Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2016 – 06:16 PM EST

PDB ID	:	5HMF
Title	:	Crystal structure of triazine hydrolase variant (P214T/Y215H/E241Q)
Authors	:	Sugrue, E.; Carr, P.D.; Jackson, C.J.
Deposited on	:	2016-01-16
Resolution	:	1.84 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
http://wwpdb.org/validation/2016/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:

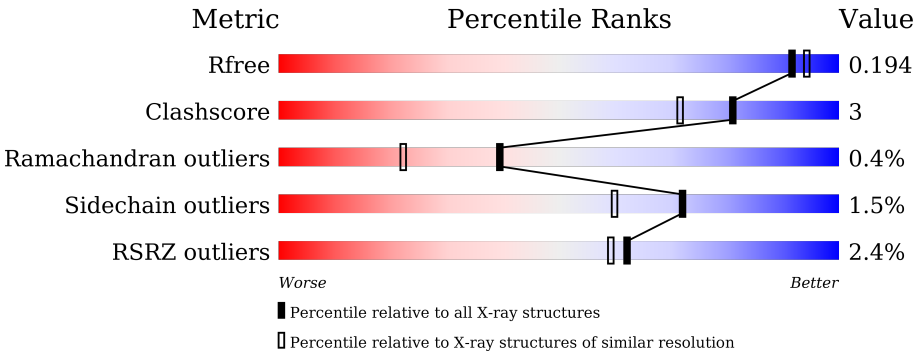
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.84 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))
R_{free}	91344	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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. 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	458	2% 91% 8%
1	B	458	3% 92% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14787 atoms, of which 6917 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 Triazine hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	H	N	O	S	0	14	0
			7047	2242	3491	629	668	17			
1	B	455	Total	C	H	N	O	S	0	4	0
			6916	2200	3426	621	653	16			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ASN	ASP	conflict	UNP Q6SJY7
A	131	PRO	LEU	conflict	UNP Q6SJY7
A	159	VAL	ALA	conflict	UNP Q6SJY7
A	214	THR	PRO	engineered mutation	UNP Q6SJY7
A	215	HIS	TYR	engineered mutation	UNP Q6SJY7
A	241	GLN	GLU	engineered mutation	UNP Q6SJY7
A	303	LEU	MET	conflict	UNP Q6SJY7
B	38	ASN	ASP	conflict	UNP Q6SJY7
B	131	PRO	LEU	conflict	UNP Q6SJY7
B	159	VAL	ALA	conflict	UNP Q6SJY7
B	214	THR	PRO	engineered mutation	UNP Q6SJY7
B	215	HIS	TYR	engineered mutation	UNP Q6SJY7
B	241	GLN	GLU	engineered mutation	UNP Q6SJY7
B	303	LEU	MET	conflict	UNP Q6SJY7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

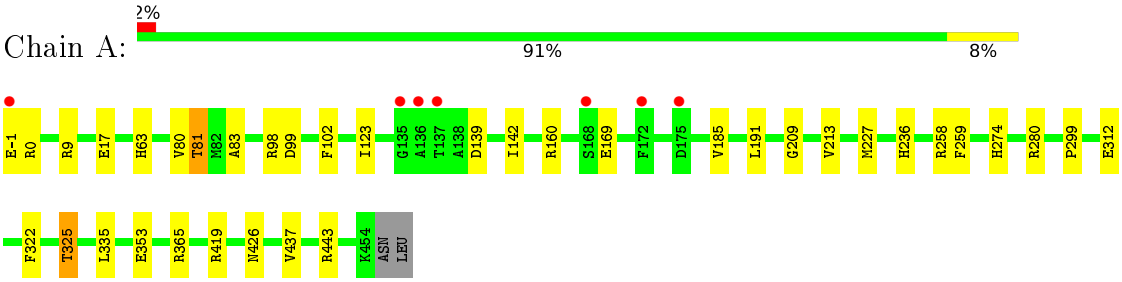
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	456	Total O 456 456	0	0
3	B	366	Total O 366 366	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

