Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 05:02 PM JST

PDB ID	:	5XOC
Title	:	Crystal structure of human Smad3-FoxH1 complex
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Deposited on	:	2017-05-27
Resolution	:	2.40 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:

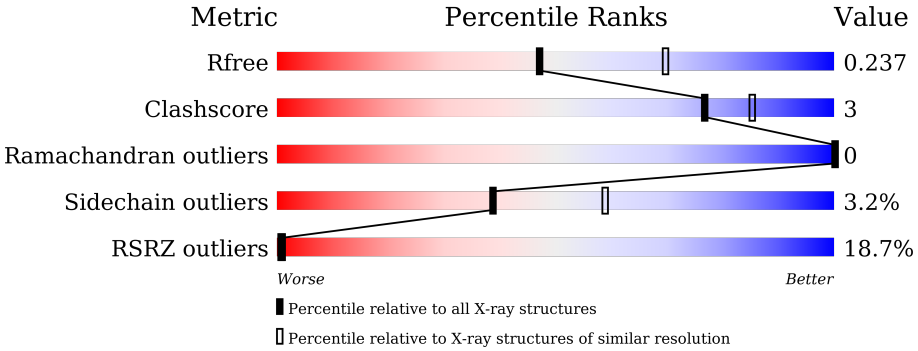
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	199	4%, 87%, 10%, • •
2	B	141	38%, 84%, 9%, • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2596 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 Mothers against decapentaplegic homolog 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	1547	982	271	281	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	GLY	-	expression tag	UNP P84022
A	219	PRO	-	expression tag	UNP P84022

- Molecule 2 is a protein called Thioredoxin 1,Forkhead box protein H1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	133	1013	654	161	194	4	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	205	MET	-	initiating methionine	UNP P0AA25
B	206	HIS	-	expression tag	UNP P0AA25
B	207	HIS	-	expression tag	UNP P0AA25
B	208	HIS	-	expression tag	UNP P0AA25
B	209	HIS	-	expression tag	UNP P0AA25
B	210	HIS	-	expression tag	UNP P0AA25
B	211	HIS	-	expression tag	UNP P0AA25
B	320	GLY	-	linker	UNP P0AA25
B	321	SER	-	linker	UNP P0AA25

- Molecule 3 is water.

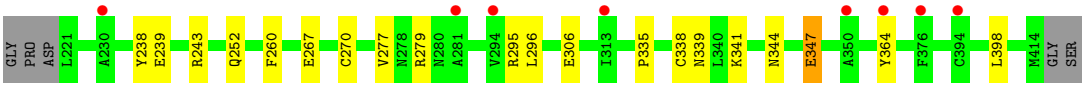
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	32	32	32	0	0
			Total	O		
3	B	4	4	4	0	0

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.

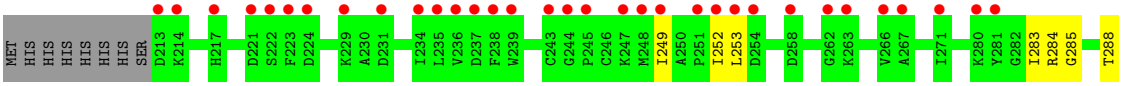
- Molecule 1: Mothers against decapentaplegic homolog 3

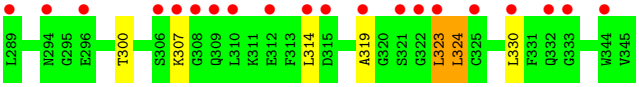
Chain A:



- Molecule 2: Thioredoxin 1,Forkhead box protein H1

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.87Å 131.87Å 91.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 2.40 19.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.88-2.40) 99.2 (19.88-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.41Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.196 , 0.235 0.200 , 0.237	Depositor DCC
R_{free} test set	963 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2596	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	0.28	0/1588	0.44	0/2160
2	B	0.23	0/1034	0.44	0/1405
All	All	0.26	0/2622	0.44	0/3565

There are no bond length outliers.

There are no bond angle outliers.

