wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2017 – 07:09 PM EST

PDB ID	:	5IJ7
Title	:	Structure of Hs/AcPRC2 in complex with a pyridone inhibitor
Authors	:	Gajiwala, K.S.; Brooun, A.; Deng, Y.-L.; Liu, W.
Deposited on	:	unknown
Resolution	:	2.62 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
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:

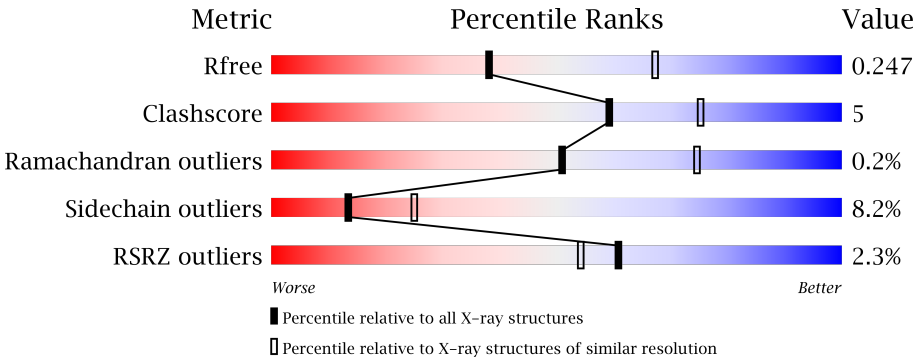
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.62 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}	100719	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (2.64-2.60)

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	643	.% 60% 11% • 28%
1	B	643	3% 60% 12% • 27%
2	E	362	.% 81% 15% • •
2	F	362	2% 80% 17% • •
3	S	191	2% 52% 13% • 34%

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Mol	Chain	Length	Quality of chain
3	T	191	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ZN	A	9002	-	-	-	X
5	ZN	A	9004	-	-	-	X
5	ZN	A	9005	-	-	-	X
5	ZN	B	9005	-	-	-	X
5	ZN	B	9006	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15642 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 Enhancer of Zeste Homolog 2 (EZH2),Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3782	2372	680	691	39			
1	B	469	Total	C	N	O	S	0	1	0
			3823	2398	687	699	39			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	linker	UNP Q15910
A	?	-	PRO	linker	UNP Q15910
A	?	-	ARG	linker	UNP Q15910
A	?	-	LYS	linker	UNP Q15910
A	492	LEU	LYS	linker	UNP Q15910
A	493	GLY	LYS	linker	UNP Q15910
A	494	GLY	ARG	linker	UNP Q15910
A	495	GLY	LYS	linker	UNP Q15910
A	496	GLY	HIS	linker	UNP Q15910
A	497	SER	ARG	linker	UNP Q15910
A	498	GLY	LEU	linker	UNP Q15910
A	499	GLY	TRP	linker	UNP Q15910
A	500	GLY	ALA	linker	UNP Q15910
A	501	GLY	ALA	linker	UNP Q15910
A	502	SER	HIS	linker	UNP Q15910
A	503	GLY	CYS	linker	UNP Q15910
A	504	GLY	ARG	linker	UNP Q15910
A	505	GLY	LYS	linker	UNP Q15910
A	506	GLY	ILE	linker	UNP Q15910
A	507	SER	GLN	linker	UNP Q15910
A	508	ALA	LEU	linker	UNP Q15910
A	509	ALA	LYS	linker	UNP Q15910
A	510	ALA	LYS	linker	UNP Q15910
A	532	ASN	SER	engineered mutation	UNP Q15910

