wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 03:09 PM EDT

PDB ID	:	1OXG
Title	:	Crystal structure of a complex formed between organic solvent treated bovine alpha-chymotrypsin and its autocatalytically produced highly potent 14-residue peptide at 2.2 resolution
Authors	:	Singh, N.; Jabeen, T.; Sharma, S.; Roy, I.; Gupta, M.N.; Bilgrami, S.; Singh, T.P.
Deposited on	:	2003-04-02
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

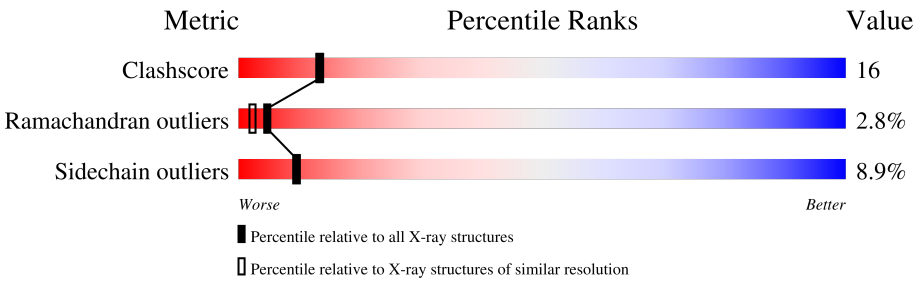
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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	245	76% 18% • •
2	B	14	43% 43% 14%

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
3	SO4	A	1004	-	X	-	-
3	SO4	B	1006	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2115 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.

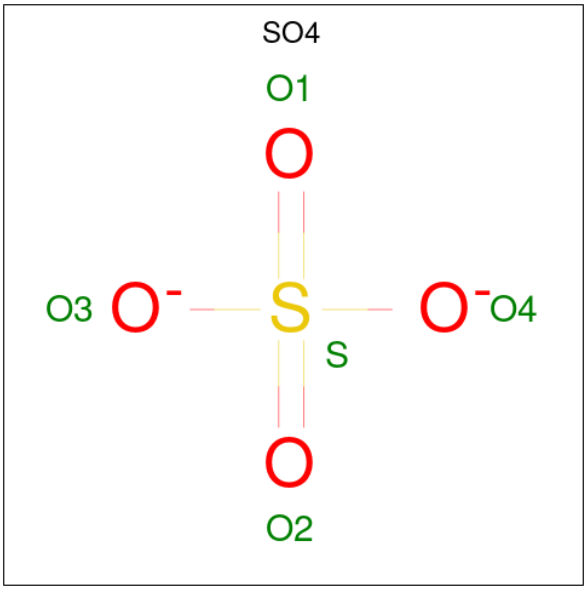
- Molecule 1 is a protein called Chymotrypsinogen A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	1767	1110	299	346	12	0	0	0

- Molecule 2 is a protein called Chymotrypsinogen A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	14	88	57	16	15	0	0	0

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



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	221	Total O 221 221	0	0
4	B	9	Total O 9 9	0	0

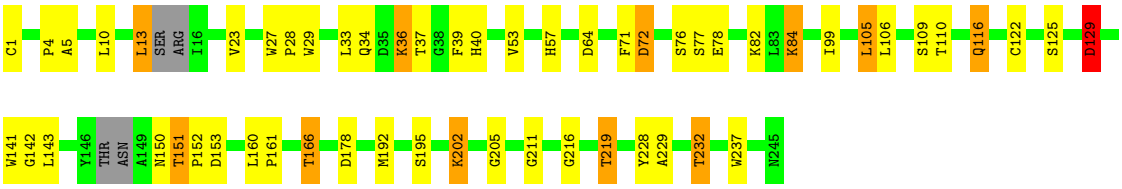
3 Residue-property plots (i)

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.

