wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2021 – 03:04 pm GMT

PDB ID	:	7P47
Title	:	Structure of the E3 ligase Smc5/Nse2 in complex with Ubc9-SUMO thioester mimetic
Authors	:	Lascorz, J.; Varejao, N.; Reverter, D.
Deposited on	:	2021-07-09
Resolution	:	3.31 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

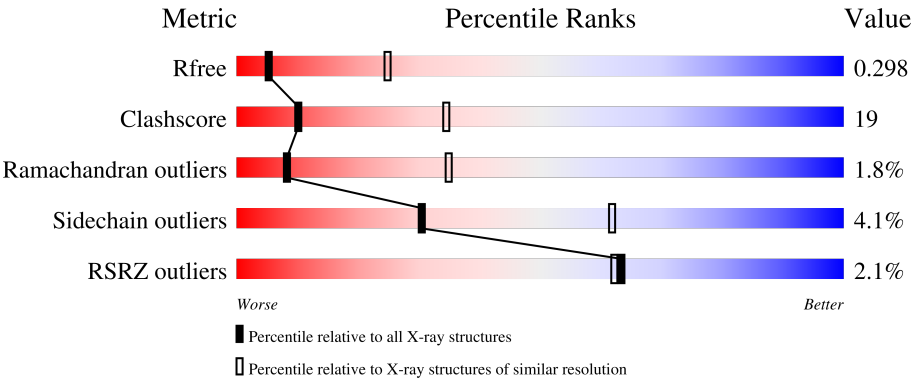
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	B	84	% 48% 33% · 18%
2	C	165	65% 27% · 6%
3	A	214	5% 49% 34% · 13%
4	D	121	47% 16% · 36%
4	E	121	40% 17% · 40%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4561 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 Structural maintenance of chromosomes protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	69	Total	C	N	O	S	0	0	0
			583	369	103	109	2			

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	326	MET	-	initiating methionine	UNP Q08204
B	327	GLY	-	expression tag	UNP Q08204
B	328	THR	-	expression tag	UNP Q08204
B	329	ASP	-	expression tag	UNP Q08204
B	330	GLU	-	expression tag	UNP Q08204
B	331	PHE	-	expression tag	UNP Q08204
B	332	LEU	-	expression tag	UNP Q08204
B	333	LYS	-	expression tag	UNP Q08204
B	334	ALA	-	expression tag	UNP Q08204
B	335	LYS	-	expression tag	UNP Q08204
B	336	GLU	-	expression tag	UNP Q08204
B	337	LYS	-	expression tag	UNP Q08204
B	338	ILE	-	expression tag	UNP Q08204
B	339	ASN	-	expression tag	UNP Q08204
B	340	GLU	-	expression tag	UNP Q08204
B	341	ILE	-	expression tag	UNP Q08204
B	342	PHE	-	expression tag	UNP Q08204
B	343	GLU	-	expression tag	UNP Q08204
B	344	LYS	-	expression tag	UNP Q08204
B	345	LEU	-	expression tag	UNP Q08204
B	346	ASN	-	expression tag	UNP Q08204
B	347	THR	-	expression tag	UNP Q08204
B	348	ILE	-	expression tag	UNP Q08204
B	349	ARG	-	expression tag	UNP Q08204
B	350	ASP	-	expression tag	UNP Q08204
B	351	GLU	-	expression tag	UNP Q08204
B	352	VAL	-	expression tag	UNP Q08204

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Chain	Residue	Modelled	Actual	Comment	Reference
B	353	ILE	-	expression tag	UNP Q08204
B	354	LYS	-	expression tag	UNP Q08204
B	355	LYS	-	expression tag	UNP Q08204
B	356	LYS	-	expression tag	UNP Q08204
B	357	ASN	-	expression tag	UNP Q08204
B	358	GLN	-	expression tag	UNP Q08204
B	359	ASN	-	expression tag	UNP Q08204
B	360	GLU	-	expression tag	UNP Q08204
B	361	TYR	-	expression tag	UNP Q08204
B	362	TYR	-	expression tag	UNP Q08204
B	363	ARG	-	expression tag	UNP Q08204
B	732	GLY	-	expression tag	UNP Q08204
B	733	ARG	-	expression tag	UNP Q08204
B	734	THR	-	expression tag	UNP Q08204
B	735	GLY	-	expression tag	UNP Q08204
B	736	THR	-	expression tag	UNP Q08204

