



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:06 PM GMT

PDB ID : 1WHT
Title : STRUCTURE OF THE COMPLEX OF L-BENZYL SUCCINATE WITH
WHEAT SERINE CARBOXYPEPTIDASE II AT 2.0 ANGSTROMS RES-
OLUTION
Authors : Bullock, T.L.; Remington, S.J.
Deposited on : 1994-03-07
Resolution : 2.00 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

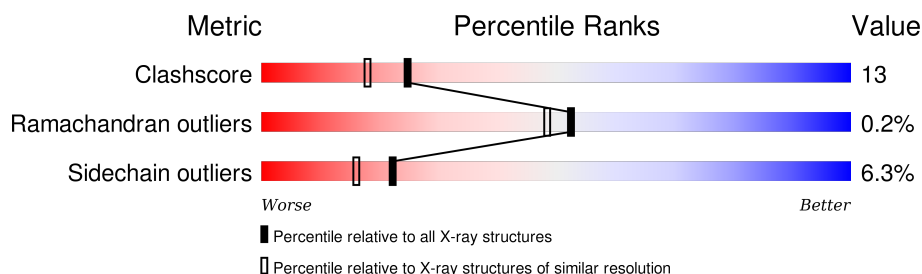
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	
2	B	153	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NDG	A	1134	X	-	-	-
5	NAG	B	2912	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3741 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 SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2003	1282	335	379	7			

- Molecule 2 is a protein called SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1213	778	208	221	6			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

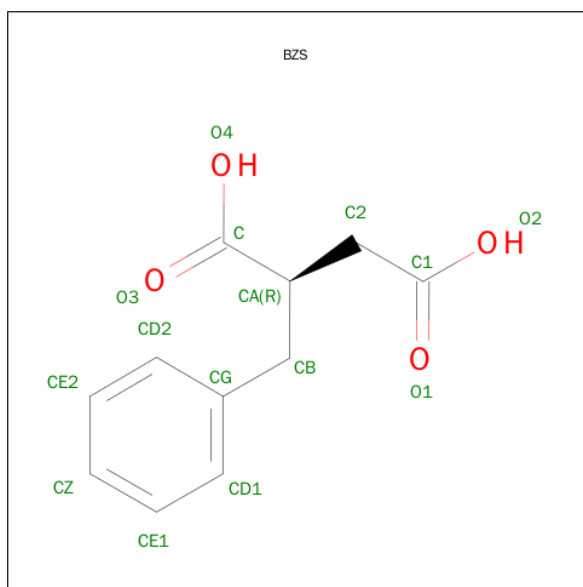
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is L-BENZYLsuccinic ACID (three-letter code: BZS) (formula: C₁₁H₁₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	11	4		

- Molecule 7 is water.

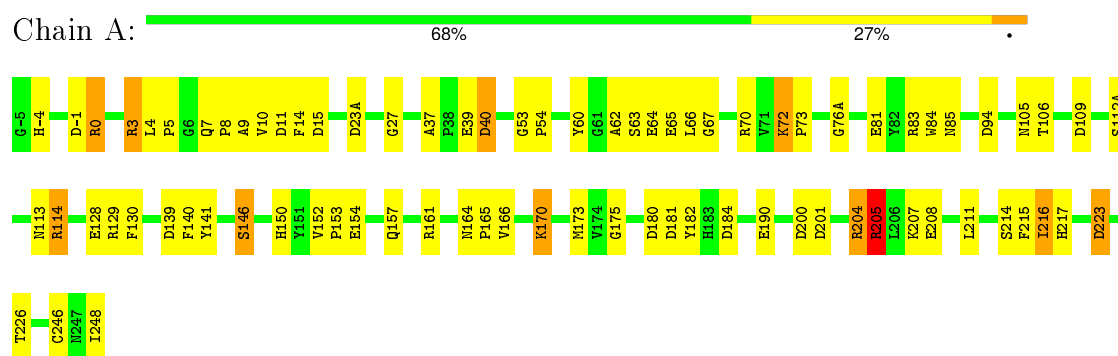
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	259	Total	O	0	0
			259	259		
7	B	171	Total	O	0	0
			171	171		

3 Residue-property plots

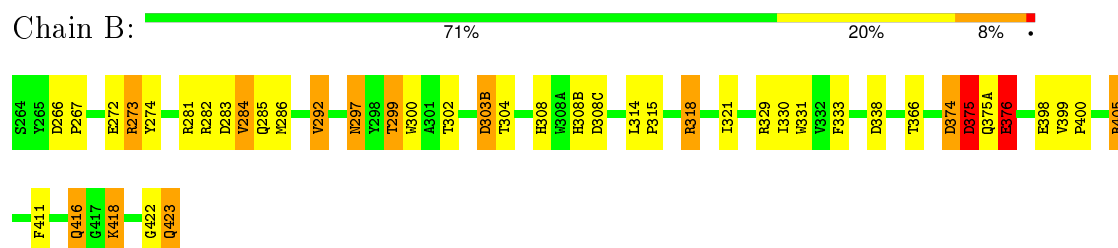
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: SERINE CARBOXYPEPTIDASE II



• Molecule 2: SERINE CARBOXYPEPTIDASE II



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.50Å 95.50Å 208.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3741	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: BZS, NAG, NDG, FUC

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	1.15	9/2066 (0.4%)	1.60	38/2819 (1.3%)
2	B	1.17	5/1253 (0.4%)	1.58	21/1718 (1.2%)
All	All	1.16	14/3319 (0.4%)	1.59	59/4537 (1.3%)

