



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:06 PM UTC

PDB ID : 5IJ8 / pdb_00005ij8
Title : Structure of the primary oncogenic mutant Y641N Hs/AcPRC2 in complex with a pyridone inhibitor
Authors : Gajiwala, K.S.; Brooun, A.; Deng, Y.-L.; Liu, W.
Deposited on : 2016-03-01
Resolution : 2.99 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

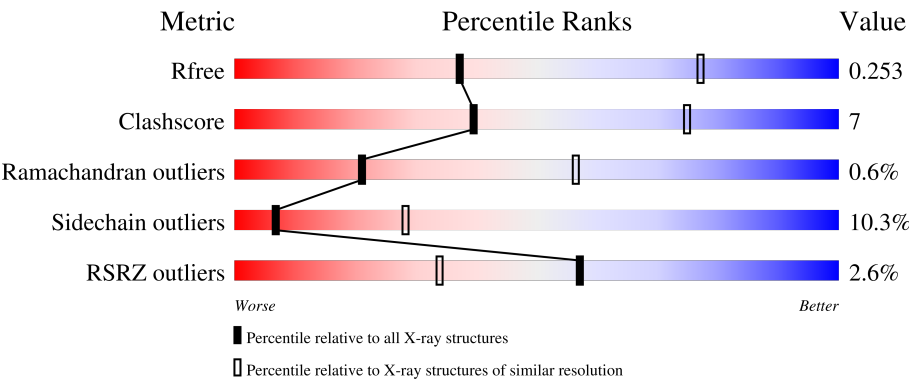
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.99 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	3% 55% 14% • 28%
1	B	643	3% 56% 14% • 28%
2	E	362	% 73% 23% • •
2	F	362	% 75% 22% • •
3	S	191	% 44% 20% • 33%

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Mol	Chain	Length	Quality of chain
3	T	191	3% 45% 19% • 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15580 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	464	Total	C	N	O	S	0	0	0
			3771	2363	680	689	39			
1	B	466	Total	C	N	O	S	0	0	0
			3779	2366	681	693	39			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP Q15910
A	?	-	PRO	deletion	UNP Q15910
A	?	-	ARG	deletion	UNP Q15910
A	?	-	LYS	deletion	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	linker	UNP Q15910

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Chain	Residue	Modelled	Actual	Comment	Reference
A	641	ASN	TYR	engineered mutation	UNP Q15910
B	?	-	PRO	deletion	UNP Q15910
B	?	-	PRO	deletion	UNP Q15910
B	?	-	ARG	deletion	UNP Q15910
B	?	-	LYS	deletion	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	linker	UNP Q15910
B	641	ASN	TYR	engineered mutation	UNP Q15910

- Molecule 2 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	358	Total	C	N	O	S	0	0	0
			2898	1834	509	534	21			
2	F	359	Total	C	N	O	S	0	0	0
			2906	1840	510	535	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

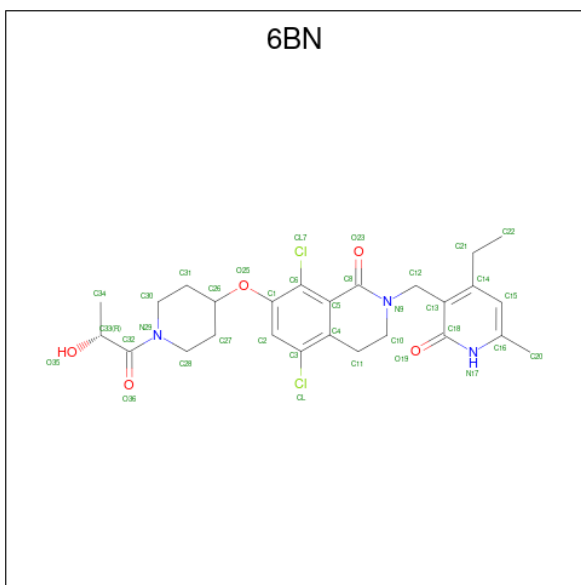
- Molecule 3 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	128	Total	C	N	O	S	0	0	0
			1070	675	185	198	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 (CCD ID: 6BN) (formula: C₂₆H₃₁Cl₂N₃O₅).



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

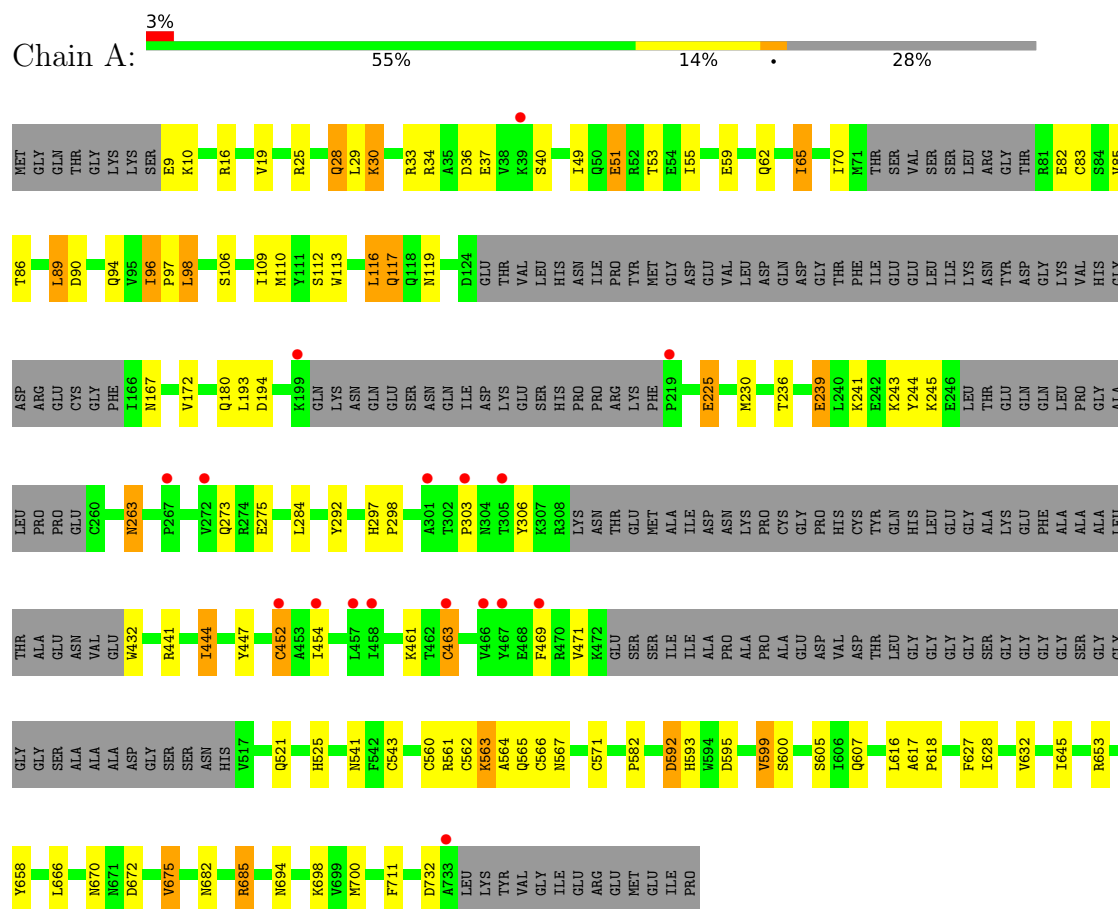
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