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	linker	UNP Q15910
B	?	-	PRO	linker	UNP Q15910
B	?	-	ARG	linker	UNP Q15910
B	?	-	LYS	linker	UNP Q15910
B	492	LEU	LYS	linker	UNP Q15910
B	493	GLY	LYS	linker	UNP Q15910
B	494	GLY	ARG	linker	UNP Q15910
B	495	GLY	LYS	linker	UNP Q15910
B	496	GLY	HIS	linker	UNP Q15910
B	497	SER	ARG	linker	UNP Q15910
B	498	GLY	LEU	linker	UNP Q15910
B	499	GLY	TRP	linker	UNP Q15910
B	500	GLY	ALA	linker	UNP Q15910
B	501	GLY	ALA	linker	UNP Q15910
B	502	SER	HIS	linker	UNP Q15910
B	503	GLY	CYS	linker	UNP Q15910
B	504	GLY	ARG	linker	UNP Q15910
B	505	GLY	LYS	linker	UNP Q15910
B	506	GLY	ILE	linker	UNP Q15910
B	507	SER	GLN	linker	UNP Q15910
B	508	ALA	LEU	linker	UNP Q15910
B	509	ALA	LYS	linker	UNP Q15910
B	510	ALA	LYS	linker	UNP Q15910
B	532	ASN	SER	engineered mutation	UNP Q15910

- Molecule 2 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	355	Total	C	N	O	S	0	0	0
			2873	1819	503	530	21			
2	F	360	Total	C	N	O	S	0	0	0
			2912	1843	511	537	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	66	MET	-	initiating methionine	UNP O75530
F	66	MET	-	initiating methionine	UNP O75530

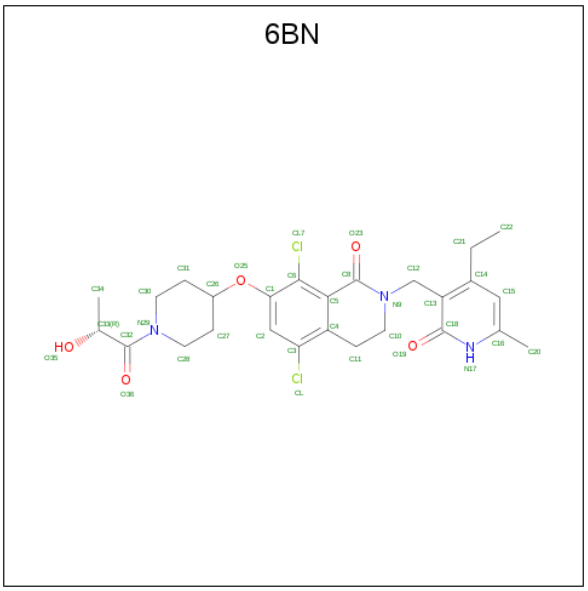
- Molecule 3 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	127	Total	C	N	O	S	0	0	0
			1060	669	182	197	12			
3	T	128	Total	C	N	O	S	0	0	0
			1070	675	185	198	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	535	MET	-	initiating methionine	UNP Q15022
S	536	ASP	-	expression tag	UNP Q15022
S	537	TYR	-	expression tag	UNP Q15022
S	538	LYS	-	expression tag	UNP Q15022
S	539	ASP	-	expression tag	UNP Q15022
S	540	ASP	-	expression tag	UNP Q15022
S	541	ASP	-	expression tag	UNP Q15022
S	542	ASP	-	expression tag	UNP Q15022
S	543	LYS	-	expression tag	UNP Q15022
S	544	GLY	-	expression tag	UNP Q15022
S	583	ASP	SER	engineered mutation	UNP Q15022
T	535	MET	-	initiating methionine	UNP Q15022
T	536	ASP	-	expression tag	UNP Q15022
T	537	TYR	-	expression tag	UNP Q15022
T	538	LYS	-	expression tag	UNP Q15022
T	539	ASP	-	expression tag	UNP Q15022
T	540	ASP	-	expression tag	UNP Q15022
T	541	ASP	-	expression tag	UNP Q15022
T	542	ASP	-	expression tag	UNP Q15022
T	543	LYS	-	expression tag	UNP Q15022
T	544	GLY	-	expression tag	UNP Q15022
T	583	ASP	SER	engineered mutation	UNP Q15022