- Molecule 2 is a protein called SUMO-conjugating enzyme UBC9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	155	Total	C	N	O	S	0	0	0
			1258	810	218	227	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	129	LYS	ALA	engineered mutation	UNP P50623
C	153	ARG	LYS	engineered mutation	UNP P50623
C	158	GLY	-	expression tag	UNP P50623
C	159	TYR	-	expression tag	UNP P50623
C	160	HIS	-	expression tag	UNP P50623
C	161	HIS	-	expression tag	UNP P50623
C	162	HIS	-	expression tag	UNP P50623
C	163	HIS	-	expression tag	UNP P50623
C	164	HIS	-	expression tag	UNP P50623
C	165	HIS	-	expression tag	UNP P50623

- Molecule 3 is a protein called E3 SUMO-protein ligase MMS21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	187	Total	C	N	O	S	0	0	0
			1487	921	249	305	12			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P38632
A	5	GLY	-	expression tag	UNP P38632
A	6	SER	-	expression tag	UNP P38632
A	7	SER	-	expression tag	UNP P38632
A	8	HIS	-	expression tag	UNP P38632
A	9	HIS	-	expression tag	UNP P38632
A	10	HIS	-	expression tag	UNP P38632
A	11	HIS	-	expression tag	UNP P38632
A	12	HIS	-	expression tag	UNP P38632
A	13	HIS	-	expression tag	UNP P38632
A	14	SER	-	expression tag	UNP P38632
A	15	SER	-	expression tag	UNP P38632
A	16	GLY	-	expression tag	UNP P38632
A	17	LEU	-	expression tag	UNP P38632
A	18	VAL	-	expression tag	UNP P38632
A	19	PRO	-	expression tag	UNP P38632
A	20	ARG	-	expression tag	UNP P38632
A	21	GLY	-	expression tag	UNP P38632
A	22	SER	-	expression tag	UNP P38632
A	23	HIS	-	expression tag	UNP P38632
A	24	MET	-	expression tag	UNP P38632
A	25	LEU	-	expression tag	UNP P38632
A	26	GLU	-	expression tag	UNP P38632
A	?	-	PHE	deletion	UNP P38632
A	?	-	ASP	deletion	UNP P38632
A	?	-	GLU	deletion	UNP P38632
A	?	-	HIS	deletion	UNP P38632
A	?	-	ILE	deletion	UNP P38632
A	?	-	LYS	deletion	UNP P38632
A	?	-	ASP	deletion	UNP P38632
A	?	-	LEU	deletion	UNP P38632
A	?	-	LYS	deletion	UNP P38632
A	?	-	LYS	deletion	UNP P38632
A	?	-	ASN	deletion	UNP P38632
A	?	-	PHE	deletion	UNP P38632
A	?	-	LYS	deletion	UNP P38632
A	?	-	GLN	deletion	UNP P38632
A	?	-	SER	deletion	UNP P38632
A	?	-	SER	deletion	UNP P38632
A	?	-	ASP	deletion	UNP P38632
A	?	-	ALA	deletion	UNP P38632
A	?	-	CYS	deletion	UNP P38632

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P38632
A	?	-	GLN	deletion	UNP P38632
A	?	-	ILE	deletion	UNP P38632
A	?	-	ASP	deletion	UNP P38632
A	?	-	LEU	deletion	UNP P38632
A	?	-	SER	deletion	UNP P38632
A	?	-	THR	deletion	UNP P38632
A	?	-	TRP	deletion	UNP P38632
A	?	-	ASP	deletion	UNP P38632
A	?	-	LYS	deletion	UNP P38632
A	?	-	TYR	deletion	UNP P38632
A	?	-	ARG	deletion	UNP P38632
A	?	-	THR	deletion	UNP P38632
A	?	-	GLY	deletion	UNP P38632
A	?	-	GLU	deletion	UNP P38632
A	?	-	LEU	deletion	UNP P38632
A	?	-	THR	deletion	UNP P38632
A	?	-	ALA	deletion	UNP P38632
A	?	-	PRO	deletion	UNP P38632
A	?	-	LYS	deletion	UNP P38632
A	?	-	LEU	deletion	UNP P38632
A	?	-	SER	deletion	UNP P38632
A	?	-	GLU	deletion	UNP P38632
A	?	-	LEU	deletion	UNP P38632
A	?	-	TYR	deletion	UNP P38632
A	?	-	LEU	deletion	UNP P38632
A	?	-	ASN	deletion	UNP P38632
A	?	-	MET	deletion	UNP P38632
A	?	-	PRO	deletion	UNP P38632
A	?	-	THR	deletion	UNP P38632
A	?	-	PRO	deletion	UNP P38632
A	133	GLY	GLU	conflict	UNP P38632
A	134	THR	PRO	conflict	UNP P38632