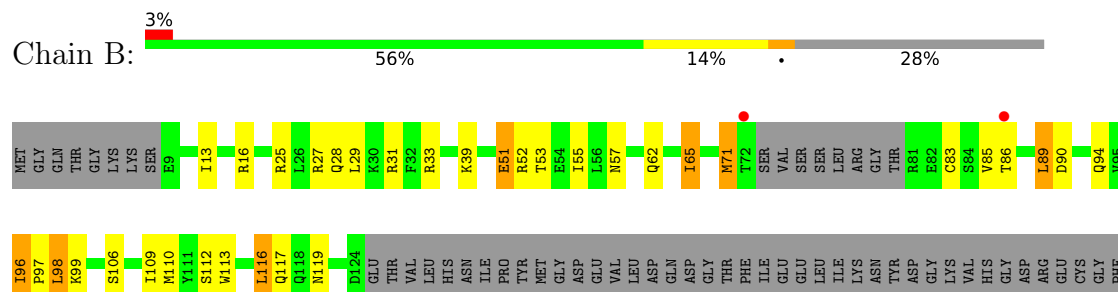
3 Residue-property plots

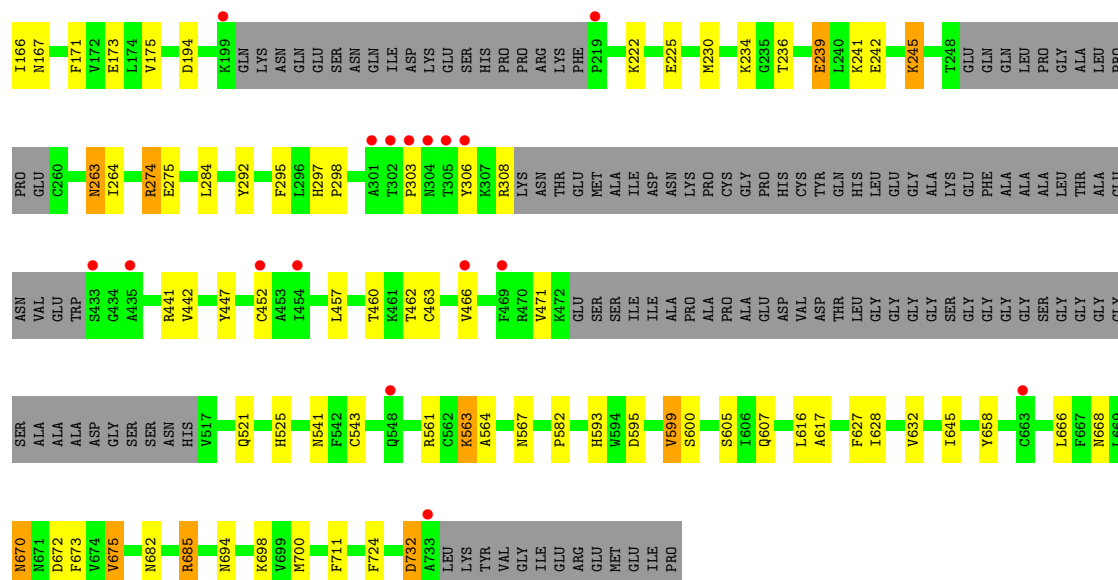
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Enhancer of Zeste Homolog 2 (EZH2), Histone-lysine N-methyltransferase EZH2

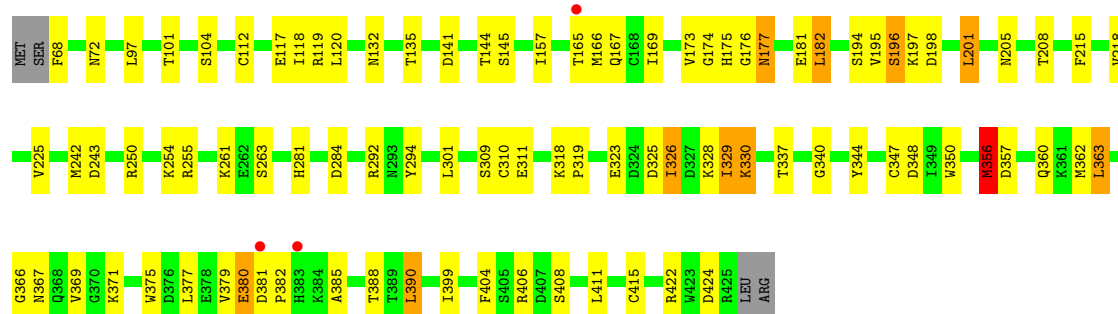
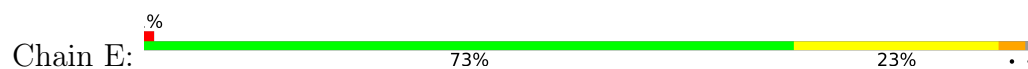


- Molecule 1: Enhancer of Zeste Homolog 2 (EZH2), Histone-lysine N-methyltransferase EZH2

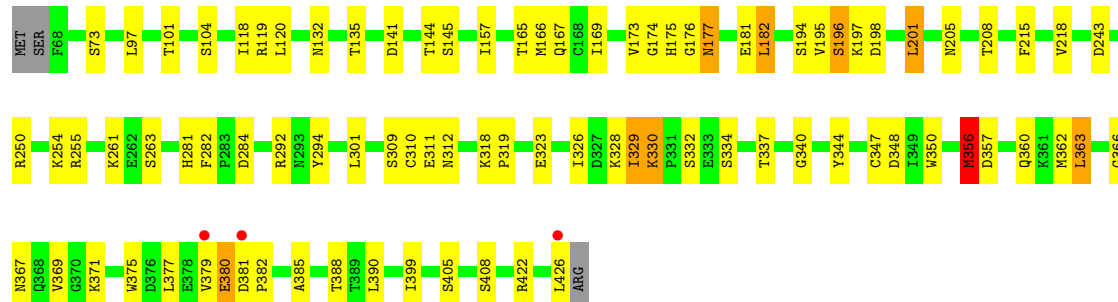
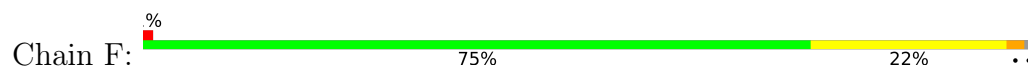




