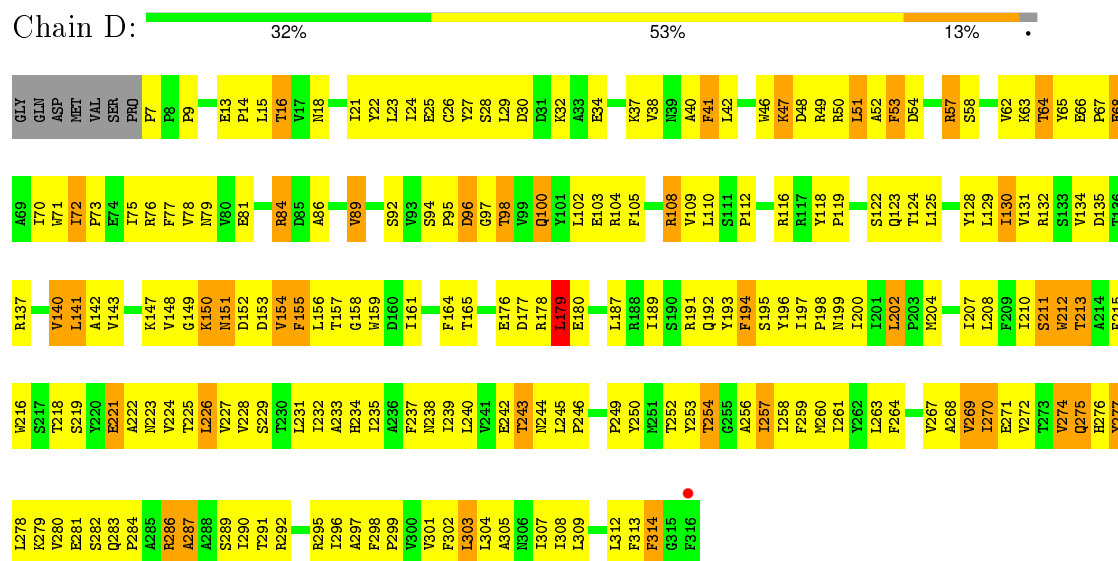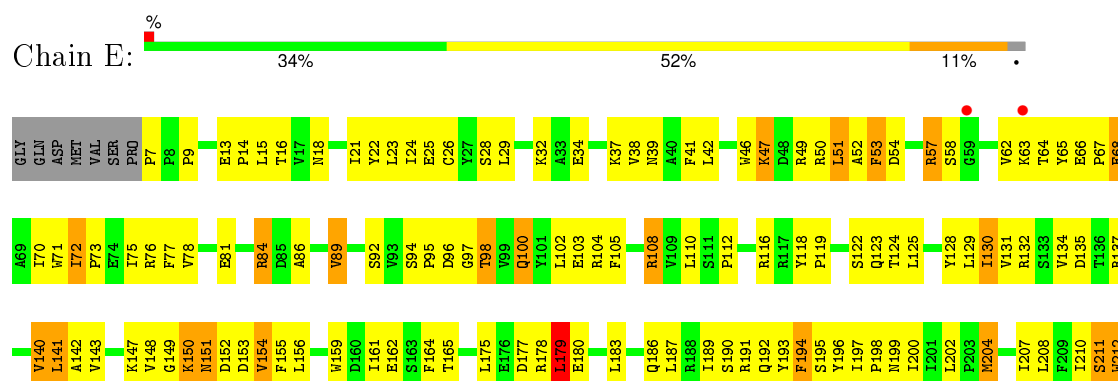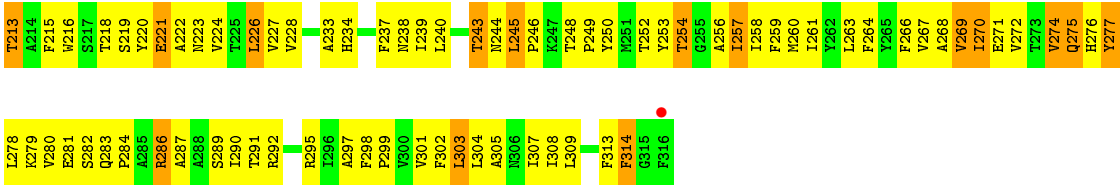
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	183.31Å 128.31Å 164.37Å 90.00° 104.04° 90.00°	Depositor
Resolution (Å)	40.20 – 3.50 40.20 – 3.38	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.20-3.50) 95.6 (40.20-3.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.86 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.249 , 0.266 0.243 , 0.261	Depositor DCC
R_{free} test set	2299 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	98.3	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 82.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|>$ = 0.45, $<L^2>$ = 0.28	Xtriage
Outliers	1 of 51417 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12606	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ARS