- Molecule 4 is 5,8-dichloro-2-[(4-ethyl-6-methyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-7-({1-[(2R)-2-hydroxypropanoyl]piperidin-4-yl}oxy)-3,4-dihydroisoquinolin-1(2H)-one (three-letter code: 6BN) (formula: $C_{26}H_{31}Cl_2N_3O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N O 36 26 2 3 5	0	0
4	B	1	Total C Cl N O 36 26 2 3 5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	7	Total Zn 7 7	0	0
5	A	7	Total Zn 7 7	0	0

- Molecule 6 is water.

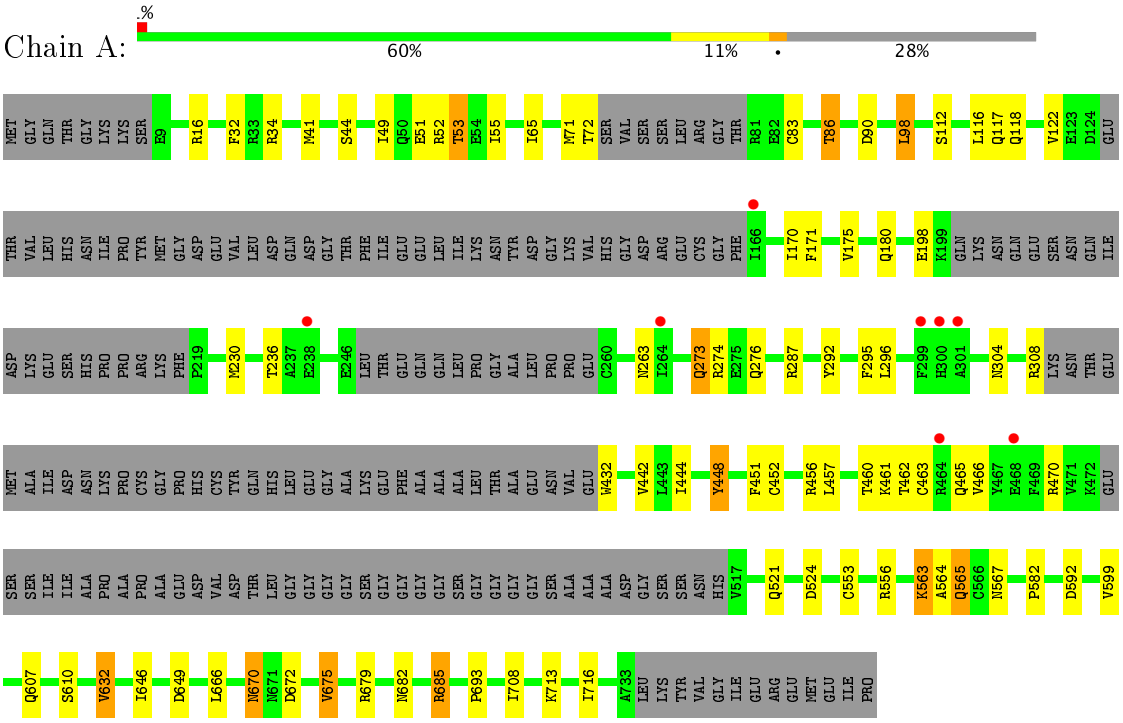
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	14	Total O 14 14	0	0
6	B	8	Total O 8 8	0	0
6	E	8	Total O 8 8	0	0
6	F	6	Total O 6 6	0	0

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 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.