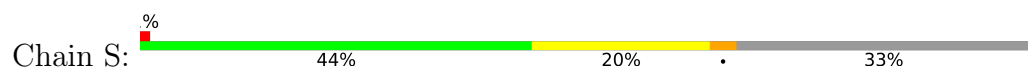
• Molecule 2: Polycomb protein EED

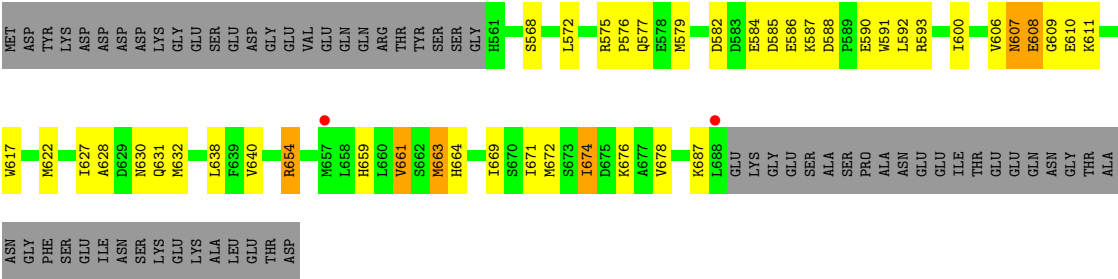


• Molecule 2: Polycomb protein EED

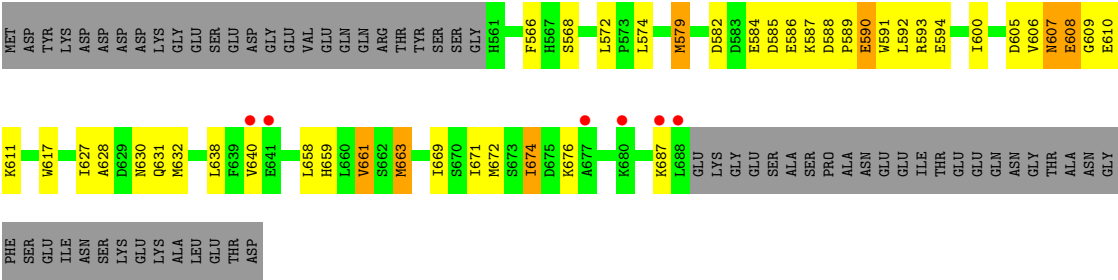
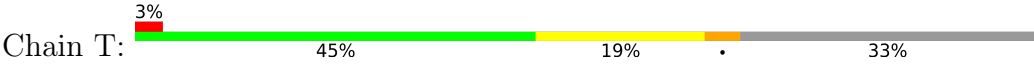


• Molecule 3: Polycomb protein SUZ12





● Molecule 3: Polycomb protein SUZ12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.33Å 115.13Å 153.94Å 90.00° 103.35° 90.00°	Depositor
Resolution (Å)	91.28 – 2.99 91.28 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (91.28-2.99) 99.7 (91.28-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.188 , 0.240 0.198 , 0.253	Depositor DCC
R_{free} test set	2497 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15580	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6BN, 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	0.88	0/3851	1.39	38/5177 (0.7%)
1	B	0.87	0/3857	1.40	25/5185 (0.5%)
2	E	0.85	1/2972 (0.0%)	1.25	10/4026 (0.2%)
2	F	0.85	0/2980	1.28	9/4037 (0.2%)
3	S	0.86	0/1091	1.48	8/1464 (0.5%)
3	T	0.86	0/1091	1.50	6/1464 (0.4%)
All	All	0.86	1/15842 (0.0%)	1.36	96/21353 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	242	MET	SD-CE	5.68	1.93	1.79

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	675	VAL	N-CA-CB	9.87	121.48	110.72
1	A	675	VAL	N-CA-CB	9.44	121.00	110.72
2	F	356	MET	CA-C-N	9.04	134.40	120.75
2	F	356	MET	C-N-CA	9.04	134.40	120.75
1	B	447	TYR	N-CA-C	-6.87	100.36	110.52
2	F	243	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	447	TYR	N-CA-C	-6.82	100.43	110.52
1	A	732	ASP	N-CA-C	-6.79	102.29	111.87
3	T	582	ASP	CA-CB-CG	6.53	119.13	112.60
1	B	599	VAL	CA-C-N	6.48	129.26	120.38
1	B	599	VAL	C-N-CA	6.48	129.26	120.38
2	F	196	SER	N-CA-C	6.48	119.56	109.52
2	F	357	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	51	GLU	CA-C-N	6.30	128.72	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	GLU	C-N-CA	6.30	128.72	120.28
1	A	89	LEU	CA-C-N	6.24	131.26	122.08
1	A	89	LEU	C-N-CA	6.24	131.26	122.08
3	T	588	ASP	CA-CB-CG	6.17	118.78	112.60
1	A	599	VAL	CA-C-N	6.09	128.44	120.28
1	A	599	VAL	C-N-CA	6.09	128.44	120.28
1	A	694	ASN	CA-CB-CG	6.03	118.63	112.60
3	S	588	ASP	CA-CB-CG	6.03	118.62	112.60
2	E	243	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	592	ASP	CA-C-N	6.00	133.00	121.54
1	A	592	ASP	C-N-CA	6.00	133.00	121.54
3	S	584	GLU	CA-C-N	5.96	131.43	122.67
3	S	584	GLU	C-N-CA	5.96	131.43	122.67
2	E	377	LEU	CA-C-N	5.87	128.74	120.28
2	E	377	LEU	C-N-CA	5.87	128.74	120.28
2	E	196	SER	N-CA-C	5.87	119.12	109.85
2	F	377	LEU	CA-C-N	5.82	128.66	120.28
2	F	377	LEU	C-N-CA	5.82	128.66	120.28
3	T	608	GLU	CB-CG-CD	5.81	122.48	112.60
1	B	89	LEU	CA-C-N	5.80	130.61	122.08
1	B	89	LEU	C-N-CA	5.80	130.61	122.08
1	A	30	LYS	CA-C-N	5.76	128.27	120.44
1	A	30	LYS	C-N-CA	5.76	128.27	120.44
1	B	194	ASP	CA-C-N	5.75	128.26	120.44
1	B	194	ASP	C-N-CA	5.75	128.26	120.44
3	S	582	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	37	GLU	CA-C-N	5.68	127.72	120.56
1	A	37	GLU	C-N-CA	5.68	127.72	120.56
2	E	325	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	441	ARG	CA-C-N	5.62	127.58	120.72
1	B	441	ARG	C-N-CA	5.62	127.58	120.72
2	F	357	ASP	N-CA-CB	-5.60	101.81	110.04
1	B	65	ILE	CA-C-N	5.57	128.59	120.51
1	B	65	ILE	C-N-CA	5.57	128.59	120.51
1	B	543	CYS	N-CA-C	-5.56	101.42	110.20
1	A	441	ARG	CA-C-N	5.54	127.48	120.72
1	A	441	ARG	C-N-CA	5.54	127.48	120.72
1	A	65	ILE	CA-C-N	5.52	128.06	120.39
1	A	65	ILE	C-N-CA	5.52	128.06	120.39
1	B	694	ASN	CA-CB-CG	5.49	118.08	112.60
2	E	356	MET	CA-C-N	5.48	130.94	120.97
2	E	356	MET	C-N-CA	5.48	130.94	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	605	ASP	CA-CB-CG	5.47	118.07	112.60
3	T	630	ASN	CA-CB-CG	5.44	118.04	112.60
3	T	584	GLU	N-CA-C	-5.43	106.44	112.57
1	A	167	ASN	CA-CB-CG	5.41	118.00	112.60
1	B	167	ASN	CA-CB-CG	5.37	117.97	112.60
3	S	630	ASN	CA-CB-CG	5.37	117.97	112.60
1	A	194	ASP	CA-C-N	5.36	127.73	120.44
1	A	194	ASP	C-N-CA	5.36	127.73	120.44
1	A	40	SER	CA-C-N	5.33	127.74	120.54
1	A	40	SER	C-N-CA	5.33	127.74	120.54
1	B	173	GLU	CA-C-N	5.32	127.67	120.65
1	B	173	GLU	C-N-CA	5.32	127.67	120.65
1	B	31	ARG	CA-C-N	5.29	127.64	120.44
1	B	31	ARG	C-N-CA	5.29	127.64	120.44
1	A	51	GLU	CA-C-N	5.29	127.80	120.29
1	A	51	GLU	C-N-CA	5.29	127.80	120.29
1	A	263	ASN	CA-CB-CG	5.22	117.83	112.60
1	A	543	CYS	N-CA-C	-5.20	101.98	110.20
1	A	541	ASN	CA-CB-CG	5.18	117.78	112.60
2	F	323	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	19	VAL	CA-C-N	5.18	127.17	120.44
1	A	19	VAL	C-N-CA	5.18	127.17	120.44
2	E	357	ASP	CA-CB-CG	5.16	117.76	112.60
3	S	576	PRO	CA-C-N	5.16	127.19	120.28
3	S	576	PRO	C-N-CA	5.16	127.19	120.28
1	A	653	ARG	CA-C-N	5.15	127.14	120.44
1	A	653	ARG	C-N-CA	5.15	127.14	120.44
1	B	724	PHE	CA-CB-CG	5.10	118.90	113.80
2	E	323	GLU	CB-CG-CD	5.08	121.23	112.60
1	B	263	ASN	CA-CB-CG	5.06	117.66	112.60
1	B	673	PHE	N-CA-C	5.05	117.36	109.52
1	B	541	ASN	CA-CB-CG	5.05	117.65	112.60
3	S	608	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	225	GLU	CB-CG-CD	5.03	121.16	112.60
1	A	59	GLU	CA-C-N	5.03	127.43	120.29
1	A	59	GLU	C-N-CA	5.03	127.43	120.29
1	A	49	ILE	N-CA-CB	5.02	116.10	110.62
1	A	469	PHE	CA-C-N	5.01	126.95	120.44
1	A	469	PHE	C-N-CA	5.01	126.95	120.44
2	E	225	VAL	N-CA-CB	5.00	116.18	110.72