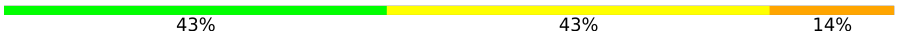
• Molecule 1: Chymotrypsinogen A

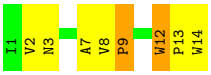
Chain A:



• Molecule 2: Chymotrypsinogen A

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	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	56.19Å 76.38Å 105.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.69 – 2.20	Depositor
% Data completeness (in resolution range)	98.8 (19.69-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.192 , 0.207	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2115	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: 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	A	0.80	0/1801	1.01	3/2453 (0.1%)
2	B	1.32	1/93 (1.1%)	3.01	7/127 (5.5%)
All	All	0.83	1/1894 (0.1%)	1.19	10/2580 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	12	TRP	CB-CG	-5.02	1.41	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	8	VAL	C-N-CD	-15.55	86.40	120.60
2	B	9	PRO	CA-N-CD	-15.21	90.21	111.50
2	B	9	PRO	N-CA-CB	13.17	119.10	103.30
2	B	8	VAL	C-N-CA	12.86	176.00	122.00
2	B	9	PRO	N-CD-CG	9.68	117.72	103.20

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	A	1767	0	1743	54	0
2	B	88	0	66	5	0
3	A	25	0	0	1	0
3	B	5	0	0	0	0
4	A	221	0	0	9	0
4	B	9	0	0	2	0
All	All	2115	0	1809	58	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 16.

The worst 5 of 58 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:A:84:LYS:HE3	1:A:110:THR:HB	1.32	1.08
1:A:141:TRP:HB3	1:A:152:PRO:HB3	1.13	1.08
1:A:143:LEU:HD23	1:A:150:ASN:ND2	1.72	1.04
1:A:143:LEU:CD2	1:A:150:ASN:ND2	2.26	0.99
1:A:84:LYS:HE2	1:A:84:LYS:H	1.27	0.99

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	A	235/245 (96%)	221 (94%)	10 (4%)	4 (2%)	9 6
2	B	12/14 (86%)	8 (67%)	1 (8%)	3 (25%)	0 0
All	All	247/259 (95%)	229 (93%)	11 (4%)	7 (3%)	5 2

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	SER
2	B	2	VAL
2	B	3	ASN
2	B	9	PRO
1	A	142	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	A	196/200 (98%)	178 (91%)	18 (9%)	9 9
2	B	6/11 (54%)	6 (100%)	0	100 100
All	All	202/211 (96%)	184 (91%)	18 (9%)	9 9

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	MET
1	A	232	THR
1	A	219	THR
1	A	125	SER
1	A	166	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	236	ASN
1	A	240	GLN
1	A	150	ASN
1	A	18	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	A	1005	-	4,4,4	2.12	2 (50%)	6,6,6	0.35	0
3	SO4	B	1006	-	4,4,4	3.80	3 (75%)	6,6,6	1.65	1 (16%)
3	SO4	A	1002	-	4,4,4	1.41	1 (25%)	6,6,6	0.91	0
3	SO4	A	1004	-	4,4,4	1.27	0	6,6,6	3.68	4 (66%)
3	SO4	A	1001	-	4,4,4	2.12	2 (50%)	6,6,6	0.51	0
3	SO4	A	1003	-	4,4,4	2.12	2 (50%)	6,6,6	0.22	0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1006	SO4	O1-S	5.42	1.75	1.46
3	B	1006	SO4	O2-S	4.45	1.70	1.46
3	A	1003	SO4	O1-S	3.53	1.65	1.46
3	A	1005	SO4	O1-S	3.52	1.65	1.46
3	A	1001	SO4	O1-S	3.37	1.64	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1004	SO4	O4-S-O1	-4.82	84.16	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1004	SO4	O4-S-O2	-4.79	84.30	109.31
3	A	1004	SO4	O4-S-O3	-4.79	88.63	109.06
3	A	1004	SO4	O3-S-O2	2.92	124.54	109.31
3	B	1006	SO4	O3-S-O1	-2.34	97.09	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	SO4	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 (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.