- Molecule 4 is a protein called Ubiquitin-like protein SMT3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	73	Total	C	N	O	S	0	0	0
			599	373	106	117	3			
4	D	78	Total	C	N	O	S	0	0	0
			633	393	112	125	3			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	MET	-	initiating methionine	UNP Q12306
E	-21	GLY	-	expression tag	UNP Q12306
E	-20	SER	-	expression tag	UNP Q12306
E	-19	SER	-	expression tag	UNP Q12306
E	-18	HIS	-	expression tag	UNP Q12306
E	-17	HIS	-	expression tag	UNP Q12306
E	-16	HIS	-	expression tag	UNP Q12306
E	-15	HIS	-	expression tag	UNP Q12306
E	-14	HIS	-	expression tag	UNP Q12306
E	-13	HIS	-	expression tag	UNP Q12306
E	-12	SER	-	expression tag	UNP Q12306
E	-11	SER	-	expression tag	UNP Q12306
E	-10	GLY	-	expression tag	UNP Q12306
E	-9	LEU	-	expression tag	UNP Q12306
E	-8	VAL	-	expression tag	UNP Q12306
E	-7	PRO	-	expression tag	UNP Q12306
E	-6	ARG	-	expression tag	UNP Q12306
E	-5	GLY	-	expression tag	UNP Q12306
E	-4	SER	-	expression tag	UNP Q12306
E	-3	HIS	-	expression tag	UNP Q12306
E	-2	MET	-	expression tag	UNP Q12306
E	-1	ALA	-	expression tag	UNP Q12306
E	0	SER	-	expression tag	UNP Q12306
D	-22	MET	-	initiating methionine	UNP Q12306
D	-21	GLY	-	expression tag	UNP Q12306
D	-20	SER	-	expression tag	UNP Q12306
D	-19	SER	-	expression tag	UNP Q12306
D	-18	HIS	-	expression tag	UNP Q12306
D	-17	HIS	-	expression tag	UNP Q12306
D	-16	HIS	-	expression tag	UNP Q12306
D	-15	HIS	-	expression tag	UNP Q12306
D	-14	HIS	-	expression tag	UNP Q12306
D	-13	HIS	-	expression tag	UNP Q12306
D	-12	SER	-	expression tag	UNP Q12306
D	-11	SER	-	expression tag	UNP Q12306
D	-10	GLY	-	expression tag	UNP Q12306
D	-9	LEU	-	expression tag	UNP Q12306
D	-8	VAL	-	expression tag	UNP Q12306
D	-7	PRO	-	expression tag	UNP Q12306
D	-6	ARG	-	expression tag	UNP Q12306
D	-5	GLY	-	expression tag	UNP Q12306
D	-4	SER	-	expression tag	UNP Q12306
D	-3	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP Q12306
D	-1	ALA	-	expression tag	UNP Q12306
D	0	SER	-	expression tag	UNP Q12306

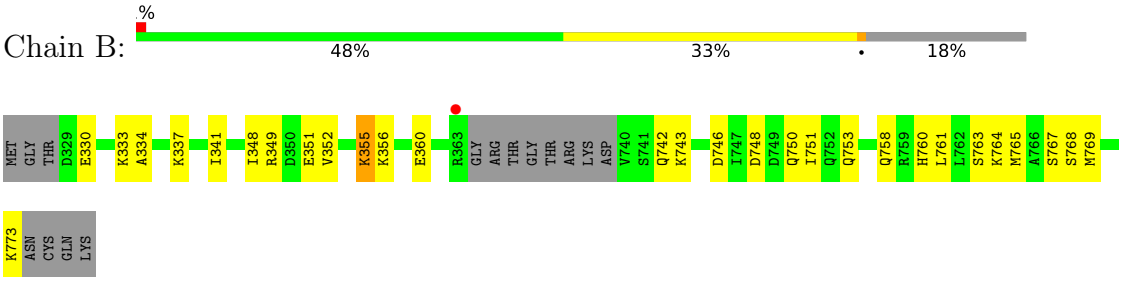
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0

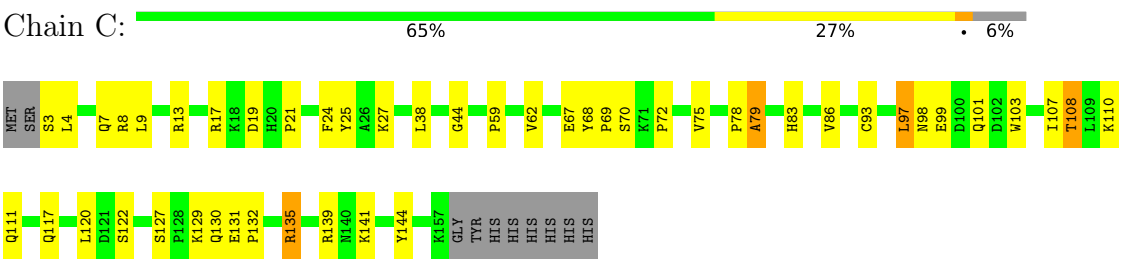
3 Residue-property plots (i)

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.