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	3771	0	3661	41	0
1	B	3779	0	3674	48	0
2	E	2898	0	2812	49	0
2	F	2906	0	2823	41	0
3	S	1070	0	1052	26	0
3	T	1070	0	1052	27	0
4	A	36	0	0	0	0
4	B	36	0	0	0	0
5	A	7	0	0	0	0
5	B	7	0	0	0	0
All	All	15580	0	15074	202	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 7.

All (202) 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:B:16:ARG:HD2	1:B:230:MET:HE3	1.58	0.85
3:S:628:ALA:H	3:S:631:GLN:HE21	1.26	0.83
3:T:628:ALA:H	3:T:631:GLN:HE21	1.26	0.82
1:B:670:ASN:HD22	1:B:672:ASP:H	1.28	0.79
3:T:627:ILE:H	3:T:631:GLN:NE2	1.81	0.79
3:T:606:VAL:HG13	3:T:610:GLU:HG3	1.65	0.78
2:F:330:LYS:HE2	2:F:330:LYS:H	1.48	0.78
2:E:330:LYS:H	2:E:330:LYS:HE2	1.48	0.77
3:S:627:ILE:H	3:S:631:GLN:NE2	1.81	0.77
1:B:57:ASN:HD22	2:E:406:ARG:HH21	1.33	0.75
1:B:263:ASN:HB3	3:S:607:ASN:ND2	2.02	0.74
1:B:71:MET:HE1	1:B:99:LYS:HB2	1.70	0.74
3:T:607:ASN:HD22	3:T:609:GLY:H	1.34	0.73
2:E:379:VAL:HG21	2:E:385:ALA:HA	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:379:VAL:HG21	2:F:385:ALA:HA	1.69	0.72
1:A:106:SER:HB3	2:F:157:ILE:HD11	1.73	0.71
2:E:201:LEU:HB2	2:E:215:PHE:HB2	1.74	0.70
3:S:607:ASN:HD22	3:S:609:GLY:H	1.36	0.70
2:E:294:TYR:CZ	2:E:350:TRP:HB3	2.27	0.69
2:F:294:TYR:OH	2:F:310:CYS:HB3	1.93	0.69
2:F:201:LEU:HB2	2:F:215:PHE:HB2	1.75	0.68
3:S:661:VAL:HA	3:S:674:ILE:HD11	1.76	0.68
3:T:663:MET:HB3	3:T:669:ILE:HG12	1.76	0.68
2:E:294:TYR:OH	2:E:310:CYS:HB3	1.93	0.68
2:F:294:TYR:CZ	2:F:350:TRP:HB3	2.29	0.67
1:B:94:GLN:HE22	2:E:119:ARG:HA	1.56	0.67
3:S:663:MET:HB3	3:S:669:ILE:HG12	1.75	0.67
3:T:661:VAL:HA	3:T:674:ILE:HD11	1.76	0.67
1:A:96:ILE:HD13	1:A:97:PRO:HD2	1.77	0.67
1:B:96:ILE:HD13	1:B:97:PRO:HD2	1.75	0.67
1:B:110:MET:O	2:E:176:GLY:HA3	1.95	0.66
1:A:263:ASN:HB3	3:T:607:ASN:ND2	2.10	0.66
1:A:292:TYR:OH	3:T:659:HIS:HD2	1.80	0.65
3:T:617:TRP:HZ2	3:T:632:MET:HE1	1.62	0.65
3:S:628:ALA:HB3	3:S:631:GLN:HG3	1.80	0.63
3:T:628:ALA:HB3	3:T:631:GLN:HG3	1.80	0.63
2:E:165:THR:HG22	2:E:167:GLN:HG2	1.80	0.63
2:E:319:PRO:HB2	2:E:329:ILE:HD13	1.81	0.63
3:S:617:TRP:HZ2	3:S:632:MET:HE1	1.64	0.62
1:B:292:TYR:OH	3:S:659:HIS:HD2	1.83	0.62
2:E:175:HIS:HE1	2:E:194:SER:OG	1.82	0.61
3:S:627:ILE:H	3:S:631:GLN:HE22	1.48	0.61
1:B:682:ASN:O	1:B:685:ARG:HG2	2.01	0.61
3:T:627:ILE:H	3:T:631:GLN:HE22	1.49	0.61
1:A:682:ASN:O	1:A:685:ARG:HG2	2.01	0.60
1:B:106:SER:HB3	2:E:157:ILE:HD11	1.83	0.60
1:A:16:ARG:HB3	1:A:230:MET:HE3	1.84	0.60
1:A:670:ASN:ND2	1:A:672:ASP:H	2.00	0.59
1:B:71:MET:CE	1:B:99:LYS:HB2	2.32	0.59
2:F:319:PRO:HB2	2:F:329:ILE:HD13	1.82	0.59
2:F:165:THR:HG22	2:F:167:GLN:HG2	1.84	0.59
3:S:606:VAL:HG13	3:S:610:GLU:HG3	1.86	0.57
1:B:242:GLU:HA	1:B:245:LYS:HB2	1.87	0.57
1:B:599:VAL:HG12	1:B:600:SER:H	1.70	0.57
1:A:582:PRO:HD3	1:A:607:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:VAL:HG12	1:A:600:SER:H	1.69	0.56
1:B:582:PRO:HD3	1:B:607:GLN:HE22	1.70	0.56
1:B:670:ASN:ND2	1:B:672:ASP:H	2.01	0.56
1:B:57:ASN:HD22	2:E:406:ARG:NH2	2.00	0.56
2:F:195:VAL:HG22	2:F:201:LEU:HD13	1.87	0.56
1:B:274:ARG:HB2	1:B:442:VAL:HA	1.87	0.55
1:A:110:MET:O	2:F:176:GLY:HA3	2.06	0.55
2:E:195:VAL:HG22	2:E:201:LEU:HD13	1.87	0.55
2:F:97:LEU:HD13	2:F:405:SER:HB2	1.88	0.55
1:B:85:VAL:HG23	2:E:120:LEU:HD22	1.90	0.54
1:A:452:CYS:HG	1:A:463:CYS:HG	1.32	0.53
2:E:366:GLY:HA3	2:E:399:ILE:HB	1.91	0.53
1:B:222:LYS:HA	1:B:225:GLU:HG2	1.90	0.53
3:S:606:VAL:HG12	3:S:611:LYS:HG3	1.91	0.53
2:F:157:ILE:HG12	2:F:173:VAL:HG22	1.91	0.53
2:E:157:ILE:HG12	2:E:173:VAL:HG22	1.92	0.52
2:F:218:VAL:HG22	2:F:281:HIS:HB3	1.91	0.52
1:B:698:LYS:HB3	1:B:711:PHE:HE2	1.75	0.51
2:F:366:GLY:HA3	2:F:399:ILE:HB	1.92	0.51
3:T:607:ASN:ND2	3:T:609:GLY:H	2.07	0.51
2:F:356:MET:HE3	2:F:360:GLN:HG2	1.92	0.51
3:T:589:PRO:HG2	3:T:592:LEU:HD12	1.92	0.51
1:A:94:GLN:HE22	2:F:119:ARG:HA	1.76	0.51
2:E:356:MET:HE3	2:E:360:GLN:HG2	1.93	0.51
1:A:698:LYS:HB3	1:A:711:PHE:HE2	1.75	0.50
1:B:563:LYS:HE2	1:B:564:ALA:H	1.77	0.50
3:S:607:ASN:ND2	3:S:610:GLU:H	2.09	0.50
2:E:218:VAL:HG22	2:E:281:HIS:HB3	1.93	0.49
1:B:616:LEU:HD22	3:S:568:SER:HA	1.94	0.49
1:A:117:GLN:HG2	3:T:587:LYS:HA	1.94	0.49
1:A:563:LYS:HE2	1:A:564:ALA:H	1.77	0.49
2:E:301:LEU:HA	2:E:360:GLN:HE22	1.77	0.49
1:A:698:LYS:HB3	1:A:711:PHE:CE2	2.47	0.49
1:B:658:TYR:HD2	1:B:666:LEU:HD21	1.78	0.49
2:E:68:PHE:HA	2:E:424:ASP:O	2.13	0.49
1:A:303:PRO:HA	1:A:306:TYR:CZ	2.48	0.49
3:T:607:ASN:ND2	3:T:610:GLU:H	2.11	0.49
1:B:698:LYS:HB3	1:B:711:PHE:CE2	2.48	0.48
2:F:301:LEU:HA	2:F:360:GLN:NE2	2.29	0.48
2:E:301:LEU:HA	2:E:360:GLN:NE2	2.28	0.48
1:A:28:GLN:HE21	1:A:28:GLN:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:MET:HE3	1:B:113:TRP:HE1	1.79	0.48
2:F:340:GLY:HA3	2:F:382:PRO:HG2	1.96	0.48
2:F:301:LEU:HA	2:F:360:GLN:HE22	1.79	0.48
1:A:658:TYR:HD2	1:A:666:LEU:HD21	1.79	0.47
1:B:303:PRO:HA	1:B:306:TYR:CZ	2.49	0.47
1:A:566:CYS:SG	1:A:571:CYS:SG	3.11	0.47
1:A:172:VAL:HG13	1:A:244:TYR:HE1	1.79	0.47
2:E:340:GLY:HA3	2:E:382:PRO:HG2	1.97	0.47