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	1547	0	1497	9	0
2	B	1013	0	1015	6	0
3	A	32	0	0	0	0
3	B	4	0	0	0	0
All	All	2596	0	2512	15	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 (15) 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:344:ASN:HB3	1:A:347:GLU:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:ALA:HB1	2:B:330:LEU:HD21	1.87	0.57
1:A:238:TYR:CZ	1:A:243:ARG:HD3	2.40	0.56
2:B:323:LEU:CB	2:B:324:LEU:HA	2.38	0.54
2:B:283:ILE:HD12	2:B:288:THR:HG21	1.93	0.51
2:B:252:ILE:HG23	2:B:307:LYS:HG2	1.94	0.50
1:A:239:GLU:OE1	1:A:279:ARG:HD3	2.12	0.50
2:B:285:GLY:O	2:B:288:THR:OG1	2.29	0.49
1:A:252:GLN:HG3	1:A:267:GLU:HG2	1.98	0.45
1:A:295:ARG:NH1	1:A:306:GLU:OE2	2.46	0.45
1:A:260:PHE:O	1:A:270:CYS:HB3	2.17	0.45
2:B:249:ILE:O	2:B:253:LEU:HG	2.19	0.43
1:A:341:LYS:HD3	1:A:344:ASN:HB2	2.03	0.41
1:A:296:LEU:HD13	1:A:398:LEU:HD21	2.02	0.40
1:A:335:PRO:HG2	1:A:338:CYS:SG	2.61	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	192/199 (96%)	186 (97%)	6 (3%)	0	100	100
2	B	131/141 (93%)	126 (96%)	5 (4%)	0	100	100
All	All	323/340 (95%)	312 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	169/172 (98%)	165 (98%)	4 (2%)	49	68
2	B	108/116 (93%)	103 (95%)	5 (5%)	27	43
All	All	277/288 (96%)	268 (97%)	9 (3%)	39	59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	VAL
1	A	339	ASN
1	A	347	GLU
1	A	364	TYR
2	B	284	ARG
2	B	300	THR
2	B	314	LEU
2	B	323	LEU
2	B	324	LEU

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

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)

There are no ligands in this entry.

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, 95th 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	194/199 (97%)	0.28	8 (4%)	37	36	34, 46, 87, 102	0
2	B	133/141 (94%)	1.71	53 (39%)	0	0	39, 104, 135, 151	0
All	All	327/340 (96%)	0.86	61 (18%)	1	1	34, 62, 125, 151	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	235	LEU	8.0
2	B	244	GLY	5.8
2	B	236	VAL	5.4
2	B	263	LYS	5.3
2	B	248	MET	5.1
2	B	223	PHE	4.8
2	B	213	ASP	4.8
2	B	237	ASP	4.7
2	B	262	GLY	4.6
2	B	231	ASP	4.1
2	B	221	ASP	4.0
1	A	281	ALA	3.9
2	B	266	VAL	3.8
2	B	249	ILE	3.6
2	B	280	LYS	3.6
2	B	308	GLY	3.6
2	B	296	GLU	3.6
2	B	229	LYS	3.5
2	B	267	ALA	3.5
2	B	247	LYS	3.5
2	B	281	TYR	3.4
2	B	224	ASP	3.4
1	A	376	PHE	3.3
2	B	332	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	234	ILE	3.2
2	B	239	TRP	3.2
2	B	243	CYS	3.1
2	B	253	LEU	3.1
2	B	319	ALA	3.1
2	B	312	GLU	3.1
2	B	289	LEU	2.9
1	A	230	ALA	2.8
2	B	251	PRO	2.8
2	B	294	ASN	2.7
2	B	238	PHE	2.7
1	A	350	ALA	2.7
2	B	252	ILE	2.6
2	B	323	LEU	2.6
1	A	394	CYS	2.6
2	B	325	CYS	2.6
2	B	306	SER	2.5
2	B	214	LYS	2.5
2	B	315	ASP	2.5
2	B	258	ASP	2.4
2	B	333	GLY	2.4
2	B	310	LEU	2.4
2	B	322	GLY	2.4
2	B	217	HIS	2.3
2	B	271	ILE	2.3
2	B	245	PRO	2.3
2	B	254	ASP	2.2
1	A	364	TYR	2.2
2	B	321	SER	2.2
2	B	307	LYS	2.2
2	B	344	TRP	2.1
2	B	330	LEU	2.1
1	A	313	ILE	2.1
2	B	309	GLN	2.0
1	A	294	VAL	2.0
2	B	222	SER	2.0
2	B	314	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.