

Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 12:38 AM EDT

PDB ID : 3K65

Title: Crystal Structure of Prethombin-2/Fragment-2 Complex

Authors : Adams, T.E.; Huntington, J.A.

Deposited on : 2009-10-08

Resolution : 1.85 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
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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

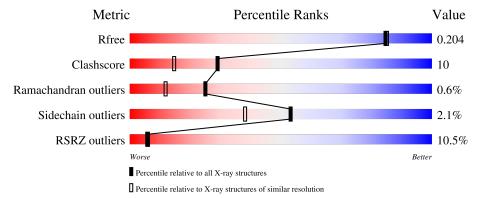
Validation Pipeline (wwPDB-VP) : 2.35

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 1.85 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 $(\# \mathrm{Entries})$	Similar resolution $(\#\text{Entries, resolution range}(\mathring{A}))$		
R_{free}	130704	2469 (1.86-1.86)		
Clashscore	141614	2625 (1.86-1.86)		
Ramachandran outliers	138981	2592 (1.86-1.86)		
Sidechain outliers	138945	2592 (1.86-1.86)		
RSRZ outliers	127900	2436 (1.86-1.86)		

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% 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	A	116	14%	61%	7% •	31%			
2	В	308	7%	70%		18% • 11%			



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3172 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 Prothrombin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	80	Total 618	C 386	N 108	O 118	S 6	0	1	0

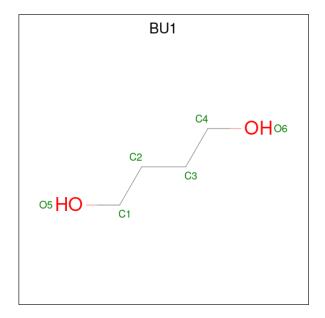
• Molecule 2 is a protein called Prothrombin.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
2	В	274	Total 2272	C 1465	N 395	O 398	S 14	0	10	0	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	525	ALA	SER	engineered mutation	UNP P00734

• Molecule 3 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: $C_4H_{10}O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 4 2	0	0
3	A	1	Total C O 6 4 2	0	0

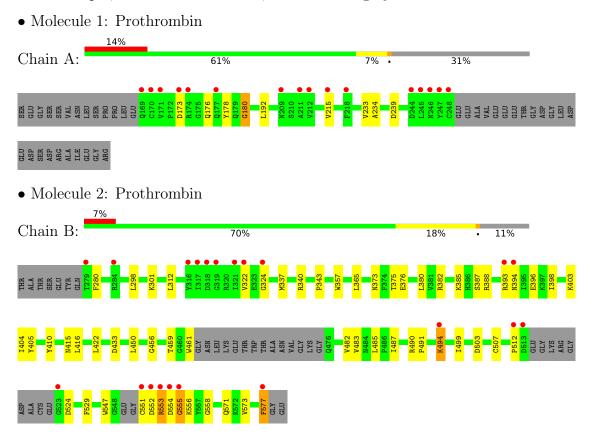
\bullet Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	84	Total O 84 84	0	0
4	В	186	Total O 186 186	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 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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	73.53Å 73.53Å 205.88Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.20 - 1.85	Depositor
resolution (A)	50.17 - 1.85	EDS
% Data completeness	98.7 (51.20-1.85)	Depositor
(in resolution range)	98.7 (50.17-1.85)	EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	$3.20 \; (at \; 1.86 \text{Å})$	Xtriage
Refinement program	CNS	Depositor
P.P.	0.213 , 0.229	Depositor
R, R_{free}	0.209 , 0.204	DCC
R_{free} test set	2467 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 61.1	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3172	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: BU1

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.31	0/634	0.53	0/863	
2	В	0.32	0/2330	0.69	4/3151 (0.1%)	
All	All	0.32	0/2964	0.66	4/4014 (0.1%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	553	ARG	N-CA-C	8.28	133.35	111.00
2	В	554	ASP	N-CA-C	-7.19	91.60	111.00
2	В	555	GLY	N-CA-C	-6.65	96.48	113.10
2	В	552	ASP	N-CA-C	6.27	127.94	111.00

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	A	618	0	556	4	0
2	В	2272	0	2217	50	0
3	A	12	0	20	2	0
4	A	84	0	0	1	0
4	В	186	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3172	0	2793	55	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 10.

