wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 08:38 pm BST

PDB ID	:	1NGP
Title	:	N1G9 (IGG1-LAMBDA) FAB FRAGMENT COMPLEXED WITH (4-HYD ROXY-3-NITROPHENYL) ACETATE
Authors	:	Mizutani, R.; Satow, Y.
Deposited on	:	1995-06-23
Resolution	:	2.40 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 (i) symbol.

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

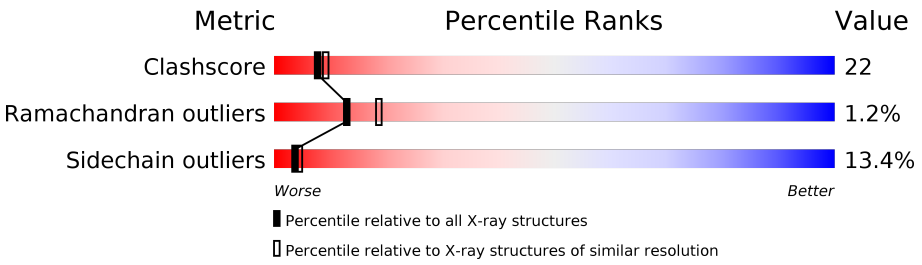
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 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	L	215	53% 33% 10% • •
2	H	222	59% 30% 6% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3380 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 N1G9 (IGG1-LAMBDA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1584	995	265	318	6	0	1	0

- Molecule 2 is a protein called N1G9 (IGG1-LAMBDA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	215	1646	1051	268	319	8	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLN	GLU	CONFLICT	UNP P01751
H	3	GLN	LYS	CONFLICT	UNP P01751
H	5	GLN	HIS	CONFLICT	UNP P01751
H	6	GLN	GLU	CONFLICT	UNP P01751
H	7	PRO	SER	CONFLICT	UNP P01751
H	9	ALA	PRO	CONFLICT	UNP P01751
H	10	GLU	GLY	CONFLICT	UNP P01751
H	13	LYS	ARG	CONFLICT	UNP P01751
H	16	ALA	THR	CONFLICT	UNP P01751
H	20	LEU	ILE	CONFLICT	UNP P01751
H	31	SER	ASN	CONFLICT	UNP P01751
H	34	MET	LEU	CONFLICT	UNP P01751
H	35	HIS	GLY	CONFLICT	UNP P01751
H	43	ARG	HIS	CONFLICT	UNP P01751
H	50	ARG	ASP	CONFLICT	UNP P01751
H	52	ASP	TYR	CONFLICT	UNP P01751
H	54	ASN	GLY	CONFLICT	UNP P01751
H	55	SER	GLY	CONFLICT	UNP P01751
H	57	GLY	TYR	CONFLICT	UNP P01751
H	59	LYS	ASN	CONFLICT	UNP P01751