2:E:177:ASN:HB3	2:E:197:LYS:HB3	1.96	0.47
3:S:607:ASN:HD22	3:S:609:GLY:N	2.09	0.47
1:A:85:VAL:HG23	2:F:120:LEU:HD22	1.95	0.47
3:T:590:GLU:O	3:T:593:ARG:HB2	2.14	0.47
1:A:82:GLU:HG2	1:A:97:PRO:HA	1.97	0.47
2:F:208:THR:HG21	2:F:263:SER:O	2.15	0.47
3:T:606:VAL:HG12	3:T:611:LYS:HG3	1.97	0.47
1:B:563:LYS:HD3	1:B:563:LYS:H	1.80	0.46
1:B:668:ASN:HD22	1:B:732:ASP:HB3	1.80	0.46
2:F:135:THR:HG23	2:F:182:LEU:HD22	1.97	0.46
2:F:309:SER:HB3	2:F:311:GLU:HG2	1.97	0.46
2:E:135:THR:HG23	2:E:182:LEU:HD22	1.97	0.46
1:B:264:ILE:HG12	3:S:654:ARG:HB3	1.97	0.46
1:A:30:LYS:HZ2	1:A:33:ARG:HH12	1.62	0.46
1:B:599:VAL:HG12	1:B:600:SER:N	2.31	0.46
2:E:208:THR:HG21	2:E:263:SER:O	2.15	0.46
3:T:607:ASN:HD22	3:T:609:GLY:N	2.08	0.46
1:A:616:LEU:HD22	3:T:568:SER:HA	1.98	0.46
1:A:560:CYS:SG	1:A:566:CYS:SG	3.13	0.46
2:F:141:ASP:HB3	2:F:144:THR:HB	1.98	0.46
2:F:196:SER:HB3	2:F:198:ASP:OD1	2.15	0.46
2:E:309:SER:HB3	2:E:311:GLU:HG2	1.99	0.45
3:S:607:ASN:ND2	3:S:609:GLY:H	2.07	0.45
2:E:141:ASP:HB3	2:E:144:THR:HB	1.99	0.45
1:A:110:MET:HE3	1:A:113:TRP:HE1	1.81	0.45
2:F:218:VAL:HG11	3:T:591:TRP:CE3	2.51	0.45
3:T:672:MET:HE3	3:T:676:LYS:HD2	1.99	0.45
1:B:52:ARG:HA	1:B:55:ILE:HD12	1.99	0.45
1:A:297:HIS:HA	1:A:298:PRO:HD3	1.86	0.44
1:A:599:VAL:HG12	1:A:600:SER:N	2.32	0.44
1:B:617:ALA:HB3	1:B:627:PHE:CE2	2.52	0.44
1:B:94:GLN:NE2	2:E:120:LEU:H	2.16	0.44
1:B:308:ARG:HH21	3:S:664:HIS:CE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:672:MET:HE3	3:S:676:LYS:HD2	1.99	0.44
1:B:57:ASN:ND2	2:E:406:ARG:HH21	2.08	0.44
1:A:563:LYS:HD3	1:A:563:LYS:H	1.81	0.44
2:F:177:ASN:HB3	2:F:197:LYS:HB3	2.00	0.44
2:F:344:TYR:HE1	2:F:347:CYS:HB3	1.83	0.43
2:E:196:SER:HB3	2:E:198:ASP:OD1	2.17	0.43
2:E:344:TYR:HE1	2:E:347:CYS:HB3	1.83	0.43
1:A:89:LEU:HD13	2:F:73:SER:HB3	2.01	0.43
2:E:404:PHE:CE1	2:E:411:LEU:HD13	2.54	0.43
1:A:119:ASN:HB3	1:A:645:ILE:HG12	2.00	0.43
2:E:104:SER:O	2:E:132:ASN:HA	2.18	0.43
2:F:282:PHE:CE2	3:T:594:GLU:HB3	2.54	0.43
1:A:444:ILE:HG22	1:A:454:ILE:HD13	2.00	0.43
2:F:104:SER:O	2:F:132:ASN:HA	2.19	0.43
1:B:171:PHE:O	1:B:175:VAL:HG23	2.19	0.42
1:A:670:ASN:HD22	1:A:672:ASP:H	1.67	0.42
1:B:119:ASN:HB3	1:B:645:ILE:HG12	2.00	0.42
2:E:218:VAL:HG11	3:S:591:TRP:CE3	2.54	0.42
2:E:367:ASN:HB2	2:E:371:LYS:H	1.85	0.42
1:A:617:ALA:HB3	1:A:627:PHE:CE2	2.54	0.42
2:F:363:LEU:HD23	2:F:375:TRP:CE3	2.55	0.42
3:S:600:ILE:HG22	3:S:611:LYS:HG2	2.01	0.42
2:E:97:LEU:HB2	2:E:112:CYS:HB2	2.02	0.42
2:E:318:LYS:HG2	2:E:337:THR:HB	2.01	0.42
2:E:330:LYS:H	2:E:330:LYS:CE	2.26	0.42
1:A:236:THR:HG23	1:A:239:GLU:H	1.85	0.42
1:B:263:ASN:HB3	3:S:607:ASN:HD21	1.82	0.42
1:B:295:PHE:CE2	3:S:592:LEU:HD22	2.55	0.42
1:B:297:HIS:HA	1:B:298:PRO:HD3	1.87	0.42
1:B:236:THR:HG23	1:B:239:GLU:H	1.84	0.42
2:E:165:THR:HG22	2:E:167:GLN:CG	2.50	0.42
2:F:205:ASN:CG	2:F:208:THR:HG22	2.45	0.42
2:F:318:LYS:HG2	2:F:337:THR:HB	2.02	0.42
3:T:590:GLU:HB3	3:T:593:ARG:NH2	2.34	0.42
2:F:118:ILE:HD11	2:F:422:ARG:HB2	2.02	0.42
2:E:205:ASN:CG	2:E:208:THR:HG22	2.45	0.41
2:F:312:ASN:HA	2:F:344:TYR:CE1	2.56	0.41
3:T:590:GLU:H	3:T:590:GLU:HG3	1.70	0.41
3:S:593:ARG:HA	3:S:622:MET:HE1	2.02	0.41
2:F:250:ARG:HG3	2:F:284:ASP:CG	2.45	0.41
2:F:367:ASN:HB3	2:F:369:VAL:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:HD12	1:B:116:LEU:HA	1.91	0.41
1:B:166:ILE:HG23	1:B:234:LYS:HD3	2.02	0.41
2:F:367:ASN:HB2	2:F:371:LYS:H	1.85	0.41
3:S:607:ASN:HD22	3:S:607:ASN:C	2.28	0.41
1:B:83:CYS:HB3	1:B:98:LEU:HG	2.01	0.41
2:F:175:HIS:HE1	2:F:194:SER:OG	2.02	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.90	0.41
1:A:432:TRP:CE2	1:A:461:LYS:HD2	2.56	0.41
1:A:461:LYS:HA	1:A:461:LYS:HD3	1.92	0.41
2:F:294:TYR:CD1	2:F:294:TYR:C	2.99	0.41
1:A:618:PRO:HD3	3:T:566:PHE:CE2	2.56	0.40
2:E:68:PHE:HB2	2:E:390:LEU:HD11	2.03	0.40
1:B:462:THR:O	1:B:466:VAL:HG23	2.20	0.40
2:E:294:TYR:CD1	2:E:294:TYR:C	2.99	0.40
2:E:367:ASN:HB3	2:E:369:VAL:H	1.85	0.40
1:B:89:LEU:HD22	2:E:72:ASN:HA	2.04	0.40
2:E:250:ARG:HG3	2:E:284:ASP:CG	2.46	0.40
2:E:363:LEU:HD23	2:E:375:TRP:CE3	2.56	0.40
3:T:600:ILE:HG22	3:T:611:LYS:HG2	2.02	0.40
3:T:607:ASN:HD22	3:T:607:ASN:C	2.29	0.40
1:A:83:CYS:HB3	1:A:98:LEU:HG	2.02	0.40
1:B:457:LEU:HD23	3:S:678:VAL:HG11	2.03	0.40
2:E:118:ILE:HD11	2:E:422:ARG:HB2	2.03	0.40
2:E:319:PRO:HG2	2:E:326:ILE:HD12	2.04	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	450/643 (70%)	413 (92%)	33 (7%)	4 (1%)	14 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	452/643 (70%)	418 (92%)	32 (7%)	2 (0%)	30	65
2	E	356/362 (98%)	343 (96%)	11 (3%)	2 (1%)	21	56
2	F	357/362 (99%)	344 (96%)	11 (3%)	2 (1%)	21	56
3	S	126/191 (66%)	112 (89%)	13 (10%)	1 (1%)	16	50
3	T	126/191 (66%)	116 (92%)	9 (7%)	1 (1%)	16	50
All	All	1867/2392 (78%)	1746 (94%)	109 (6%)	12 (1%)	21	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593	HIS
1	B	593	HIS
2	F	380	GLU
1	A	245	LYS
1	B	460	THR
2	E	380	GLU
3	S	579	MET
3	T	579	MET
1	A	273	GLN
1	A	565	GLN
2	E	174	GLY
2	F	174	GLY

