



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2016 – 11:38 PM EDT

PDB ID : 5DFX
Title : Structure of the parental state of GAF3 from Slr1393 of *Synechocystis* sp. PCC6803 (in vivo assembled protein/chromophore)
Authors : Xu, X.-L.; Zhao, K.-H.; Gaertner, W.; Hoepfner, A.
Deposited on : 2015-08-27
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

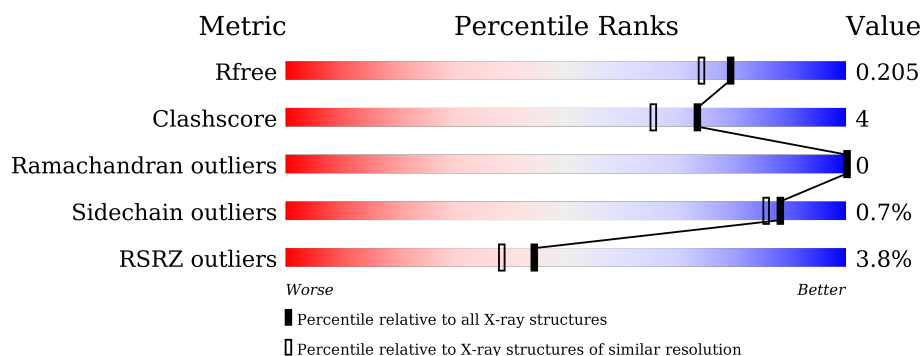
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 $\leq 5\%$. 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	215	<div> <div>3%</div> <div>62%</div> <div>11%</div> <div>•</div> <div>27%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1530 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 Histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	4	0
			1319	839	239	238	3			

There are 58 discrepancies between the modelled and reference sequences:

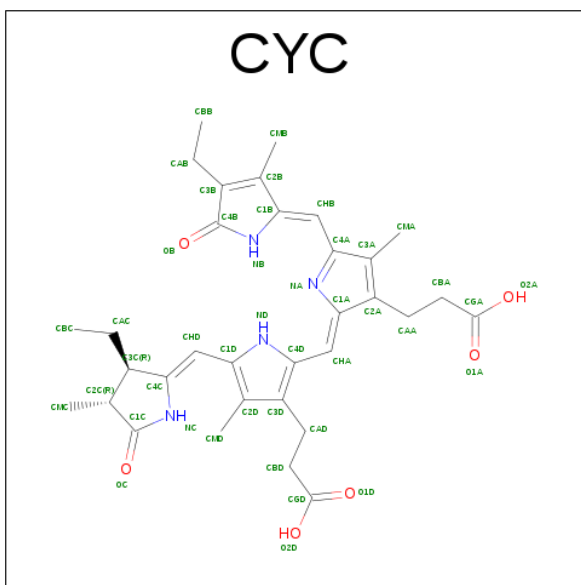
Chain	Residue	Modelled	Actual	Comment	Reference
A	391	MET	-	initiating methionine	UNP P73184
A	392	HIS	-	expression tag	UNP P73184
A	393	HIS	-	expression tag	UNP P73184
A	394	HIS	-	expression tag	UNP P73184
A	395	HIS	-	expression tag	UNP P73184
A	396	HIS	-	expression tag	UNP P73184
A	397	HIS	-	expression tag	UNP P73184
A	398	SER	-	expression tag	UNP P73184
A	399	SER	-	expression tag	UNP P73184
A	400	GLY	-	expression tag	UNP P73184
A	401	LEU	-	expression tag	UNP P73184
A	402	VAL	-	expression tag	UNP P73184
A	403	PRO	-	expression tag	UNP P73184
A	404	ARG	-	expression tag	UNP P73184
A	405	GLY	-	expression tag	UNP P73184
A	406	SER	-	expression tag	UNP P73184
A	407	GLY	-	expression tag	UNP P73184
A	408	MET	-	expression tag	UNP P73184
A	409	LYS	-	expression tag	UNP P73184
A	410	GLU	-	expression tag	UNP P73184
A	411	THR	-	expression tag	UNP P73184
A	412	ALA	-	expression tag	UNP P73184
A	413	ALA	-	expression tag	UNP P73184
A	414	ALA	-	expression tag	UNP P73184
A	415	LYS	-	expression tag	UNP P73184
A	416	PHE	-	expression tag	UNP P73184
A	417	GLU	-	expression tag	UNP P73184