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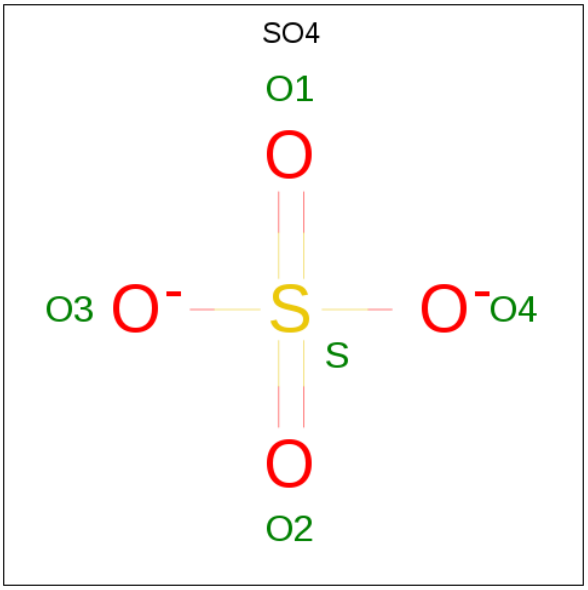
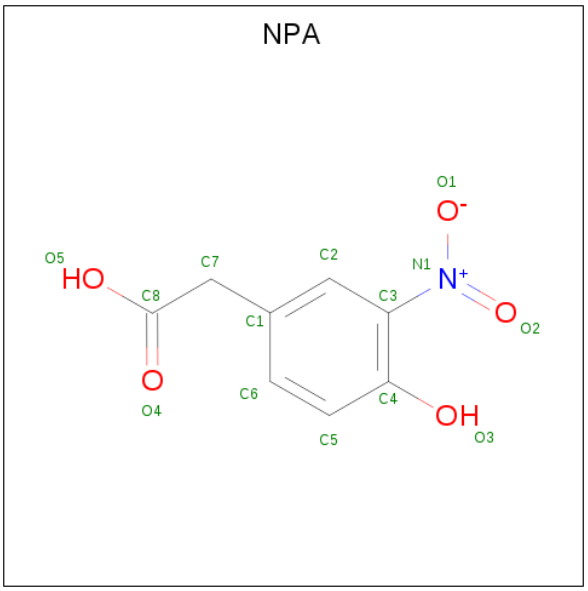
Chain	Residue	Modelled	Actual	Comment	Reference
H	66	SER	GLY	CONFLICT	UNP P01751
H	72	VAL	ALA	CONFLICT	UNP P01751
H	74	LYS	THR	CONFLICT	UNP P01751
H	75	PRO	SER	CONFLICT	UNP P01751
H	95	TYR	PHE	CONFLICT	UNP P01751
H	99	TYR	-	INSERTION	UNP P01751
H	100	ASP	PHE	CONFLICT	UNP P01751
H	?	-	TYR	DELETION	UNP P01751
H	?	-	TRP	DELETION	UNP P01751
H	109	TYR	VAL	CONFLICT	UNP P01751
H	116	LEU	VAL	CONFLICT	UNP P01751
H	194	PRO	THR	CONFLICT	UNP P01751

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	H	1	5	4	1	0	0

- Molecule 4 is 2-(4-HYDROXY-3-NITROPHENYL)ACETIC ACID (three-letter code: NPA) (formula: $C_8H_7NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	H	1	14	8	1	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	L	58	58	58	0	0
			Total	O		
5	H	73	73	73	0	0

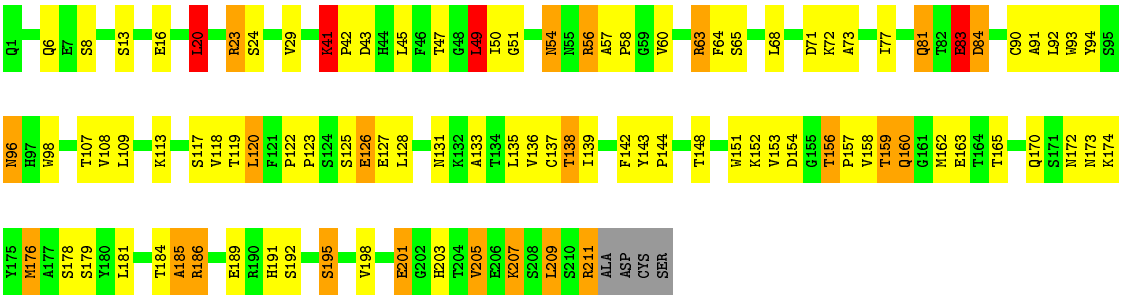
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