5.3.2 Protein sidechains ⓘ

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	419/560 (75%)	372 (89%)	47 (11%)	6	24
1	B	421/560 (75%)	378 (90%)	43 (10%)	7	29
2	E	321/325 (99%)	294 (92%)	27 (8%)	10	37
2	F	322/325 (99%)	294 (91%)	28 (9%)	9	35
3	S	122/175 (70%)	105 (86%)	17 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	122/175 (70%)	106 (87%)	16 (13%)	4	19
All	All	1727/2120 (82%)	1549 (90%)	178 (10%)	7	28

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	10	LYS
1	A	25	ARG
1	A	28	GLN
1	A	29	LEU
1	A	34	ARG
1	A	36	ASP
1	A	51	GLU
1	A	53	THR
1	A	55	ILE
1	A	62	GLN
1	A	65	ILE
1	A	70	ILE
1	A	86	THR
1	A	90	ASP
1	A	96	ILE
1	A	98	LEU
1	A	109	ILE
1	A	112	SER
1	A	116	LEU
1	A	117	GLN
1	A	180	GLN
1	A	193	LEU
1	A	225	GLU
1	A	239	GLU
1	A	241	LYS
1	A	243	LYS
1	A	275	GLU
1	A	284	LEU
1	A	444	ILE
1	A	452	CYS
1	A	463	CYS
1	A	471	VAL
1	A	521	GLN
1	A	525	HIS
1	A	561	ARG

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Mol	Chain	Res	Type
1	A	562	CYS
1	A	563	LYS
1	A	567	ASN
1	A	592	ASP
1	A	595	ASP
1	A	605	SER
1	A	628	ILE
1	A	632	VAL
1	A	675	VAL
1	A	685	ARG
1	A	700	MET
1	B	13	ILE
1	B	25	ARG
1	B	27	ARG
1	B	28	GLN
1	B	29	LEU
1	B	33	ARG
1	B	39	LYS
1	B	51	GLU
1	B	53	THR
1	B	62	GLN
1	B	65	ILE
1	B	71	MET
1	B	86	THR
1	B	90	ASP
1	B	96	ILE
1	B	98	LEU
1	B	109	ILE
1	B	112	SER
1	B	116	LEU
1	B	117	GLN
1	B	239	GLU
1	B	241	LYS
1	B	245	LYS
1	B	274	ARG
1	B	275	GLU
1	B	284	LEU
1	B	452	CYS
1	B	463	CYS
1	B	471	VAL
1	B	521	GLN
1	B	525	HIS

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Mol	Chain	Res	Type
1	B	561	ARG
1	B	563	LYS
1	B	567	ASN
1	B	595	ASP
1	B	605	SER
1	B	628	ILE
1	B	632	VAL
1	B	670	ASN
1	B	675	VAL
1	B	685	ARG
1	B	700	MET
1	B	732	ASP
2	E	101	THR
2	E	117	GLU
2	E	145	SER
2	E	166	MET
2	E	169	ILE
2	E	177	ASN
2	E	181	GLU
2	E	182	LEU
2	E	201	LEU
2	E	254	LYS
2	E	255	ARG
2	E	261	LYS
2	E	292	ARG
2	E	326	ILE
2	E	328	LYS
2	E	329	ILE
2	E	330	LYS
2	E	348	ASP
2	E	356	MET
2	E	362	MET
2	E	363	LEU
2	E	380	GLU
2	E	381	ASP
2	E	388	THR
2	E	390	LEU
2	E	408	SER
2	E	415	CYS
2	F	101	THR
2	F	145	SER
2	F	166	MET

