



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 01:48 AM EST

PDB ID : 1YNL
Title : Identification of Key residues of the NC6.8 Fab antibody fragment binding to synthetic sweeteners: Crystal structure of NC6.8 co-crystallized with high potency sweetener compound SC45647
Authors : Gokulan, K.; Khare, S.; Ronning, D.R.; Linthicum, S.D.; Sacchettini, J.C.; Rupp, B.
Deposited on : 2005-01-24
Resolution : 1.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

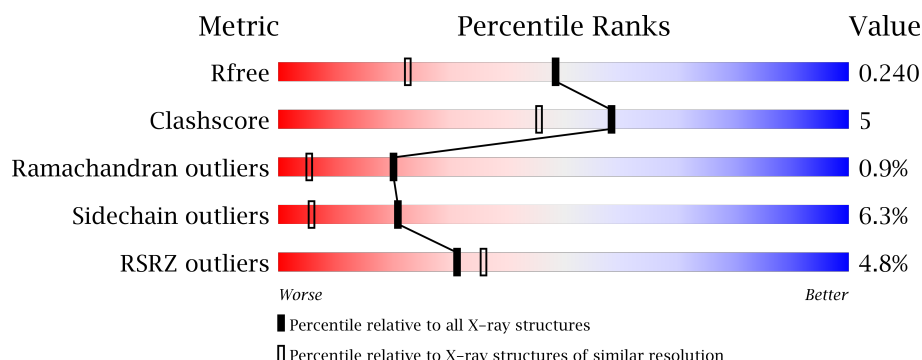
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	L	219	<div> <div>4%</div> <div>86%</div> <div>11%</div> <div>•</div> </div>
2	H	219	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3699 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.

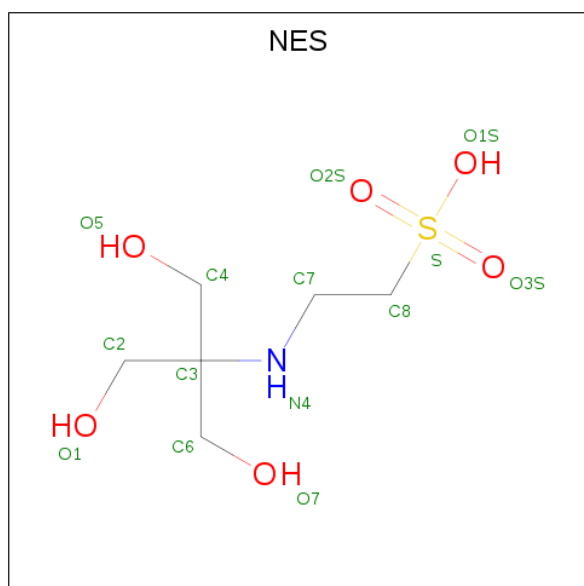
- Molecule 1 is a protein called Ig gamma light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1696	1059	291	339	7			

- Molecule 2 is a protein called Ig gamma heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1642	1037	265	331	9			

- Molecule 3 is 2-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-ETHANESULFONIC ACID (three-letter code: NES) (formula: C₆H₁₅NO₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	L	1	Total	C	N	O	S	0	0
			14	6	1	6	1		

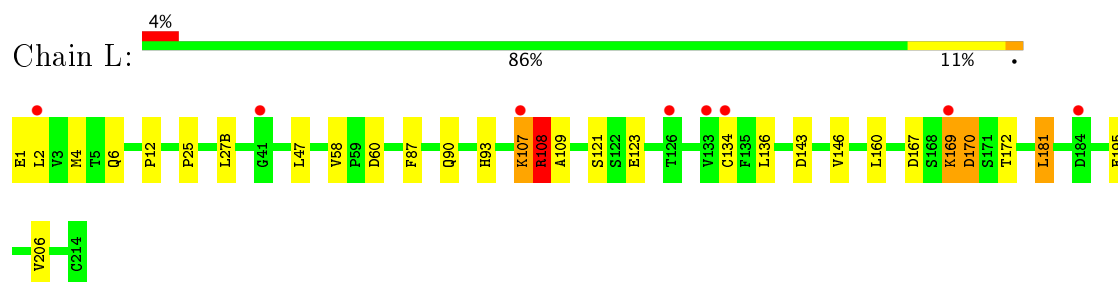
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	195	Total 195	O 195	0	0
4	H	152	Total 152	O 152	0	0

