

Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 02:12 AM EDT

PDB ID : 3UD6

Title : Structural analyses of covalent enzyme-substrate analogue complexes reveal

strengths and limitations of de novo enzyme design

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Deposited on : 2011-10-27

Resolution : 2.09 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

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 : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

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

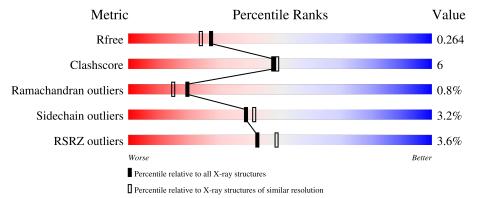
Validation Pipeline (wwPDB-VP) : 2.35

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 2.09 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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		
			3%		
1	A	258	80%	14%	• •



2 Entry composition (i)

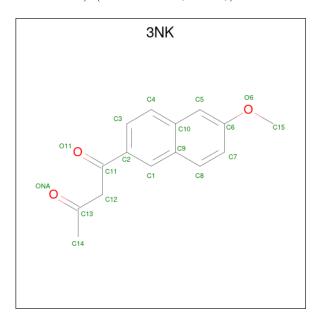
There are 4 unique types of molecules in this entry. The entry contains 2101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETRO-ALDOLASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	248	Total	С	N	О	S	0	9	0
1	Λ	240	2009	1273	349	379	8	0	2	

• Molecule 2 is 1-(6-METHOXYNAPHTHALEN-2-YL)BUTANE-1,3-DIONE (three-letter code: 3NK) (formula: C₁₅H₁₄O₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total 17	C 15		0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





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

• Molecule 4 is water.

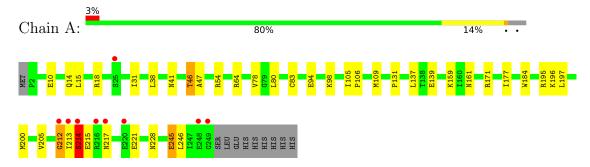
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	65	Total O 65 65	0	0



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.

• Molecule 1: RETRO-ALDOLASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	62.68Å 62.68Å 123.68Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.47 - 2.09	Depositor
rtesolution (A)	19.47 - 2.09	EDS
% Data completeness	99.3 (19.47-2.09)	Depositor
(in resolution range)	99.3 (19.47-2.09)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	6.75 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
P. P.	0.227 , 0.258	Depositor
R, R_{free}	0.212 , 0.264	DCC
R_{free} test set	868 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39 , 40.8	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2101	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.55% 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: 3NK, 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).

Mal	Chain	Bond	lengths	Bo	nd angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	1.05	0/2044	0.79	4/2755 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	54	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	64	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	64	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	18	ARG	NE-CZ-NH1	-5.11	117.75	120.30

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	A	2009	0	2075	23	0
2	A	17	0	14	4	0
3	A	10	0	0	0	0
4	A	65	0	0	2	0
All	All	2101	0	2089	25	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 6.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:A:46:THR:HG21	4:A:337:HOH:O	1.66	0.95
1:A:213:ILE:O	1:A:214:SER:HB3	1.72	0.88
1:A:161:ASN:HD21	1:A:184:TRP:HE1	1.38	0.72
2:A:300:3NK:H142	2:A:300:3NK:O11	1.93	0.68
2:A:300:3NK:O11	2:A:300:3NK:C14	2.42	0.68
1:A:10:GLU:O	1:A:14:GLN:HG2	1.97	0.64
1:A:139:GLU:OE2	1:A:171[A]:ARG:HD2	2.05	0.57
1:A:109:MET:O	1:A:131:PRO:HD3	2.05	0.56
1:A:94:GLU:HG3	1:A:98:LYS:HE3	1.88	0.56
1:A:177:ILE:HD12	1:A:205:VAL:HG11	1.89	0.54
1:A:83:CYS:SG	2:A:300:3NK:H153	2.49	0.52
1:A:212:GLY:O	1:A:215:GLU:OE2	2.30	0.49
1:A:245:GLU:HG3	1:A:246:LEU:N	2.27	0.49
1:A:41:ASN:ND2	1:A:228:ASN:HD22	2.11	0.49
1:A:159:LYS:HD3	2:A:300:3NK:C12	2.45	0.46
1:A:214:SER:OG	1:A:215:GLU:N	2.46	0.46
1:A:41:ASN:HD21	1:A:228:ASN:HB3	1.81	0.46
1:A:31:ILE:HG22	1:A:106:PRO:HG3	1.97	0.45
1:A:47:ALA:HB1	1:A:78:VAL:HG11	1.99	0.44
1:A:215:GLU:O	1:A:217:ASN:N	2.48	0.44
1:A:80:LEU:HG	1:A:105:ILE:HD11	2.00	0.43
1:A:197:LEU:HA	1:A:200:MET:HE3	2.00	0.43
1:A:139:GLU:OE2	1:A:171[B]:ARG:HD3	2.18	0.43
1:A:195:ARG:NH2	1:A:221[B]:GLU:OE1	2.52	0.42
1:A:217:ASN:HB3	4:A:381:HOH:O	2.20	0.41

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	248/258 (96%)	240 (97%)	6 (2%)	2 (1%)	19 15	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	SER
1	A	212	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	224/232 (97%)	217 (97%)	7 (3%)	40 43

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	38	LEU
1	A	46	THR
1	A	137	LEU
1	A	196	LYS
1	A	214	SER
1	A	245	GLU

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	41	ASN
1	A	124	ASN
1	A	161	ASN
1	A	194	GLN



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)

3 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	Type Chain Res Link		Link	Bo	nd leng	ths	Bond angles		
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	401	-	4,4,4	0.24	0	6,6,6	0.35	0
3	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.25	0
2	3NK	A	300	1	11,18,19	2.78	2 (18%)	11,24,26	1.89	3 (27%)

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	3NK	A	300	1	-	4/6/31/32	0/0/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
2	A	300	3NK	C10-C9	-8.47	1.39	1.48

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(\AA)$	$\operatorname{Ideal}(ext{\AA})$
2	A	300	3NK	C2-C11	2.73	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	A	300	3NK	C13-C12-C11	-3.83	106.49	113.87
2	A	300	3NK	C9-C10-C4	3.23	121.27	117.38
2	A	300	3NK	C3-C2-C11	-2.28	115.38	119.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	3NK	C11-C12-C13-C14
2	A	300	3NK	O11-C11-C2-C3
2	A	300	3NK	O11-C11-C2-C1
2	A	300	3NK	C12-C11-C2-C3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	3NK	4	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	<RSRZ $>$	#R5	$\mathrm{SRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	248/258 (96%)	-0.07	9 (3%)	42 49	16, 26, 40, 62	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	GLY	5.6
1	A	214	SER	5.0
1	A	216	ARG	4.5
1	A	217	ASN	2.9
1	A	25	SER	2.8
1	A	248	GLU	2.7
1	A	213	ILE	2.7
1	A	212	GLY	2.1
1	A	220	GLU	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
2	3NK	A	300	17/18	0.50	0.23	40,55,60,61	0
3	SO4	A	401	5/5	0.94	0.19	52,53,55,55	0
3	SO4	A	402	5/5	0.98	0.15	39,42,44,45	0

6.5 Other polymers (i)

There are no such residues in this entry.