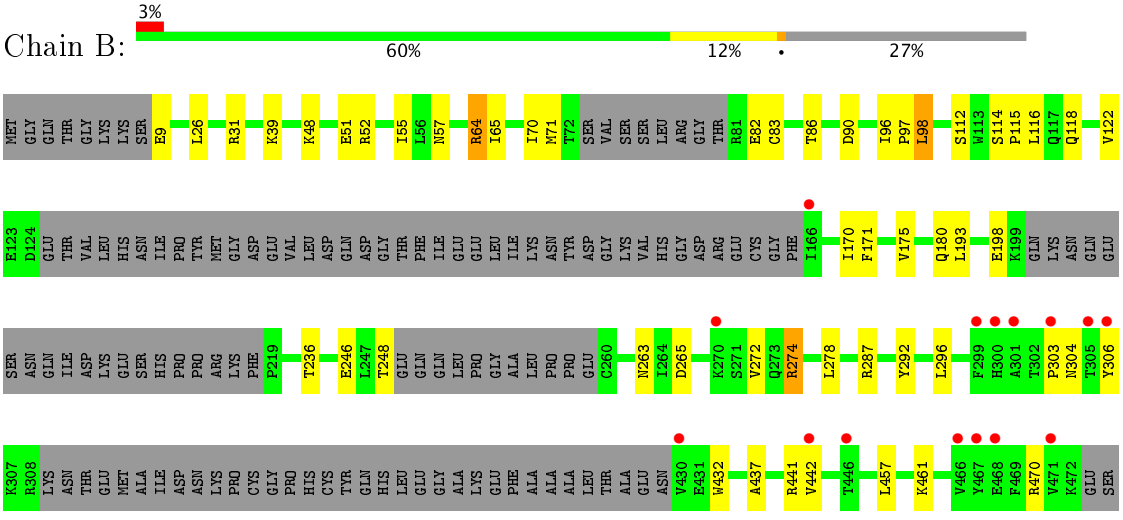
• Molecule 1: Enhancer of Zeste Homolog 2 (EZH2),Histone-lysine N-methyltransferase EZH2

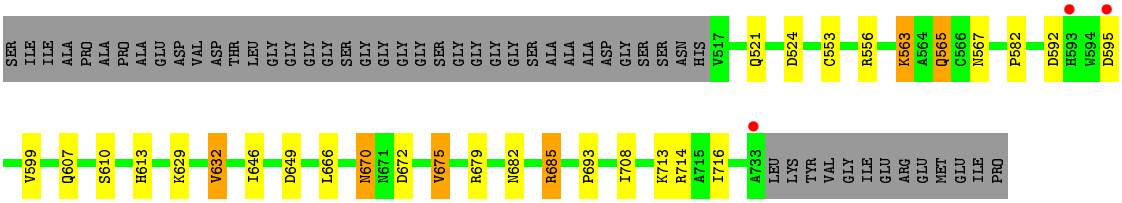
Chain A:

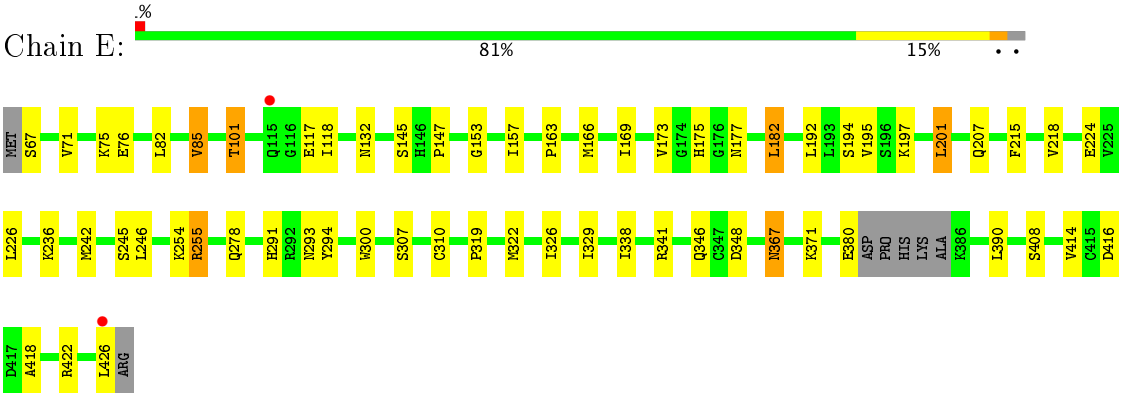


• Molecule 1: Enhancer of Zeste Homolog 2 (EZH2),Histone-lysine N-methyltransferase EZH2