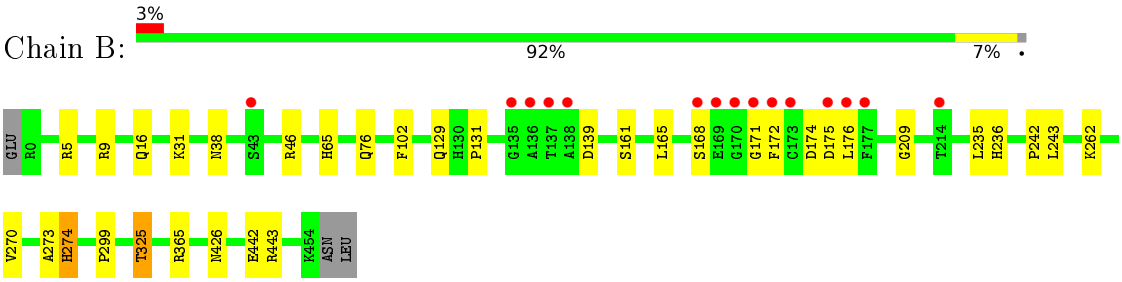
- Molecule 1: Triazine hydrolase

Chain A:



- Molecule 1: Triazine hydrolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.25Å 101.67Å 80.43Å 90.00° 104.02° 90.00°	Depositor
Resolution (Å)	45.97 – 1.84 55.54 – 1.84	Depositor EDS
% Data completeness (in resolution range)	93.5 (45.97-1.84) 88.8 (55.54-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.84Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.164 , 0.195 0.164 , 0.194	Depositor DCC
R_{free} test set	3428 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	14.3	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 51.6	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	14787	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.37 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.7742e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

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

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	0.49	0/3669	0.69	2/4994 (0.0%)
1	B	0.47	0/3582	0.62	0/4877
All	All	0.48	0/7251	0.66	2/9871 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	258	ARG	CG-CD-NE	-6.88	97.35	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	VAL	Mainchain,Peptide
1	A	81[A]	THR	Peptide
1	B	172	PHE	Peptide

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	3556	3491	3447	27	0
1	B	3490	3426	3408	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	456	0	0	7	0
3	B	366	0	0	8	0
All	All	7870	6917	6855	46	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 3.