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Mol	Chain	Res	Type
2	F	169	ILE
2	F	177	ASN
2	F	181	GLU
2	F	182	LEU
2	F	201	LEU
2	F	254	LYS
2	F	255	ARG
2	F	261	LYS
2	F	292	ARG
2	F	326	ILE
2	F	328	LYS
2	F	329	ILE
2	F	330	LYS
2	F	332	SER
2	F	334	SER
2	F	348	ASP
2	F	356	MET
2	F	362	MET
2	F	363	LEU
2	F	380	GLU
2	F	381	ASP
2	F	388	THR
2	F	390	LEU
2	F	408	SER
2	F	426	LEU
3	S	572	LEU
3	S	575	ARG
3	S	577	GLN
3	S	585	ASP
3	S	586	GLU
3	S	587	LYS
3	S	590	GLU
3	S	607	ASN
3	S	608	GLU
3	S	638	LEU
3	S	640	VAL
3	S	654	ARG
3	S	661	VAL
3	S	663	MET
3	S	671	ILE
3	S	674	ILE
3	S	687	LYS

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Mol	Chain	Res	Type
3	T	572	LEU
3	T	574	LEU
3	T	579	MET
3	T	585	ASP
3	T	586	GLU
3	T	590	GLU
3	T	607	ASN
3	T	608	GLU
3	T	638	LEU
3	T	640	VAL
3	T	658	LEU
3	T	661	VAL
3	T	663	MET
3	T	671	ILE
3	T	674	ILE
3	T	687	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	47	GLN
1	A	50	GLN
1	A	102	ASN
1	A	263	ASN
1	A	548	GLN
1	A	607	GLN
1	A	635	ASN
1	A	648	GLN
1	A	670	ASN
1	A	671	ASN
1	A	717	GLN
1	B	57	ASN
1	B	94	GLN
1	B	102	ASN
1	B	263	ASN
1	B	548	GLN
1	B	567	ASN
1	B	607	GLN
1	B	648	GLN
1	B	668	ASN
1	B	670	ASN

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Mol	Chain	Res	Type
1	B	671	ASN
1	B	706	HIS
1	B	717	GLN
2	E	86	GLN
2	E	132	ASN
2	E	143	ASN
2	E	175	HIS
2	E	244	HIS
2	E	258	ASN
2	E	291	HIS
2	E	293	ASN
2	E	360	GLN
2	E	383	HIS
2	F	86	GLN
2	F	132	ASN
2	F	143	ASN
2	F	175	HIS
2	F	244	HIS
2	F	258	ASN
2	F	291	HIS
2	F	293	ASN
2	F	360	GLN
2	F	383	HIS
3	S	562	ASN
3	S	567	HIS
3	S	607	ASN
3	S	631	GLN
3	S	642	ASN
3	S	645	GLN
3	S	659	HIS
3	S	664	HIS
3	T	607	ASN
3	T	631	GLN
3	T	642	ASN
3	T	645	GLN
3	T	651	ASN
3	T	659	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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	-	38,39,39	0.43	0	46,57,57	0.91	2 (4%)
4	6BN	B	9001	-	38,39,39	0.34	0	46,57,57	0.87	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	-	-	2/18/41/41	0/4/4/4
4	6BN	B	9001	-	-	2/18/41/41	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	9001	6BN	C15-C14-C13	-2.69	117.28	120.26
4	A	9001	6BN	C4-C5-C8	-2.41	116.31	119.58
4	B	9001	6BN	C15-C14-C13	-2.39	117.61	120.26
4	B	9001	6BN	C4-C5-C8	-2.38	116.35	119.58

There are no chirality outliers.

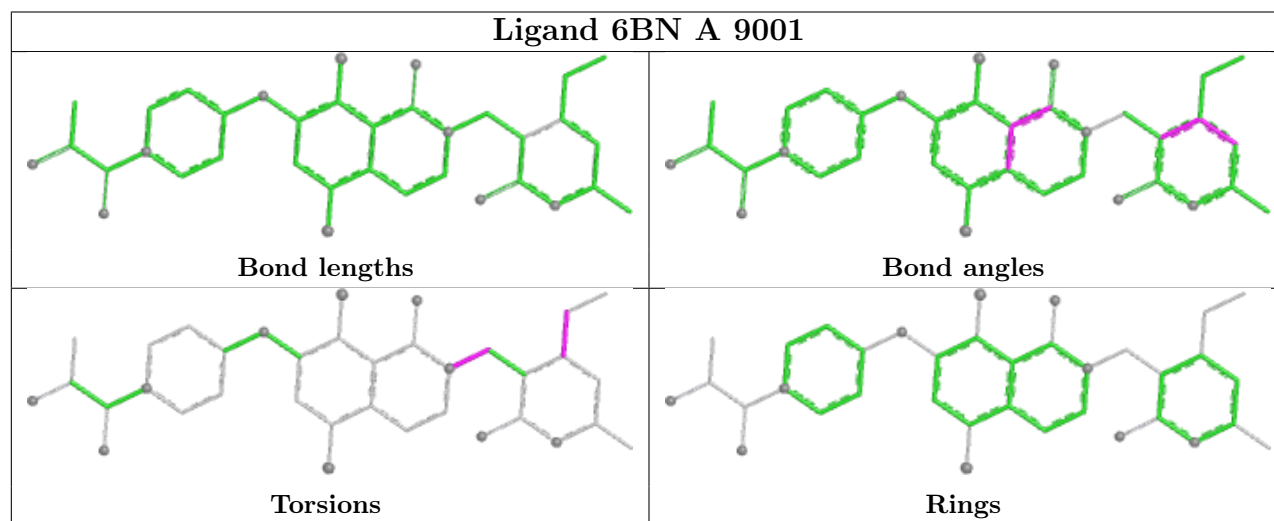
All (4) torsion outliers are listed below:

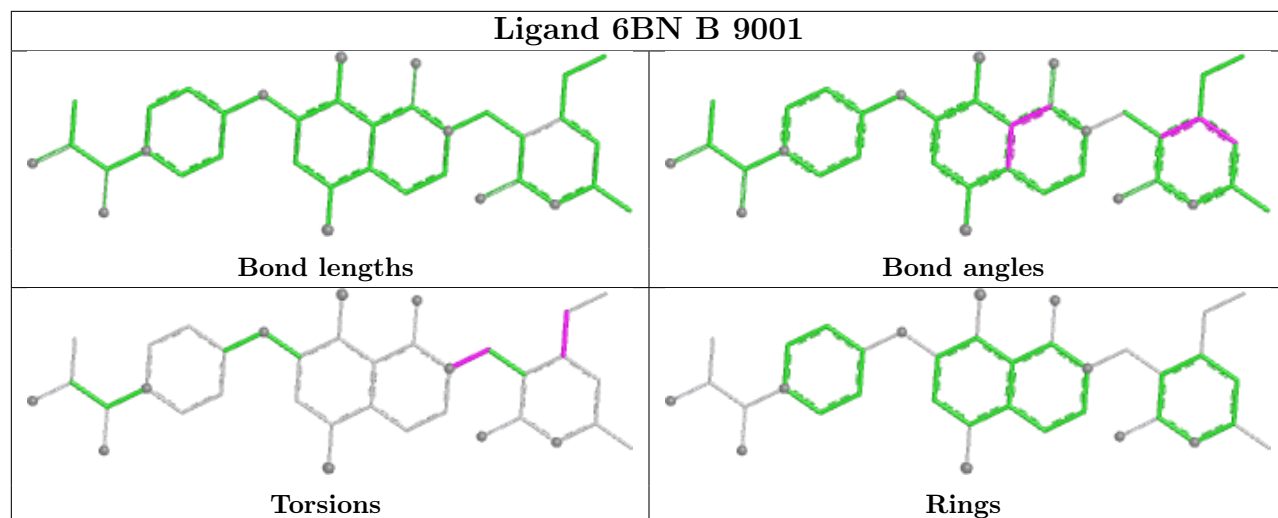
Mol	Chain	Res	Type	Atoms
4	A	9001	6BN	C13-C14-C21-C22
4	B	9001	6BN	C13-C14-C21-C22
4	A	9001	6BN	C13-C12-N9-C8
4	B	9001	6BN	C13-C12-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