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Chain	Residue	Modelled	Actual	Comment	Reference
A	418	ARG	-	expression tag	UNP P73184
A	419	GLN	-	expression tag	UNP P73184
A	420	HIS	-	expression tag	UNP P73184
A	421	MET	-	expression tag	UNP P73184
A	422	ASP	-	expression tag	UNP P73184
A	423	SER	-	expression tag	UNP P73184
A	424	PRO	-	expression tag	UNP P73184
A	425	ASP	-	expression tag	UNP P73184
A	426	LEU	-	expression tag	UNP P73184
A	427	GLY	-	expression tag	UNP P73184
A	428	THR	-	expression tag	UNP P73184
A	429	ASP	-	expression tag	UNP P73184
A	430	ASP	-	expression tag	UNP P73184
A	431	ASP	-	expression tag	UNP P73184
A	432	ASP	-	expression tag	UNP P73184
A	433	LYS	-	expression tag	UNP P73184
A	434	ALA	-	expression tag	UNP P73184
A	435	MET	-	expression tag	UNP P73184
A	436	ALA	-	expression tag	UNP P73184
A	437	ASP	-	expression tag	UNP P73184
A	438	ILE	-	expression tag	UNP P73184
A	439	GLY	-	expression tag	UNP P73184
A	440	SER	-	expression tag	UNP P73184
A	598	LEU	-	expression tag	UNP P73184
A	599	GLU	-	expression tag	UNP P73184
A	600	HIS	-	expression tag	UNP P73184
A	601	HIS	-	expression tag	UNP P73184
A	602	HIS	-	expression tag	UNP P73184
A	603	HIS	-	expression tag	UNP P73184
A	604	HIS	-	expression tag	UNP P73184
A	605	HIS	-	expression tag	UNP P73184

- Molecule 2 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: C₃₃H₄₀N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		

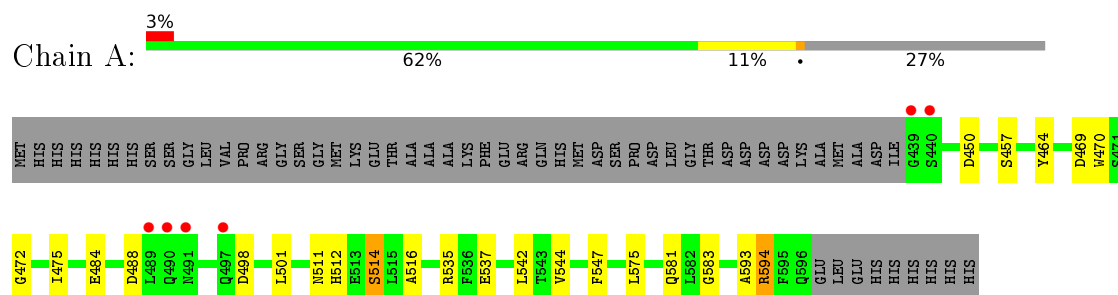
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	168	Total O 168 168	0	0

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: Histidine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.12Å 63.12Å 118.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 1.80 19.83 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.96-1.80) 99.6 (19.83-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.164 , 0.199 0.175 , 0.205	Depositor DCC
R_{free} test set	1039 reflections (4.75%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1530	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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

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	1.18	4/1366 (0.3%)	1.13	12/1855 (0.6%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	GLU	CD-OE1	-7.52	1.17	1.25
1	A	501	LEU	C-N	-5.84	1.20	1.34
1	A	537	GLU	CD-OE2	5.75	1.31	1.25
1	A	514	SER	CB-OG	-5.01	1.35	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594[A]	ARG	CA-C-O	7.63	136.13	120.10
1	A	594[B]	ARG	CA-C-O	7.63	136.13	120.10
1	A	450	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	593	ALA	C-N-CA	-7.00	104.20	121.70
1	A	469	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	535	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	594[A]	ARG	CA-C-N	-6.21	103.53	117.20
1	A	594[B]	ARG	CA-C-N	-6.21	103.53	117.20
1	A	488	ASP	CB-CG-OD2	-5.97	112.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	594[A]	ARG	N-CA-C	5.11	124.81	111.00
1	A	594[B]	ARG	N-CA-C	5.11	124.81	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	470	TRP	Peptide
1	A	594[B]	ARG	Mainchain

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	1319	0	1263	10	0
2	A	43	0	36	2	0
3	A	168	0	0	1	0
All	All	1530	0	1299	11	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 4.