Chain B:

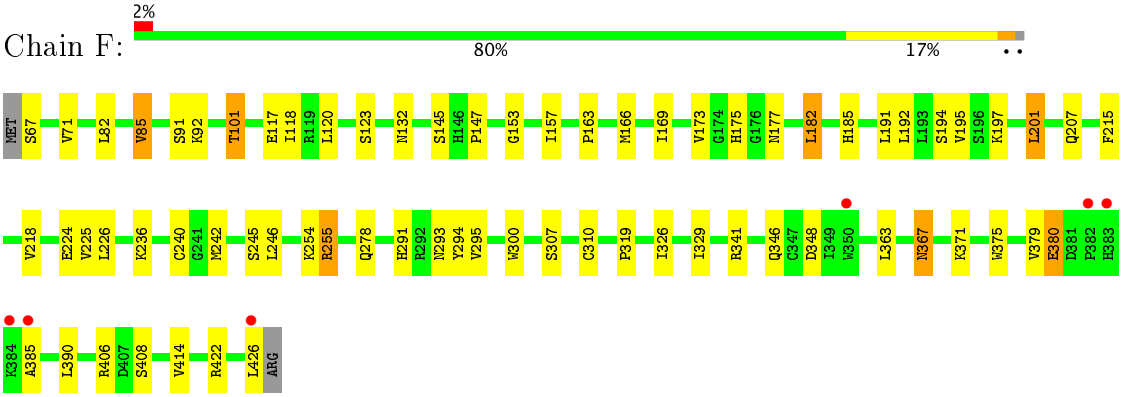




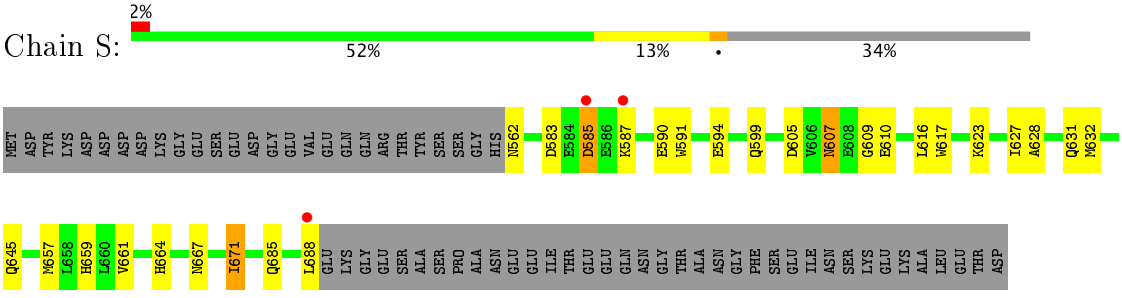


• Molecule 2: Polycomb protein EED

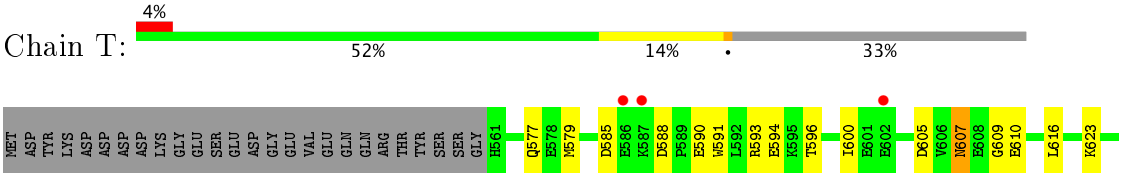
• Molecule 2: Polycomb protein EED

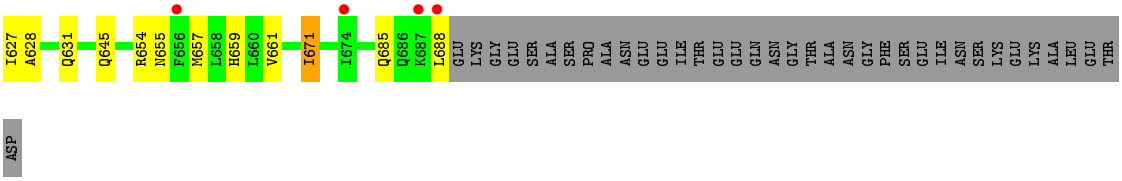


• Molecule 3: Polycomb protein SUZ12



• Molecule 3: Polycomb protein SUZ12




I627
A628
Q631
Q645
R654
N655
F656
M657
L658
H659
L660
V661
I671
I674
Q685
Q686
K687
L688
GLU LYS GLY GLU SER ALA SER PRO ALA ASN GLU GLU ILE THR GLU GLU GLN ASN GLY THR ALA ASN GLY PHE SER GLU ILE ASN SER LYS GLU LYS ALA LEU GLU THR
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.58Å 115.04Å 153.03Å 90.00° 102.53° 90.00°	Depositor
Resolution (Å)	91.15 – 2.62 91.15 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.6 (91.15-2.62) 99.6 (91.15-2.62)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.191 , 0.238 0.200 , 0.247	Depositor DCC
R_{free} test set	3591 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15642	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 6BN

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	0.53	0/3863	0.70	0/5194
1	B	0.51	0/3905	0.70	0/5252
2	E	0.50	0/2944	0.75	0/3986
2	F	0.50	0/2986	0.75	0/4045
3	S	0.49	0/1080	0.67	0/1449
3	T	0.51	0/1091	0.68	0/1464
All	All	0.51	0/15869	0.71	0/21390

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

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	3782	0	3669	43	0
1	B	3823	0	3708	41	0
2	E	2873	0	2791	30	0
