

wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2020 – 09:19 PM BST

PDB ID : 4TY8

Title : An Ligand-observed Mass Spectrometry-based Approach Integrated into the

Fragment Based Lead Discovery Pipeline

Authors: Shui, W.; Yang, C.; Lin, J.; Chen, X.; Qin, S.; Chen, S.

Deposited on : 2014-07-08

Resolution : 2.78 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 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 : 2.13.1

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

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

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

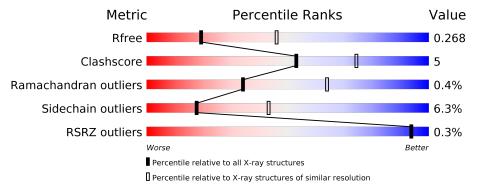
Validation Pipeline (wwPDB-VP) : 2.13.1

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 2.78 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 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	566	80%	14%	•	-
1	С	566	82%	12%	•	-
1	D	566	81%	13%	•	-
2	В	566	83%	12%	-	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16942 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 Polyprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	544	Total	С	Ν	О	S	0	0	0
1	A	944	4222	2664	744	783	31	U	0	
1	C	545	Total	С	N	О	S	0	0	0
1		040	4229	2669	745	784	31	U	U	
1	D	546	Total	С	N	О	S	0	0	0
1	ש	040	4234	2672	746	785	31			

• Molecule 2 is a protein called Polyprotein.

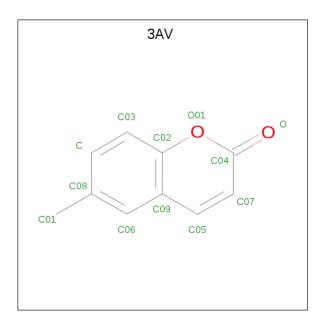
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	D	547	Total	С	N	О	S	0	0	0
	Ъ	047	4233	2669	746	786	32	0	0	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	550	MET	TRP	engineered mutation	UNP D0PY27

• Molecule 3 is 6-methyl-2H-chromen-2-one (three-letter code: 3AV) (formula: $C_{10}H_8O_2$).





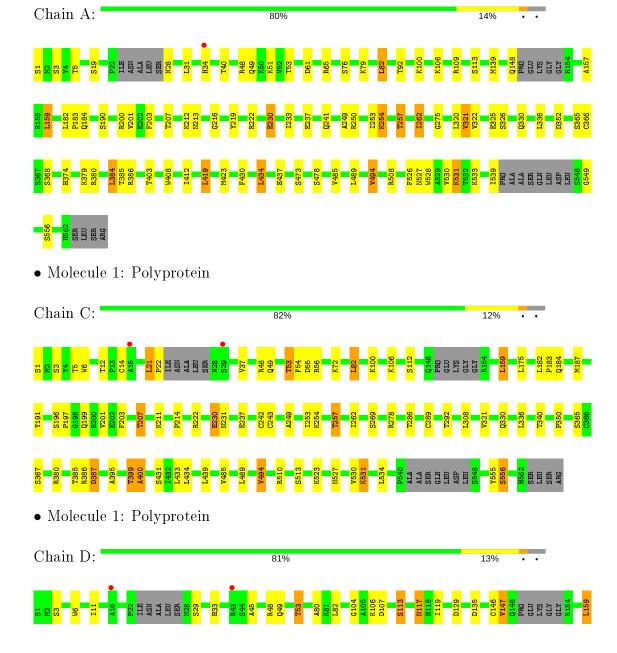
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 10 2	0	0
3	В	1	Total C O 12 10 2	0	0



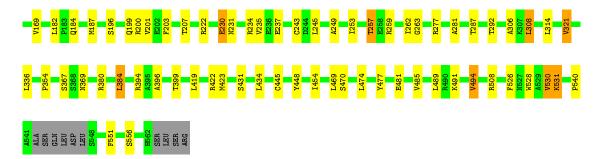
3 Residue-property plots (i)

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.

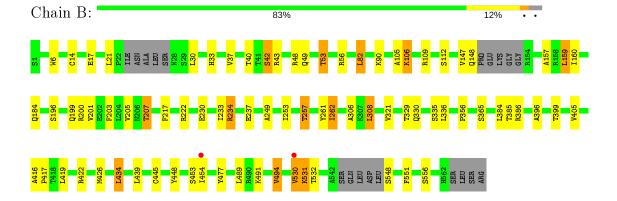
• Molecule 1: Polyprotein







• Molecule 2: Polyprotein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	101.94Å 102.07 Å 251.93 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 - 2.78	Depositor
Resolution (A)	49.96 - 2.78	EDS
% Data completeness	92.2 (50.00-2.78)	Depositor
(in resolution range)	92.2 (49.96-2.78)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.50 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0049, REFMAC 5.8.0049	Depositor
D.D.	0.207 , 0.268	Depositor
R, R_{free}	0.211 , 0.268	DCC
R_{free} test set	3119 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 18.0	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.069 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16942	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.77% 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: 3AV