All (11) 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:542:LEU:HG	1:A:575:LEU:HD23	1.77	0.66
1:A:511:ASN:O	1:A:512:HIS:HB2	2.01	0.59
1:A:498:ASP:OD2	2:A:701:CYC:NA	2.39	0.55
2:A:701:CYC:NB	2:A:701:CYC:HMA1	2.30	0.47
1:A:512:HIS:CE1	1:A:547:PHE:CD1	3.03	0.46
1:A:581:GLN:CD	3:A:804:HOH:O	2.56	0.44
1:A:514:SER:HB3	1:A:544:VAL:HG12	2.01	0.42
1:A:475:ILE:HG21	1:A:475:ILE:HD13	1.83	0.42
1:A:547:PHE:O	1:A:583:GLY:HA3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TYR:CZ	1:A:472:GLY:HA3	2.56	0.41
1:A:516:ALA:HB2	1:A:542:LEU:HD13	2.03	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	160/215 (74%)	158 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	139/183 (76%)	137 (99%)	2 (1%)	74	65

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	457[A]	SER
1	A	457[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CYC	A	701	1	35,46,46	2.88	10 (28%)	44,67,67	4.16	25 (56%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CYC	A	701	1	-	2/21/74/74	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CYC	C4C-NC	-3.00	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CYC	C1B-NB	-2.62	1.33	1.37
2	A	701	CYC	C4A-C3A	2.23	1.50	1.45
2	A	701	CYC	OB-C4B	2.40	1.28	1.23
2	A	701	CYC	C3D-C2D	3.07	1.46	1.37
2	A	701	CYC	C1B-C2B	3.15	1.50	1.45
2	A	701	CYC	CHB-C1B	3.35	1.45	1.37
2	A	701	CYC	C2A-C3A	3.90	1.45	1.36
2	A	701	CYC	C3B-C2B	4.08	1.45	1.36
2	A	701	CYC	CHA-C1A	13.39	1.47	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CYC	C4B-C3B-C2B	-8.67	103.15	108.04
2	A	701	CYC	C1A-C2A-C3A	-6.70	99.50	106.80
2	A	701	CYC	OB-C4B-C3B	-6.10	120.55	128.11
2	A	701	CYC	C1B-C2B-C3B	-5.78	101.78	107.82
2	A	701	CYC	C1B-NB-C4B	-5.30	103.05	110.73
2	A	701	CYC	C1A-NA-C4A	-4.68	97.60	106.50
2	A	701	CYC	CHB-C1B-C2B	-4.58	118.01	126.92
2	A	701	CYC	CHB-C4A-C3A	-4.39	114.22	124.71
2	A	701	CYC	CHA-C1A-C2A	-4.24	115.81	125.48
2	A	701	CYC	CHA-C1A-NA	-3.36	122.75	128.71
2	A	701	CYC	OC-C1C-C2C	-2.91	123.96	126.30
2	A	701	CYC	CBB-CAB-C3B	-2.10	105.99	112.38
2	A	701	CYC	CMD-C2D-C3D	2.03	129.49	125.24
2	A	701	CYC	CMC-C2C-C1C	2.64	118.05	112.39
2	A	701	CYC	C2D-C1D-ND	2.68	114.68	110.29
2	A	701	CYC	C3A-C4A-NA	2.69	116.51	110.65
2	A	701	CYC	C2C-C1C-NC	2.91	111.19	108.31
2	A	701	CYC	CAA-C2A-C1A	4.39	132.71	125.00
2	A	701	CYC	CAA-CBA-CGA	5.69	123.85	112.78
2	A	701	CYC	CMA-C3A-C4A	6.01	134.67	125.06
2	A	701	CYC	CMB-C2B-C1B	6.55	132.74	124.20
2	A	701	CYC	C2B-C1B-NB	6.69	116.39	106.94
2	A	701	CYC	C2A-C1A-NA	7.32	121.14	109.98
2	A	701	CYC	CAB-C3B-C4B	7.51	128.13	121.47
2	A	701	CYC	C3B-C4B-NB	9.68	115.61	106.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	CYC	C1B-CHB-C4A-C3A
2	A	701	CYC	C1B-CHB-C4A-NA

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	CYC	2	0

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	158/215 (73%)	-0.20	6 (3%) 44 38	15, 24, 46, 70	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	GLN	4.2
1	A	439	GLY	3.4
1	A	440	SER	3.0
1	A	491	ASN	2.7
1	A	489	LEU	2.3
1	A	497	GLN	2.1

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(\AA^2)	Q<0.9
2	CYC	A	701	43/43	0.91	0.10	0.13	22,31,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.