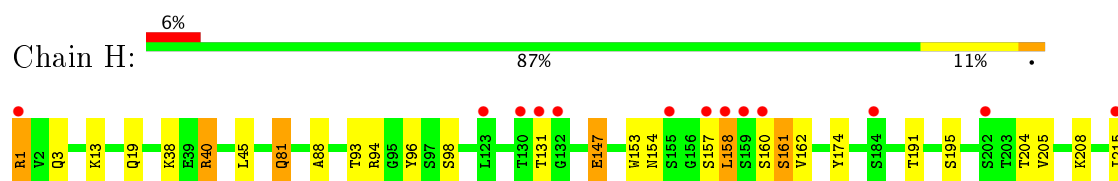
3 Residue-property plots [i](#)

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 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: Ig gamma light chain



- Molecule 2: Ig gamma heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.23Å 48.14Å 76.09Å 90.00° 109.53° 90.00°	Depositor
Resolution (Å)	23.30 – 1.70 23.25 – 1.70	Depositor EDS
% Data completeness (in resolution range)	84.5 (23.30-1.70) 84.5 (23.25-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.42 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.241 0.205 , 0.240	Depositor DCC
R_{free} test set	2217 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3699	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.75	2/1736 (0.1%)	0.83	2/2355 (0.1%)
2	H	0.72	0/1687	0.77	0/2303
All	All	0.74	2/3423 (0.1%)	0.80	2/4658 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	1	GLU	CB-CG	-6.58	1.39	1.52
1	L	134	CYS	CB-SG	-5.42	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	108	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	L	181	LEU	CA-CB-CG	5.95	128.98	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	L	1696	0	1637	21	0
2	H	1642	0	1586	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	14	0	12	0	0
4	H	152	0	0	0	0
4	L	195	0	0	0	0
All	All	3699	0	3235	36	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 5.

All (36) 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)
2:H:160:SER:HB3	2:H:162:VAL:H	1.41	0.84
1:L:108:ARG:HD3	1:L:109:ALA:O	1.80	0.81
2:H:38:LYS:HE2	2:H:40:ARG:HG3	1.69	0.75
1:L:2:LEU:HD21	1:L:25:PRO:HB2	1.75	0.69
2:H:147:GLU:HG3	2:H:174:TYR:CZ	2.33	0.64
1:L:195:GLU:HG2	1:L:206:VAL:HG12	1.80	0.63
2:H:160:SER:CB	2:H:162:VAL:H	2.11	0.63
1:L:170:ASP:HB3	1:L:172:THR:H	1.66	0.60
2:H:1:ARG:HH11	2:H:1:ARG:HB3	1.69	0.58
1:L:2:LEU:HD21	1:L:25:PRO:CB	2.33	0.57
2:H:1:ARG:NH1	2:H:1:ARG:HB3	2.20	0.57
2:H:147:GLU:HG3	2:H:174:TYR:CE1	2.41	0.56
2:H:40:ARG:HG2	2:H:88:ALA:HB2	1.89	0.55
1:L:167:ASP:OD2	1:L:170:ASP:HB2	2.07	0.54
1:L:108:ARG:CD	1:L:109:ALA:O	2.53	0.53
1:L:2:LEU:CD1	1:L:93:HIS:HD2	2.25	0.50
1:L:2:LEU:HD12	1:L:93:HIS:CD2	2.46	0.50
2:H:153:TRP:HB2	2:H:158:LEU:HD21	1.93	0.49
2:H:191:THR:HG23	2:H:208:LYS:HE2	1.94	0.49
1:L:2:LEU:HD11	1:L:27(B):LEU:CD2	2.43	0.49
1:L:121:SER:OG	1:L:123:GLU:OE1	2.30	0.48
1:L:12:PRO:HB2	1:L:107:LYS:HG2	1.96	0.48
1:L:2:LEU:CD1	1:L:93:HIS:CD2	2.97	0.48
1:L:6:GLN:HE22	1:L:87:PHE:HA	1.79	0.47
2:H:19:GLN:HB2	2:H:81:GLN:NE2	2.29	0.47
1:L:136:LEU:HD21	1:L:146:VAL:HG22	1.96	0.46
1:L:12:PRO:CB	1:L:107:LYS:HG2	2.45	0.46
2:H:19:GLN:HB2	2:H:81:GLN:HE22	1.80	0.46
1:L:2:LEU:HD11	1:L:27(B):LEU:HD23	1.97	0.45
1:L:2:LEU:CD1	1:L:27(B):LEU:CD2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:167:ASP:OD2	1:L:169:LYS:HG2	2.16	0.45
1:L:4:MET:HE2	1:L:90:GLN:HB3	2.01	0.42
2:H:160:SER:HB3	2:H:162:VAL:N	2.21	0.42
1:L:47:LEU:HA	1:L:58:VAL:HG21	2.02	0.42
2:H:215:ILE:O	2:H:215:ILE:HD12	2.21	0.41
2:H:160:SER:CA	2:H:162:VAL:H	2.34	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	L	217/219 (99%)	216 (100%)	1 (0%)	0	100	100
2	H	217/219 (99%)	207 (95%)	6 (3%)	4 (2%)	10	1
All	All	434/438 (99%)	423 (98%)	7 (2%)	4 (1%)	20	5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	98	SER
2	H	154	ASN
2	H	96	TYR
2	H	161	SER