2	F	2912	0	2828	36	0
3	S	1060	0	1045	21	0
3	T	1070	0	1052	21	0
4	A	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	36	0	0	0	0
5	A	7	0	0	0	0
5	B	7	0	0	0	0
6	A	14	0	0	0	0
6	B	8	0	0	0	0
6	E	8	0	0	0	0
6	F	6	0	0	0	0
All	All	15642	0	15093	164	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 164 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:F:195:VAL:HG22	2:F:201:LEU:HD13	1.67	0.77
2:E:195:VAL:HG22	2:E:201:LEU:HD13	1.66	0.75
3:S:628:ALA:H	3:S:631:GLN:HE21	1.35	0.73
3:T:628:ALA:H	3:T:631:GLN:HE21	1.38	0.72
1:A:16:ARG:HD2	1:A:230:MET:CE	2.20	0.72

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	451/643 (70%)	428 (95%)	21 (5%)	2 (0%)	38 61
1	B	456/643 (71%)	437 (96%)	18 (4%)	1 (0%)	51 74
2	E	351/362 (97%)	338 (96%)	13 (4%)	0	100 100
2	F	358/362 (99%)	344 (96%)	14 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	S	125/191 (65%)	120 (96%)	5 (4%)	0	100 100
3	T	126/191 (66%)	116 (92%)	9 (7%)	1 (1%)	22 42
All	All	1867/2392 (78%)	1783 (96%)	80 (4%)	4 (0%)	51 74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	TYR
3	T	579	MET
1	A	565	GLN
1	B	565	GLN

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	420/560 (75%)	388 (92%)	32 (8%)	15 29
1	B	425/560 (76%)	386 (91%)	39 (9%)	11 19
2	E	319/325 (98%)	294 (92%)	25 (8%)	15 28
2	F	323/325 (99%)	298 (92%)	25 (8%)	15 28
3	S	121/175 (69%)	111 (92%)	10 (8%)	13 24
3	T	122/175 (70%)	112 (92%)	10 (8%)	13 25
All	All	1730/2120 (82%)	1589 (92%)	141 (8%)	13 25