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		
MIOI	Chain	77 1 1		RMSZ	# Z > 5	
1	A	0.54	0/4313	0.74	1/5852~(0.0%)	
1	С	0.54	0/4321	0.75	0/5864	
1	D	0.54	0/4326	0.75	0/5871	
2	В	0.53	0/4323	0.75	2/5865~(0.0%)	
All	All	0.54	0/17283	0.75	$3/23452 \ (0.0\%)$	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
2	В	234	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	419	LEU	CA-CB-CG	5.31	127.52	115.30
2	В	234	ARG	NE-CZ-NH2	-5.18	117.71	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	4222	0	4212	39	0
1	С	4229	0	4219	47	0
1	D	4234	0	4224	50	0
2	В	4233	0	4228	46	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	8	1	0
3	В	12	0	8	1	0
All	All	16942	0	16899	182	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 5.

The worst 5 of 182 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:C:253:ILE:O	1:C:257:THR:HG23	1.63	0.96
2:B:49:GLN:O	2:B:53:THR:HG23	1.68	0.92
1:A:49:GLN:O	1:A:53:THR:HG22	1.69	0.91
2:B:49:GLN:O	2:B:53:THR:CG2	2.23	0.86
1:A:237:GLU:HG3	1:A:257:THR:HG21	1.59	0.84

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	536/566~(95%)	502 (94%)	32 (6%)	2 (0%)	34	64
1	С	537/566~(95%)	505 (94%)	30 (6%)	2 (0%)	34	64
1	D	538/566~(95%)	504 (94%)	31 (6%)	3 (1%)	25	54
2	В	539/566~(95%)	511 (95%)	27 (5%)	1 (0%)	47	76
All	All	2150/2264~(95%)	2022 (94%)	120 (6%)	8 (0%)	34	64

5 of 8 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	531	LYS
2	В	531	LYS
1	С	531	LYS
1	D	531	LYS
1	D	367	SER

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	$460/482 \; (95\%)$	426 (93%)	34 (7%)	13	34	
1	С	461/482 (96%)	433 (94%)	28 (6%)	18	45	
1	D	461/482 (96%)	436 (95%)	25 (5%)	22	50	
2	В	461/482 (96%)	432 (94%)	29 (6%)	18	43	
All	All	1843/1928 (96%)	1727 (94%)	116 (6%)	18	43	

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	329	THR
1	С	21	LEU
1	D	380	ARG
2	В	335	SER
2	В	494	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	199	GLN
1	С	28	ASN
1	D	199	GLN
2	В	273	ASN
1	С	33	HIS



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	Type	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	туре	Chain	nes	5 LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	$\mid \# Z > 2 \mid$
3	3AV	A	601	-	9,13,13	2.04	1 (11%)	10,18,18	1.59	3 (30%)
3	3AV	В	601	-	9,13,13	2.14	1 (11%)	10,18,18	1.75	3 (30%)

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	3AV	A	601	_	-	-	0/2/2/2
3	3AV	В	601	_	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\operatorname{Ideal}(ext{\AA})$
3	В	601	3AV	C07-C04	5.73	1.48	1.37

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
3	A	601	3AV	C07-C04	5.51	1.48	1.37

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
3	В	601	3AV	C05-C07-C04	3.06	122.25	118.45
3	В	601	3AV	C05-C09-C02	2.59	119.61	116.61
3	A	601	3AV	C05-C07-C04	2.55	121.62	118.45
3	A	601	3AV	O01-C02-C09	2.54	123.68	121.10
3	A	601	3AV	C05-C09-C02	2.33	119.31	116.61

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	${f Res}$	Type	Clashes	Symm-Clashes
3	A	601	3AV	1	0
3	В	601	3AV	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	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	544/566~(96%)	-0.22	1 (0%) 95 95	16, 30, 50, 71	0
1	С	545/566~(96%)	-0.27	2 (0%) 92 92	17, 30, 47, 71	0
1	D	546/566~(96%)	-0.23	2 (0%) 92 92	18, 30, 52, 81	0
2	В	547/566 (96%)	-0.26	2 (0%) 92 92	18, 29, 48, 91	0
All	All	2182/2264~(96%)	-0.24	7 (0%) 94 94	16, 30, 50, 91	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	29	SER	2.7
2	В	530	VAL	2.3
1	D	16	ALA	2.2
1	С	15	ALA	2.2
2	В	454	ILE	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	${f B-factors}({f A}^2)$	Q < 0.9
3	3AV	A	601	12/12	0.87	0.23	57,63,66,68	0
3	3AV	В	601	12/12	0.89	0.33	69,73,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.

