wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 11:50 PM EST

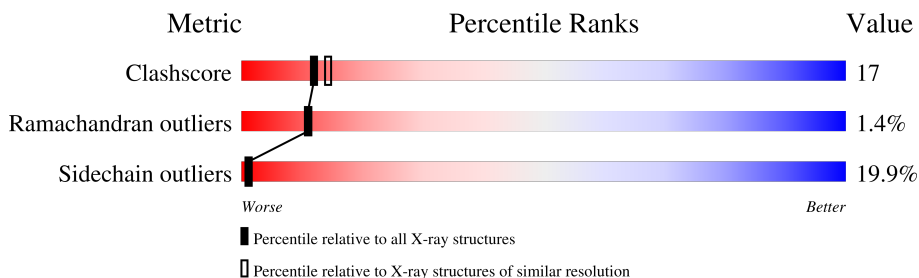|		
PDB ID	:	1GGG
Title	:	GLUTAMINE BINDING PROTEIN OPEN LIGAND-FREE STRUCTURE
Authors	:	Hsiao, C.-D.; Sun, Y.-J.; Rose, J.; Wang, B.-C.
Deposited on	:	1996-06-25
Resolution	:	2.30 Å(reported)

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 2.30 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
Clashscore		17
Ramachandran outliers		1.4%
Sidechain outliers		19.9%

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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	226	59% 31% 7% ··
1	B	226	64% 20% 11% ··

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 3587 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 GLUTAMINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1714	1098	281	332	3			
1	B	220	Total	C	N	O	S	0	0	0
			1714	1098	281	332	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	LYS	conflict	UNP P10344
B	23	LEU	LYS	conflict	UNP P10344

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		
2	B	79	Total	O	0	0
			79	79		

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. 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. 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.
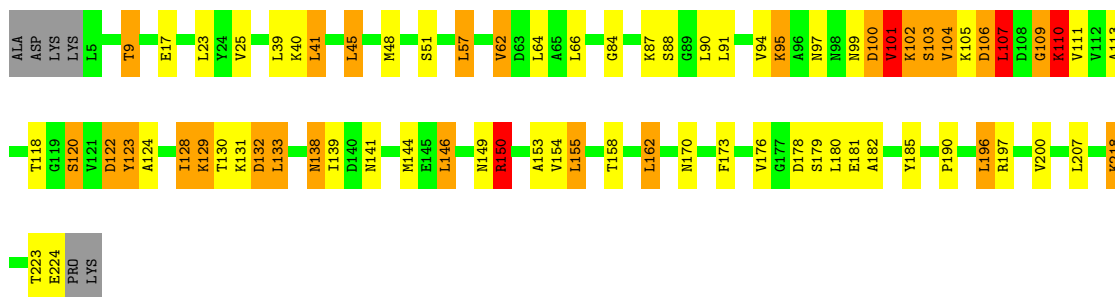
Note EDS was not executed.

• Molecule 1: GLUTAMINE BINDING PROTEIN

Chain A:
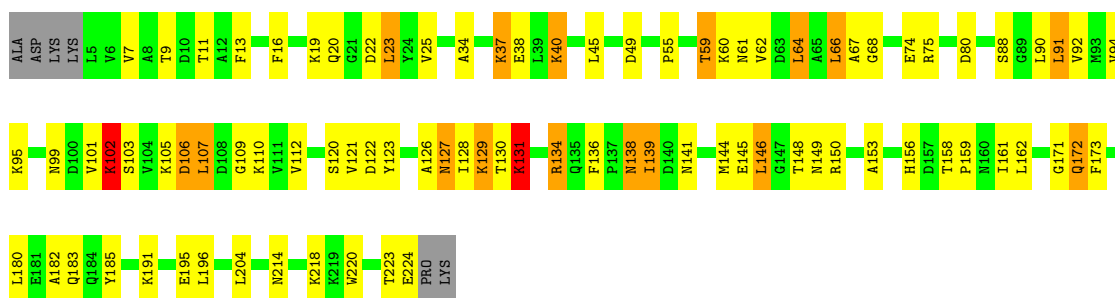
• Molecule 1: GLUTAMINE BINDING PROTEIN

Chain B:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.30Å 86.30Å 81.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	81.0 (10.00-2.30)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3587	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

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	0.63	0/1745	0.79	3/2358 (0.1%)
1	B	0.84	4/1745 (0.2%)	1.02	11/2358 (0.5%)
All	All	0.74	4/3490 (0.1%)	0.91	14/4716 (0.3%)

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	6
1	B	0	7
All	All	0	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	VAL	C-N	-16.37	0.96	1.34
1	B	150	ARG	C-N	10.63	1.58	1.34
1	B	100	ASP	C-N	9.51	1.55	1.34
1	B	104	VAL	C-N	-7.20	1.17	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	VAL	O-C-N	-17.68	94.42	122.70
1	B	101	VAL	C-N-CA	15.66	160.85	121.70
1	B	101	VAL	CA-C-N	11.35	142.18	117.20
1	B	150	ARG	O-C-N	-9.19	107.99	122.70
1	B	150	ARG	NE-CZ-NH2	7.41	124.01	120.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	TYR	Sidechain
1	A	131	LYS	Mainchain
1	A	134	ARG	Sidechain
1	A	136	PHE	Sidechain
1	A	75	ARG	Sidechain

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	1714	0	1713	52	0
1	B	1714	0	1710	66	0
2	A	80	0	0	4	0
2	B	79	0	0	2	0
All	All	3587	0	3423	118	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 17.

The worst 5 of 118 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:B:102:LYS:HG2	1:B:103:SER:H	1.10	1.16
1:B:105:LYS:HE2	1:B:153:ALA:HB3	1.38	1.02
1:B:102:LYS:HG2	1:B:103:SER:N	1.70	0.95
1:B:110:LYS:HD3	1:B:131:LYS:H	1.32	0.95
1:B:110:LYS:HB2	1:B:130:THR:OG1	1.76	0.85

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	218/226 (96%)	191 (88%)	25 (12%)	2 (1%)	17	20
1	B	218/226 (96%)	194 (89%)	20 (9%)	4 (2%)	8	7
All	All	436/452 (96%)	385 (88%)	45 (10%)	6 (1%)	11	11

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	107	LEU
1	B	101	VAL
1	B	109	GLY
1	B	110	LYS
1	A	102	LYS

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	181/186 (97%)	145 (80%)	36 (20%)	1	1
1	B	181/186 (97%)	145 (80%)	36 (20%)	1	1
All	All	362/372 (97%)	290 (80%)	72 (20%)	1	1

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	132	ASP

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Mol	Chain	Res	Type
1	B	223	THR
1	B	138	ASN
1	B	176	VAL
1	A	129	LYS

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	B	160	ASN
1	B	138	ASN
1	A	156	HIS
1	A	141	ASN
1	B	97	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 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	104:VAL	C	105:LYS	N	1.17
1	B	101:VAL	C	102:LYS	N	0.96

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.