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	0.49	0/2589	0.69	3/3535 (0.1%)
1	B	0.48	0/2589	0.70	2/3535 (0.1%)
1	C	0.48	0/2589	0.69	3/3535 (0.1%)
1	D	0.50	0/2589	0.70	3/3535 (0.1%)
1	E	0.49	0/2589	0.70	3/3535 (0.1%)
All	All	0.49	0/12945	0.70	14/17675 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	179	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	179	LEU	CA-CB-CG	5.68	128.36	115.30
1	D	179	LEU	CA-CB-CG	5.67	128.35	115.30
1	E	179	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	179	LEU	CA-CB-CG	5.66	128.32	115.30

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2521	0	2537	278	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2521	0	2537	267	0
1	C	2521	0	2537	235	0
1	D	2521	0	2537	270	0
1	E	2521	0	2537	243	0
2	C	1	0	0	0	0
All	All	12606	0	12685	1177	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 47.

The worst 5 of 1177 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:226:LEU:HD23	1:B:224:VAL:HB	1.33	1.06
1:D:155:PHE:CE1	1:E:112:PRO:HB3	1.92	1.03
1:A:155:PHE:CE1	1:B:112:PRO:HB3	1.94	1.01
1:A:222:ALA:HB2	1:B:221:GLU:HA	1.42	1.01
1:A:27:TYR:HB3	1:B:110:LEU:HD11	1.42	0.99

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	308/317 (97%)	245 (80%)	56 (18%)	7 (2%)	8	48
1	B	308/317 (97%)	250 (81%)	51 (17%)	7 (2%)	8	48
1	C	308/317 (97%)	249 (81%)	52 (17%)	7 (2%)	8	48
1	D	308/317 (97%)	253 (82%)	47 (15%)	8 (3%)	7	45
1	E	308/317 (97%)	250 (81%)	52 (17%)	6 (2%)	10	51
All	All	1540/1585 (97%)	1247 (81%)	258 (17%)	35 (2%)	8	48

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	TYR
1	A	150	LYS
1	A	194	PHE
1	B	118	TYR
1	B	150	LYS

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	278/284 (98%)	230 (83%)	48 (17%)	2	14
1	B	278/284 (98%)	228 (82%)	50 (18%)	2	12
1	C	278/284 (98%)	230 (83%)	48 (17%)	2	14
1	D	278/284 (98%)	231 (83%)	47 (17%)	2	15
1	E	278/284 (98%)	228 (82%)	50 (18%)	2	12
All	All	1390/1420 (98%)	1147 (82%)	243 (18%)	2	14

5 of 243 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	72	ILE
1	C	254	THR
1	E	204	MET
1	C	100	GLN
1	C	155	PHE

Some 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	100	GLN
1	C	151	ASN
1	E	100	GLN
1	B	244	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	244	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	310/317 (97%)	-0.25	4 (1%)	79	70	64, 106, 164, 215	0
1	B	310/317 (97%)	-0.28	2 (0%)	90	85	69, 106, 164, 215	0
1	C	310/317 (97%)	-0.28	3 (0%)	84	76	66, 106, 163, 215	0
1	D	310/317 (97%)	-0.29	1 (0%)	94	91	66, 105, 164, 215	0
1	E	310/317 (97%)	-0.30	3 (0%)	84	76	70, 106, 164, 215	0
All	All	1550/1585 (97%)	-0.28	13 (0%)	87	80	64, 106, 164, 215	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	GLY	4.7
1	A	316	PHE	3.8
1	A	58	SER	3.2
1	E	59	GLY	3.1
1	D	316	PHE	3.0

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ARS	C	1317	1/1	0.88	0.49	-	144,144,144,144	0

6.5 Other polymers (i)

There are no such residues in this entry.