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	632	VAL
2	E	169	ILE
3	S	671	ILE
1	B	666	LEU
2	E	67	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	670	ASN
2	E	293	ASN
3	T	631	GLN
1	B	706	HIS
2	E	175	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	6BN	A	9001	-	36,39,39	0.87	2 (5%)	42,57,57	1.37	2 (4%)
4	6BN	B	9001	-	36,39,39	0.86	2 (5%)	42,57,57	1.38	2 (4%)

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
4	6BN	A	9001	-	-	0/18/41/41	0/4/4/4
4	6BN	B	9001	-	-	0/18/41/41	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	9001	6BN	C15-C14	2.73	1.44	1.39
4	A	9001	6BN	C15-C14	2.87	1.44	1.39
4	B	9001	6BN	C18-N17	3.33	1.39	1.33
4	A	9001	6BN	C18-N17	3.40	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	9001	6BN	C4-C5-C8	-2.41	116.08	120.13
4	B	9001	6BN	C4-C5-C8	-2.16	116.49	120.13
4	A	9001	6BN	C18-N17-C16	6.79	124.16	117.24
4	B	9001	6BN	C18-N17-C16	7.02	124.39	117.24

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	465/643 (72%)	0.21	8 (1%) 70 65	38, 63, 103, 133	0
1	B	469/643 (72%)	0.34	18 (3%) 41 34	40, 73, 110, 148	0
2	E	355/362 (98%)	0.06	2 (0%) 89 87	39, 55, 82, 102	0
2	F	360/362 (99%)	0.16	6 (1%) 70 65	39, 61, 90, 120	0
3	S	127/191 (66%)	0.24	3 (2%) 59 52	45, 67, 111, 122	0
3	T	128/191 (67%)	0.39	7 (5%) 26 20	50, 77, 116, 127	0
All	All	1904/2392 (79%)	0.22	44 (2%) 61 54	38, 64, 104, 148	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	383	HIS	7.9
1	B	300	HIS	5.9
1	B	303	PRO	5.4
2	F	382	PRO	5.3
1	B	467	TYR	5.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
5	ZN	A	9005	1/1	0.99	0.24	5.48	36,36,36,36	1
5	ZN	A	9002	1/1	1.00	0.22	5.21	35,35,35,35	1
5	ZN	A	9004	1/1	1.00	0.22	4.02	38,38,38,38	1
5	ZN	B	9005	1/1	0.97	0.23	3.69	61,61,61,61	1
5	ZN	B	9006	1/1	0.98	0.21	2.09	56,56,56,56	1
5	ZN	A	9007	1/1	1.00	0.20	1.89	50,50,50,50	1
5	ZN	B	9004	1/1	0.98	0.21	1.77	66,66,66,66	1
5	ZN	A	9003	1/1	1.00	0.19	1.27	46,46,46,46	1
5	ZN	B	9003	1/1	0.99	0.20	1.15	53,53,53,53	1
5	ZN	A	9006	1/1	0.99	0.22	0.84	52,52,52,52	1
5	ZN	B	9002	1/1	0.97	0.18	0.71	63,63,63,63	1
5	ZN	A	9008	1/1	1.00	0.20	0.60	35,35,35,35	1
5	ZN	B	9007	1/1	0.99	0.19	0.50	45,45,45,45	1
5	ZN	B	9008	1/1	0.99	0.18	0.42	49,49,49,49	1
4	6BN	A	9001	36/36	0.97	0.17	-0.34	32,51,64,66	0
4	6BN	B	9001	36/36	0.96	0.18	-0.49	31,56,69,70	0

6.5 Other polymers

There are no such residues in this entry.