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	1	0
2	B	2	0
4	A	1	0
5	B	2	0
All	All	6	0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	376	GLU	CD-OE2	12.47	1.39	1.25
1	A	81	GLU	CD-OE1	10.51	1.37	1.25
1	A	128	GLU	CD-OE2	8.23	1.34	1.25
1	A	39	GLU	CD-OE1	8.09	1.34	1.25
1	A	154	GLU	CD-OE2	8.07	1.34	1.25

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NE-CZ-NH1	22.07	131.34	120.30
1	A	114	ARG	NE-CZ-NH1	18.39	129.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	405	ARG	NE-CZ-NH1	13.91	127.25	120.30
1	A	114	ARG	NE-CZ-NH2	-13.29	113.66	120.30
2	B	303(B)	ASP	CB-CG-OD1	-11.30	108.12	118.30

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	226	THR	CB
4	A	1134	NDG	C2
2	B	302	THR	CB
2	B	366	THR	CB
5	B	2912	NAG	C2,C5

There are no planarity outliers.

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	2003	0	1855	46	0
2	B	1213	0	1150	34	0
3	A	14	0	13	4	0
4	A	38	0	34	5	0
5	B	28	0	25	5	0
6	A	15	0	10	1	0
7	A	259	0	0	6	1
7	B	171	0	0	5	0
All	All	3741	0	3087	82	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 13.

The worst 5 of 82 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:B:297:ASN:ND2	2:B:297:ASN:H	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:ASN:N	2:B:297:ASN:HD22	1.56	0.88
2:B:285:GLN:HE22	5:B:2911:NAG:H83	1.43	0.83
4:A:1132(A):FUC:H3	4:A:1134:NDG:H6C1	1.59	0.82
2:B:297:ASN:H	2:B:297:ASN:HD22	0.86	0.80

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)
7:A:1308:HOH:O	7:A:1308:HOH:O[8_665]	1.81	0.39

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	254/256 (99%)	242 (95%)	12 (5%)	0	100	100
2	B	151/153 (99%)	144 (95%)	6 (4%)	1 (1%)	26	19
All	All	405/409 (99%)	386 (95%)	18 (4%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	ASP

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	205/208 (99%)	195 (95%)	10 (5%)	31	25
2	B	126/128 (98%)	115 (91%)	11 (9%)	13	7
All	All	331/336 (98%)	310 (94%)	21 (6%)	22	16

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	ILE
2	B	284	VAL
2	B	375	ASP
1	A	216	ILE
2	B	376	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
2	B	308	HIS
2	B	285	GLN
1	A	117	HIS
2	B	297	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 ⓘ

5 carbohydrates 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	$\# Z > 2$
4	FUC	A	1132(A)	4	10,10,11	2.79	3 (30%)	14,14,16	3.57	5 (35%)
4	NAG	A	1133	1,4	14,14,15	0.64	0	15,19,21	2.75	6 (40%)
4	NDG	A	1134	4	14,14,15	0.72	0	15,19,21	2.90	4 (26%)
5	NAG	B	2911	2,5	14,14,15	0.75	0	15,19,21	1.70	3 (20%)
5	NAG	B	2912	5	14,14,15	1.71	5 (35%)	15,19,21	2.71	7 (46%)

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	FUC	A	1132(A)	4	-	0/0/17/20	0/1/1/1
4	NAG	A	1133	1,4	-	0/6/23/26	0/1/1/1
4	NDG	A	1134	4	1/1/5/7	0/6/23/26	1/1/1/1
5	NAG	B	2911	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2912	5	2/2/5/7	0/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1132(A)	FUC	C2-C3	-2.22	1.49	1.52
5	B	2912	NAG	O3-C3	2.15	1.48	1.43
5	B	2912	NAG	C4-C3	2.35	1.58	1.52
5	B	2912	NAG	C3-C2	2.36	1.57	1.52
4	A	1132(A)	FUC	C4-C3	2.49	1.58	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1132(A)	FUC	C2-C3-C4	-7.22	98.78	111.04
4	A	1133	NAG	C3-C2-N2	-4.93	98.76	110.56
5	B	2912	NAG	O7-C7-C8	-4.78	113.29	122.06
5	B	2912	NAG	O6-C6-C5	-4.20	97.44	111.33
4	A	1133	NAG	O3-C3-C2	-4.12	100.94	109.11

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1134	NDG	C2
5	B	2912	NAG	C2
5	B	2912	NAG	C5

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1134	NDG	C1-C2-C3-C4-C5-O

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1132(A)	FUC	4	0
4	A	1133	NAG	1	0
4	A	1134	NDG	5	0
5	B	2911	NAG	4	0
5	B	2912	NAG	3	0

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	NAG	A	1131	1	14,14,15	0.83	0	15,19,21	2.14	2 (13%)
6	BZS	A	430	-	9,15,15	1.07	1 (11%)	12,19,19	1.30	2 (16%)

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	NAG	A	1131	1	-	0/6/23/26	0/1/1/1
6	BZS	A	430	-	-	0/6/12/12	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	430	BZS	CB-CA	-2.01	1.52	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1131	NAG	C2-N2-C7	-5.58	115.87	123.04
3	A	1131	NAG	C4-C3-C2	-5.21	103.12	111.23
6	A	430	BZS	CZ-CE2-CD2	-2.39	116.69	120.19
6	A	430	BZS	CB-CA-C	-2.31	106.50	111.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1131	NAG	4	0
6	A	430	BZS	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.