All (46) 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:98:ARG:NH1	1:A:99:ASP:OD1	2.12	0.83
1:A:81[A]:THR:O	1:A:83:ALA:N	2.11	0.83
1:A:426:ASN:OD1	3:A:602:HOH:O	2.01	0.78
1:A:17:GLU:OE2	1:A:365[B]:ARG:NH2	2.16	0.78
1:B:426:ASN:ND2	3:B:602:HOH:O	2.14	0.74
1:B:442:GLU:OE1	3:B:601:HOH:O	2.11	0.69
1:B:5:ARG:NH2	3:B:609:HOH:O	2.27	0.67
1:A:280:ARG:NH1	1:A:312[B]:GLU:OE2	2.28	0.67
1:B:46:ARG:NH1	3:B:615:HOH:O	2.32	0.62
1:A:419:ARG:NH1	3:A:611:HOH:O	2.34	0.60
1:A:312[A]:GLU:OE1	3:A:603:HOH:O	2.17	0.58
1:B:168:SER:OG	1:B:175:ASP:OD2	2.21	0.57
1:B:139:ASP:OD1	3:B:603:HOH:O	2.17	0.57
1:A:322:PHE:HD2	1:A:335[B]:LEU:CD2	2.18	0.56
1:A:139[B]:ASP:OD1	1:A:139[B]:ASP:N	2.40	0.55
1:A:443:ARG:NH2	3:A:614:HOH:O	2.40	0.54
1:A:419:ARG:HG3	3:A:611:HOH:O	2.09	0.53
1:A:-1:GLU:H3	1:A:0:ARG:CB	2.21	0.53
1:B:242:PRO:O	1:B:243:LEU:HB2	2.10	0.52
1:A:-1:GLU:N	1:A:0:ARG:CB	2.73	0.51
1:B:65:HIS:CE1	1:B:129:GLN:HG2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLU:OE2	3:A:604:HOH:O	2.20	0.51
1:B:131:PRO:HA	1:B:161:SER:HB3	1.94	0.50
1:B:16:GLN:OE1	3:B:604:HOH:O	2.19	0.49
1:A:63:HIS:CD2	1:A:325:THR:HG22	2.47	0.49
1:A:123:ILE:HD11	1:A:335[B]:LEU:HB2	1.96	0.48
1:B:299:PRO:HG3	1:B:325:THR:CG2	2.42	0.48
1:A:185:VAL:HG13	1:A:227:MET:CE	2.44	0.47
1:B:9:ARG:NH2	3:B:628:HOH:O	2.46	0.47
1:A:209:GLY:HA2	1:A:236:HIS:O	2.15	0.47
1:A:299:PRO:HG3	1:A:325:THR:CG2	2.45	0.47
1:A:63:HIS:HD2	1:A:325:THR:HG22	1.80	0.47
1:B:273:ALA:O	1:B:274:HIS:HB2	2.15	0.45
1:A:142[B]:ILE:HD11	1:A:160:ARG:HG2	1.97	0.45
1:B:235:LEU:HB2	1:B:270:VAL:HG22	1.99	0.44
1:A:322:PHE:HD2	1:A:335[B]:LEU:HD21	1.82	0.44
1:B:299:PRO:HG3	1:B:325:THR:HG21	1.99	0.44
1:A:142[B]:ILE:HD13	1:A:191:LEU:CD1	2.47	0.44
1:B:161:SER:HA	1:B:209:GLY:O	2.17	0.43
1:B:443:ARG:NH1	3:B:644:HOH:O	2.52	0.43
1:B:165:LEU:HG	1:B:171:GLY:HA3	2.00	0.42
1:A:142[B]:ILE:HD13	1:A:191:LEU:HD11	2.00	0.42
1:A:213:VAL:HG22	1:A:259:PHE:CD1	2.55	0.42
1:B:209:GLY:HA2	1:B:236:HIS:O	2.19	0.42
1:A:312[A]:GLU:OE1	1:A:312[A]:GLU:N	2.51	0.42
1:A:9:ARG:NH2	3:A:639:HOH:O	2.54	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	468/458 (102%)	456 (97%)	10 (2%)	2 (0%)	39 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	457/458 (100%)	437 (96%)	18 (4%)	2 (0%)	39 22
All	All	925/916 (101%)	893 (96%)	28 (3%)	4 (0%)	39 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	274	HIS
1	A	325	THR
1	A	274	HIS
1	B	325	THR

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	372/366 (102%)	369 (99%)	3 (1%)	86 81
1	B	362/366 (99%)	353 (98%)	9 (2%)	55 37
All	All	734/732 (100%)	722 (98%)	12 (2%)	72 57

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	PHE
1	A	169	GLU
1	A	437	VAL
1	B	31	LYS
1	B	38	ASN
1	B	76	GLN
1	B	102	PHE
1	B	174	ASP
1	B	176	LEU
1	B	262	LYS
1	B	365[A]	ARG
1	B	365[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules 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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

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>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	456/458 (99%)	-0.34	7 (1%) 76 74	6, 14, 35, 71	0
1	B	455/458 (99%)	-0.15	15 (3%) 50 46	7, 17, 43, 86	0
All	All	911/916 (99%)	-0.24	22 (2%) 62 59	6, 15, 39, 86	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	SER	6.6
1	B	170	GLY	6.2
1	A	172	PHE	5.5
1	B	137	THR	5.4
1	B	172	PHE	5.3
1	B	173	CYS	5.2
1	B	176	LEU	5.1
1	A	136	ALA	4.5
1	B	171	GLY	4.0
1	B	175	ASP	3.8
1	B	169	GLU	3.3
1	B	136	ALA	3.2
1	A	135	GLY	3.0
1	A	137	THR	3.0
1	B	43	SER	2.8
1	B	138	ALA	2.7
1	B	214	THR	2.7
1	B	177	PHE	2.4
1	A	-1	GLU	2.3
1	A	175	ASP	2.1
1	B	135	GLY	2.0
1	A	168	SER	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	501	1/1	1.00	0.07	-1.60	17,17,17,17	1
2	ZN	B	501	1/1	0.99	0.05	-2.34	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.