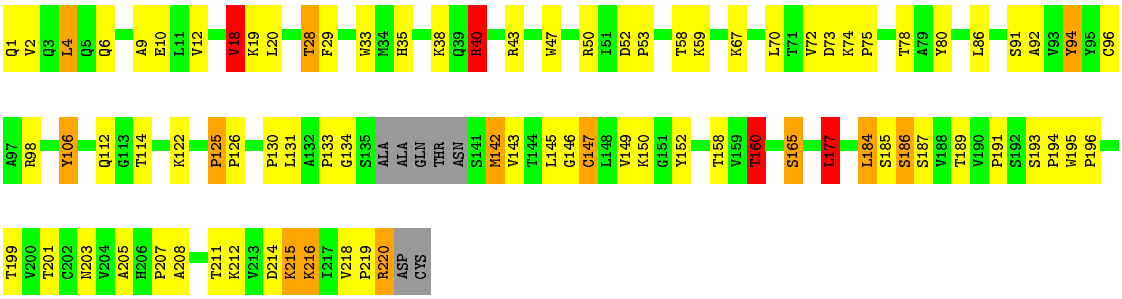
- Molecule 1: N1G9 (IGG1-LAMBDA)

Chain L:



- Molecule 2: N1G9 (IGG1-LAMBDA)

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	110.69Å 110.69Å 98.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	89.3 (15.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR 2.1	Depositor
R, R_{free}	0.196 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3380	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

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: NPA, SO4

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	L	0.95	0/1627	1.65	21/2225 (0.9%)
2	H	0.94	0/1699	1.74	28/2320 (1.2%)
All	All	0.94	0/3326	1.70	49/4545 (1.1%)

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	40	ARG	NE-CZ-NH1	16.16	128.38	120.30
2	H	94	TYR	CB-CG-CD2	11.04	127.63	121.00
1	L	56	ARG	NE-CZ-NH2	9.93	125.26	120.30
1	L	23	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	L	143	TYR	CB-CG-CD1	-8.47	115.92	121.00

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1584	0	1527	80	0
2	H	1646	0	1603	63	1
3	H	5	0	0	1	0
4	H	14	0	5	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	73	0	0	3	0
5	L	58	0	0	3	0
All	All	3380	0	3135	139	1

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 22.

The worst 5 of 139 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:L:211:ARG:HH11	1:L:211:ARG:HG2	1.14	1.06
1:L:153:VAL:HG12	1:L:158:VAL:HG22	1.40	1.02
2:H:35:HIS:CD2	2:H:47:TRP:HE1	1.87	0.91
2:H:35:HIS:HD2	2:H:47:TRP:HE1	0.94	0.89
1:L:51:GLY:HA3	2:H:106:TYR:HB3	1.56	0.88

All (1) 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)
2:H:19:LYS:NZ	2:H:19:LYS:NZ[8_665]	2.12	0.08

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	L	210/215 (98%)	190 (90%)	17 (8%)	3 (1%)	11 15
2	H	212/222 (96%)	191 (90%)	19 (9%)	2 (1%)	17 25
All	All	422/437 (97%)	381 (90%)	36 (8%)	5 (1%)	13 19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	43	ASP
2	H	133	PRO
1	L	160	GLN
1	L	185	ALA
2	H	134	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	L	175/182 (96%)	149 (85%)	26 (15%)	3 3
2	H	186/192 (97%)	163 (88%)	23 (12%)	4 5
All	All	361/374 (96%)	312 (86%)	49 (14%)	4 4

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	203	HIS
2	H	2	VAL
2	H	211	THR
1	L	207	LYS
2	H	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	54	ASN
1	L	81	GLN
1	L	96	ASN
2	H	1	GLN
2	H	35	HIS

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)

2 ligands are 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	$\#\|Z\| > 2$
3	SO4	H	301	-	4,4,4	0.62	0	6,6,6	0.54	0
4	NPA	H	302	-	10,14,14	1.39	2 (20%)	11,19,19	1.51	4 (36%)

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
4	NPA	H	302	-	-	0/4/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	302	NPA	C2-C1	-2.61	1.34	1.39
4	H	302	NPA	C3-N1	-2.58	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	302	NPA	O3-C4-C3	2.34	128.22	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	302	NPA	C6-C5-C4	-2.09	118.35	120.50
4	H	302	NPA	O2-N1-C3	-2.07	115.49	119.03
4	H	302	NPA	O3-C4-C5	-2.05	113.77	119.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	301	SO4	1	0
4	H	302	NPA	3	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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.