All (55) 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:512:PRO:HA	2:B:555:GLY:HA3	1.52	0.92
2:B:490[B]:ARG:NE	2:B:494:LYS:HE2	1.90	0.86
2:B:490[B]:ARG:HE	2:B:494:LYS:HE2	1.46	0.79
2:B:324:GLY:HA2	2:B:483[B]:VAL:HG22	1.66	0.76
2:B:551:CYS:HA	2:B:556:LYS:HE2	1.67	0.75
2:B:551:CYS:HA	2:B:556:LYS:CE	2.19	0.73
2:B:388:ARG:HB2	2:B:461[A]:TRP:CE3	2.26	0.70
2:B:490[A]:ARG:HB3	2:B:491:PRO:HD3	1.76	0.68
3:A:600:BU1:H31	2:B:373:ASN:HD21	1.59	0.67
2:B:512:PRO:HA	2:B:555:GLY:CA	2.24	0.67
2:B:376:GLU:H	2:B:376:GLU:CD	1.98	0.66
2:B:485:LEU:HD11	2:B:551:CYS:HB2	1.78	0.65
2:B:490[B]:ARG:NH2	2:B:503:ASP:OD1	2.31	0.64
1:A:178:TYR:CZ	1:A:180:GLY:HA3	2.34	0.62
2:B:388:ARG:HB2	2:B:461[B]:TRP:CD1	2.37	0.59
2:B:375:THR:HB	2:B:376:GLU:OE2	2.02	0.59
2:B:573:VAL:O	2:B:577:PHE:HD2	1.89	0.56
2:B:337:MET:HG2	2:B:461[B]:TRP:CZ3	2.40	0.56
2:B:322:VAL:HG13	2:B:322:VAL:O	2.06	0.54
2:B:301:LYS:HE3	4:B:854:HOH:O	2.06	0.54
2:B:403:LYS:HD3	2:B:405:TYR:OH	2.09	0.53
2:B:450[A]:LEU:HD12	2:B:487:ILE:HD13	1.91	0.53
2:B:393:ARG:HG2	2:B:394:ASN:ND2	2.23	0.53
2:B:551:CYS:HB3	4:B:813:HOH:O	2.09	0.52
2:B:490[B]:ARG:HE	2:B:494:LYS:CE	2.20	0.51
2:B:298:LEU:CD1	2:B:433:ASP:HB3	2.42	0.50
2:B:382:ARG:HD2	2:B:396:GLU:OE2	2.12	0.49
2:B:324:GLY:CA	2:B:483[B]:VAL:HG22	2.39	0.49
2:B:380:LEU:C	2:B:380:LEU:HD12	2.33	0.49
2:B:499:ILE:HD12	2:B:547:TRP:CZ3	2.48	0.49
1:A:173:ASP:O	1:A:176:GLN:HG3	2.13	0.49
2:B:461[B]:TRP:HZ3	4:B:651:HOH:O	1.95	0.49
2:B:490[B]:ARG:HG2	2:B:494:LYS:HD3	1.95	0.48