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, 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	464/643 (72%)	0.19	17 (3%)	45 25	39, 66, 109, 139	0
1	B	466/643 (72%)	0.28	19 (4%)	41 23	41, 72, 113, 125	0
2	E	358/362 (98%)	-0.10	3 (0%)	82 64	37, 59, 87, 127	0
2	F	359/362 (99%)	-0.18	3 (0%)	82 64	35, 56, 87, 120	0
3	S	128/191 (67%)	0.45	2 (1%)	70 47	47, 83, 111, 117	0
3	T	128/191 (67%)	0.55	6 (4%)	36 19	41, 80, 112, 128	0
All	All	1903/2392 (79%)	0.13	50 (2%)	57 34	35, 65, 108, 139	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	PRO	4.3
1	B	301	ALA	3.8
1	B	219	PRO	3.6
3	T	688	LEU	3.6
1	A	733	ALA	3.5
1	B	305	THR	3.5
1	A	466	VAL	3.4
1	B	469	PHE	3.1
1	B	452	CYS	3.0
1	B	466	VAL	3.0
1	A	458	ILE	2.9
2	F	426	LEU	2.9
1	A	452	CYS	2.7
1	A	305	THR	2.7
1	B	454	ILE	2.7
1	A	303	PRO	2.7
1	B	548	GLN	2.6
3	S	688	LEU	2.5
2	F	381	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	304	ASN	2.5
1	B	663	CYS	2.5
1	B	302	THR	2.5
1	A	39	LYS	2.4
1	B	72	THR	2.4
1	A	463	CYS	2.4
3	T	687	LYS	2.4
1	A	454	ILE	2.4
1	A	467	TYR	2.4
2	E	165	THR	2.4
1	A	199	LYS	2.3
3	T	677	ALA	2.3
1	B	435	ALA	2.3
2	E	381	ASP	2.3
1	B	433	SER	2.3
1	A	301	ALA	2.2
2	F	379	VAL	2.1
3	T	680	LYS	2.1
1	B	306	TYR	2.1
1	B	733	ALA	2.1
2	E	383	HIS	2.1
1	A	272	VAL	2.1
3	S	657	MET	2.1
1	A	267	PRO	2.1
1	B	86	THR	2.1
1	B	303	PRO	2.1
1	A	457	LEU	2.1
1	A	469	PHE	2.1
3	T	641	GLU	2.1
1	B	199	LYS	2.0
3	T	640	VAL	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 oligosaccharides in this entry.

6.4 Ligands

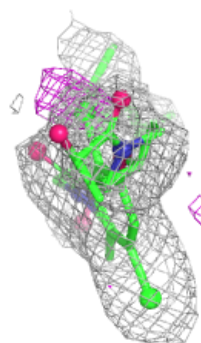
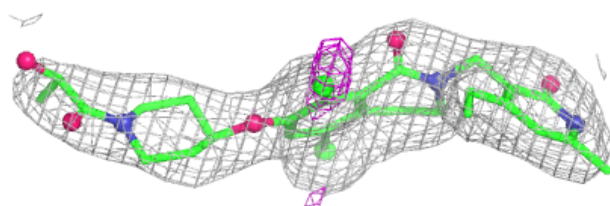
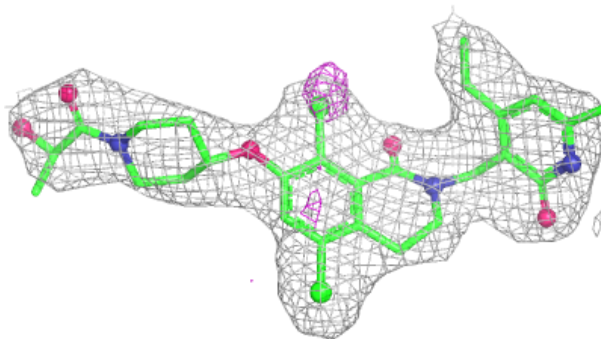
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	A	9005	1/1	0.93	0.21	300,300,300,300	1
4	6BN	B	9001	36/36	0.94	0.09	29,50,68,69	0
4	6BN	A	9001	36/36	0.95	0.08	18,46,55,56	0
5	ZN	A	9004	1/1	0.99	0.03	45,45,45,45	1
5	ZN	B	9002	1/1	0.99	0.07	53,53,53,53	1
5	ZN	B	9003	1/1	0.99	0.05	61,61,61,61	1
5	ZN	B	9004	1/1	0.99	0.08	59,59,59,59	1
5	ZN	B	9007	1/1	0.99	0.05	65,65,65,65	1
5	ZN	A	9008	1/1	1.00	0.04	35,35,35,35	1
5	ZN	A	9002	1/1	1.00	0.06	59,59,59,59	1
5	ZN	A	9003	1/1	1.00	0.03	45,45,45,45	1
5	ZN	A	9006	1/1	1.00	0.06	37,37,37,37	1
5	ZN	B	9005	1/1	1.00	0.07	42,42,42,42	1
5	ZN	B	9006	1/1	1.00	0.07	53,53,53,53	1
5	ZN	A	9007	1/1	1.00	0.06	39,39,39,39	1
5	ZN	B	9008	1/1	1.00	0.07	47,47,47,47	1

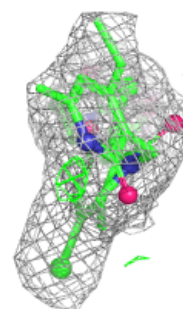
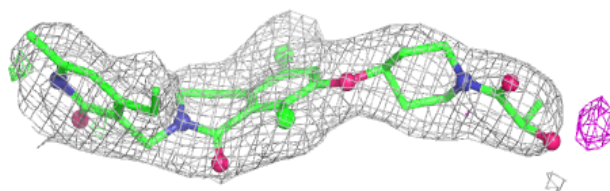
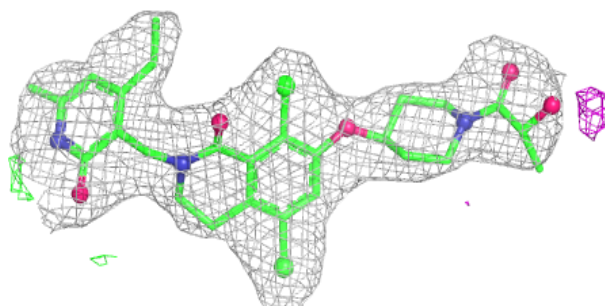
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 6BN B 9001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 6BN A 9001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.