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	195/195 (100%)	187 (96%)	8 (4%)	35	14
2	H	186/186 (100%)	170 (91%)	16 (9%)	12	2
All	All	381/381 (100%)	357 (94%)	24 (6%)	21	6

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	60	ASP
1	L	107	LYS
1	L	108	ARG
1	L	143	ASP
1	L	160	LEU
1	L	169	LYS
1	L	170	ASP
1	L	181	LEU
2	H	1	ARG
2	H	3	GLN
2	H	13	LYS
2	H	40	ARG
2	H	45	LEU
2	H	81	GLN
2	H	93	THR
2	H	94	ARG
2	H	131	THR
2	H	147	GLU
2	H	157	SER
2	H	158	LEU
2	H	161	SER
2	H	195	SER
2	H	204	THR
2	H	205	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	156	GLN
1	L	161	ASN
1	L	212	ASN

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Mol	Chain	Res	Type
2	H	3	GLN
2	H	81	GLN
2	H	154	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 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
3	NES	L	501	-	13,13,13	5.77	9 (69%)	17,18,18	3.12	6 (35%)

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
3	NES	L	501	-	-	0/17/17/17	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	501	NES	O5-C4	-5.59	1.24	1.42
3	L	501	NES	O7-C6	-5.09	1.25	1.42
3	L	501	NES	O1-C2	-4.81	1.26	1.42
3	L	501	NES	C8-S	-2.36	1.73	1.77
3	L	501	NES	O1S-S	5.28	1.65	1.47
3	L	501	NES	C6-C3	7.38	1.61	1.53
3	L	501	NES	O3S-S	9.08	1.71	1.45
3	L	501	NES	O2S-S	9.14	1.71	1.45
3	L	501	NES	C2-C3	9.89	1.64	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	501	NES	C4-C3-N4	-2.19	102.62	108.98
3	L	501	NES	O3S-S-C8	4.81	110.92	106.79
3	L	501	NES	O1-C2-C3	4.84	121.56	111.54
3	L	501	NES	O2S-S-C8	5.01	111.10	106.79
3	L	501	NES	O7-C6-C3	5.97	123.89	111.54
3	L	501	NES	O5-C4-C3	6.63	125.26	111.54

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 ⓘ

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	L	219/219 (100%)	0.05	8 (3%)	42	48	14, 23, 32, 36	0
2	H	219/219 (100%)	0.19	13 (5%)	23	26	15, 22, 38, 50	0
All	All	438/438 (100%)	0.12	21 (4%)	31	36	14, 23, 36, 50	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	159	SER	8.9
2	H	158	LEU	7.6
2	H	157	SER	5.7
2	H	155	SER	5.1
2	H	215	ILE	4.8
2	H	131	THR	3.8
2	H	1	ARG	3.7
1	L	133	VAL	3.1
1	L	169	LYS	3.0
2	H	130	THR	2.9
2	H	123	LEU	2.8
1	L	126	THR	2.6
1	L	134	CYS	2.6
2	H	184	SER	2.4
2	H	160	SER	2.4
1	L	184	ASP	2.4
2	H	132	GLY	2.1
1	L	2	LEU	2.1
1	L	41	GLY	2.1
2	H	202	SER	2.1
1	L	107	LYS	2.0

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(\AA^2)	Q<0.9
3	NES	L	501	14/14	0.85	0.15	1.77	17,19,23,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.