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A + a 1	A4 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ (\mathring{\rm A})$	overlap (Å)
2:B:524:ASP:HB3	4:B:622:HOH:O	2.13	0.48
1:A:234:ALA:HB3	1:A:239:ASP:HB3	1.96	0.47
2:B:450[B]:LEU:HD12	4:B:859:HOH:O	2.14	0.47
2:B:577:PHE:CD2	2:B:577:PHE:N	2.83	0.47
2:B:357:TRP:CE3	2:B:422[A]:LEU:HG	2.50	0.47
2:B:365:LEU:HD13	2:B:404:ILE:HG21	1.97	0.46
2:B:459:THR:HG22	2:B:482[A]:VAL:HG22	1.98	0.46
2:B:340:ARG:HD2	2:B:343:PRO:O	2.16	0.46
2:B:324:GLY:HA2	2:B:482[A]:VAL:O	2.17	0.44
2:B:415:ASN:O	2:B:416:LEU:HB2	2.18	0.44
2:B:456:GLY:HA3	2:B:529:PHE:CZ	2.54	0.43
2:B:298:LEU:HD11	2:B:433:ASP:HB3	2.01	0.43
2:B:558:GLY:HA3	4:B:813:HOH:O	2.18	0.42
1:A:192:LEU:HD13	1:A:233:VAL:HA	2.02	0.42
2:B:403:LYS:HD3	2:B:405:TYR:CZ	2.54	0.42
2:B:485:LEU:HD11	2:B:551:CYS:CB	2.49	0.42
2:B:382:ARG:HG2	2:B:398:ILE:HG12	2.02	0.41
2:B:280:PHE:HE1	2:B:571:GLN:HB2	1.85	0.41
2:B:324:GLY:HA2	2:B:483[B]:VAL:CG2	2.44	0.41
2:B:385:LYS:HE3	2:B:387:SER:O	2.22	0.40
3:A:599:BU1:H11	4:A:738:HOH:O	2.21	0.40
2:B:450[A]:LEU:HD12	2:B:487:ILE:CD1	2.52	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	A	79/116 (68%)	74 (94%)	4 (5%)	1 (1%)	12 3
2	В	275/308~(89%)	262 (95%)	12 (4%)	1 (0%)	34 19
All	All	354/424 (84%)	336 (95%)	16 (4%)	2 (1%)	25 12



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	GLY
2	В	553	ARG

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	63/94 (67%)	62 (98%)	1 (2%)	62 49
2	В	239/267 (90%)	234 (98%)	5 (2%)	53 38
All	All	302/361 (84%)	296 (98%)	6 (2%)	53 40

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	VAL
2	В	312	LEU
2	В	410	TYR
2	В	494	LYS
2	В	507	CYS
2	В	577	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	198	GLN
2	В	373	ASN
2	В	394	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)

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	Tuno	Chain	Res Link		В	ond leng	${ m gths}$	В	ond ang	gles
IVIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BU1	A	599	-	5,5,5	0.37	0	4,4,4	0.40	0
3	BU1	A	600	-	5,5,5	0.37	0	4,4,4	0.42	0

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	BU1	A	599	-	-	0/3/3/3	-
3	BU1	A	600	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	599	BU1	1	0
3	A	600	BU1	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)

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	80/116 (68%)	0.83	16 (20%) 1 1	28, 40, 59, 62	0
2	В	274/308 (88%)	0.45	21 (7%) 13 13	22, 34, 63, 83	0
All	All	354/424 (83%)	0.54	37 (10%) 6 6	22, 35, 61, 83	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	551	CYS	6.8
2	В	554	ASP	5.4
2	В	555	GLY	5.3
2	В	577	PHE	5.0
2	В	513	ASP	4.6
2	В	553	ARG	4.5
1	A	170	CYS	4.2
1	A	248	CYS	3.9
2	В	318	ASP	3.9
1	A	215	VAL	3.6
2	В	552	ASP	3.5
1	A	246	ASN	3.4
1	A	212	VAL	3.3
2	В	512	PRO	3.3
2	В	279	THR	3.2
1	A	173	ASP	3.2
1	A	218	PHE	3.1
2	В	322	VAL	3.0
2	В	319	GLY	3.0
1	A	177	GLN	3.0
2	В	317	ILE	2.9
2	В	316	TYR	2.9
2	В	284	ARG	2.9
2	В	324	GLY	2.7

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Mol	Chain	Res	$\overline{\text{Type}}$	RSRZ	
1	A	245[A]	LEU	2.7	
1	A	244	ASP	2.7	
2	В	321	ILE	2.6	
2	В	393	ARG	2.4	
2	В	394	ASN	2.4	
1	A	211	ALA	2.3	
1	A	209	ASN	2.3	
1	A	169	GLN	2.3	
1	A	171	VAL	2.2	
2	В	523	GLY	2.2	
1	A	247	TYR	2.2	
1	A	174	ARG	2.1	
2	В	494	LYS	2.1	

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	BU1	A	599	6/6	0.65	0.29	64,66,67,67	0
3	BU1	A	600	6/6	0.65	0.31	71,72,73,74	0

6.5 Other polymers (i)

There are no such residues in this entry.

