



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 10:05 PM GMT

PDB ID : 1CEB
Title : THE STRUCTURE OF THE NON-COVALENT COMPLEX OF RECOMBINANT KRINGLE 1 DOMAIN OF HUMAN PLASMINOGEN WITH AMCHA (TRANS-4-AMINOMETHYLCYCLOHEXANE-1-CARBOXYLIC ACID)
Authors : Tulinsky, A.; Mathews, I.I.
Deposited on : 1995-12-03
Resolution : 2.07 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

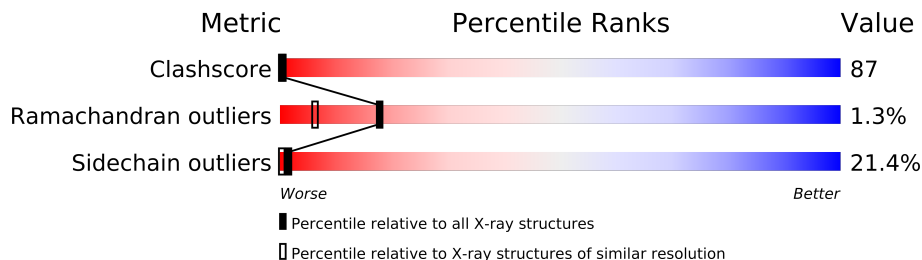
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.07 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	79885	1390 (2.08-2.04)
Ramachandran outliers	78287	1381 (2.08-2.04)
Sidechain outliers	78261	1381 (2.08-2.04)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	88	
1	B	88	

2 Entry composition i

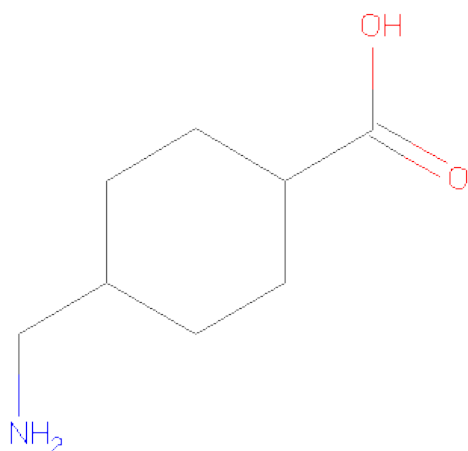
There are 3 unique types of molecules in this entry. The entry contains 1448 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PLASMINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	0	0	0
			641	390	115	129	7			
1	B	80	Total	C	N	O	S	0	0	0
			635	387	112	129	7			

- Molecule 2 is TRANS-4-AMINOMETHYLCYCLOHEXANE-1-CARBOXYLICACID (three-letter code: AMH) (formula: C₈H₁₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	8	1	2		
2	B	1	Total	C	N	O	0	0
			11	8	1	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total 81	O 81	0	0
3	B	69	Total 69	O 69	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.30Å 51.70Å 46.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.07	Depositor
% Data completeness (in resolution range)	57.0 (7.00-2.07)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1448	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.09	0/660	2.24	18/895 (2.0%)
1	B	1.21	1/654 (0.2%)	2.24	31/888 (3.5%)
All	All	1.15	1/1314 (0.1%)	2.24	49/1783 (2.7%)

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	3
1	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	CYS	CB-SG	-5.15	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	NE-CZ-NH2	27.85	134.23	120.30
1	A	46	GLU	OE1-CD-OE2	9.70	134.94	123.30
1	B	17	LYS	CA-CB-CG	9.42	134.12	113.40
1	A	51	ARG	NE-CZ-NH1	-9.17	115.72	120.30
1	A	51	ARG	NH1-CZ-NH2	-8.90	109.61	119.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	CYS	Mainchain
1	A	68	GLU	Mainchain
1	A	70	ARG	Sidechain
1	B	58	GLN	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	641	0	583	146	1
1	B	635	0	572	79	0
2	A	11	0	13	1	0
2	B	11	0	14	2	0
3	A	81	0	0	14	2
3	B	69	0	0	3	1
All	All	1448	0	1182	216	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 87.

The worst 5 of 216 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:64:THR:HG23	1:A:66:ASP:H	1.09	1.18
1:A:3:THR:HG22	1:A:79:CYS:CB	1.80	1.10
1:A:1(A):GLU:OE1	1:A:1(A):GLU:CA	1.92	1.09
1:A:28:THR:HB	1:A:32:ARG:HG3	1.22	1.09
1:A:28:THR:HB	1:A:32:ARG:CG	1.86	1.05

All (2) 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	Distance(Å)	Clash(Å)
3:A:369:HOH:O	3:B:236:HOH:O[2_544]	1.94	0.26
1:A:15:LYS:NZ	3:A:326:HOH:O[2_554]	2.10	0.10

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	78/88 (89%)	71 (91%)	6 (8%)	1 (1%)	18	6
1	B	78/88 (89%)	71 (91%)	6 (8%)	1 (1%)	18	6
All	All	156/176 (89%)	142 (91%)	12 (8%)	2 (1%)	18	6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	PRO
1	B	45	LEU

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	73/81 (90%)	55 (75%)	18 (25%)	1	0
1	B	72/81 (89%)	59 (82%)	13 (18%)	2	0
All	All	145/162 (90%)	114 (79%)	31 (21%)	1	0

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	79	CYS
1	B	35	PHE
1	A	73	TYR
1	B	2	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	31	HIS
1	B	31	HIS
1	B	55	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	$\# Z > 2$
2	AMH	A	90	-	11,11,11	1.49	2 (18%)	14,14,14	2.45	5 (35%)
2	AMH	B	90	-	11,11,11	1.78	3 (27%)	14,14,14	2.72	7 (50%)

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	AMH	A	90	-	-	0/6/16/16	0/1/1/1
2	AMH	B	90	-	-	0/6/16/16	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	90	AMH	C7-C4	4.07	1.65	1.53
2	A	90	AMH	C7-C4	2.91	1.62	1.53
2	B	90	AMH	C3-C2	-2.55	1.46	1.52
2	B	90	AMH	C5-C4	2.29	1.58	1.52
2	A	90	AMH	C2-C1	-2.10	1.47	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	90	AMH	O2-C8-O1	-6.07	110.35	124.07
2	A	90	AMH	C6-C1-C2	5.17	121.81	109.70
2	B	90	AMH	C4-C7-N	-4.59	95.66	112.88
2	A	90	AMH	C2-C1-C8	4.12	120.10	111.37
2	A	90	AMH	C5-C4-C3	3.38	117.06	109.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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.