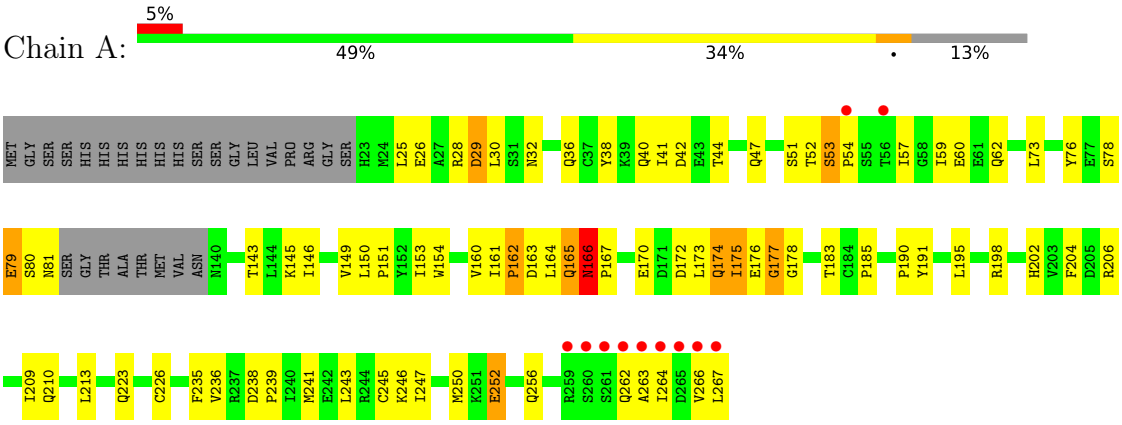
• Molecule 1: Structural maintenance of chromosomes protein 5



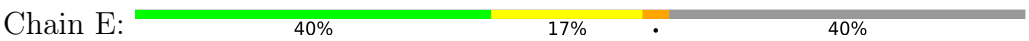
• Molecule 2: SUMO-conjugating enzyme UBC9

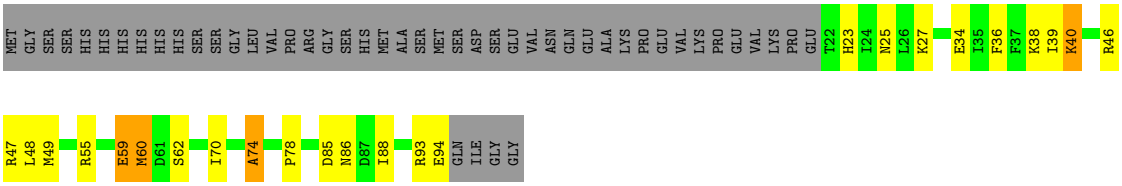


• Molecule 3: E3 SUMO-protein ligase MMS21



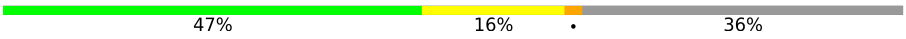
• Molecule 4: Ubiquitin-like protein SMT3

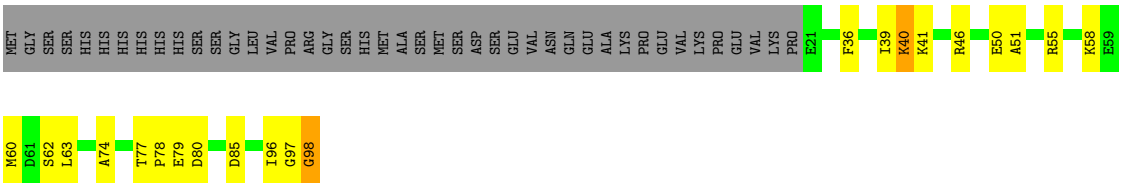




• Molecule 4: Ubiquitin-like protein SMT3

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.14Å 103.24Å 115.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.13 – 3.31 47.14 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.13-3.31) 99.2 (47.14-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.236 , 0.293 0.241 , 0.298	Depositor DCC
R_{free} test set	654 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	100.2	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4561	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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

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	B	0.44	0/586	0.76	3/774 (0.4%)
2	C	0.55	0/1298	0.67	0/1761
3	A	0.46	0/1509	0.75	1/2044 (0.0%)
4	D	0.63	2/641 (0.3%)	0.84	4/856 (0.5%)
4	E	0.43	0/607	0.74	1/811 (0.1%)
All	All	0.51	2/4641 (0.0%)	0.74	9/6246 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	98	GLY	C-O	-10.28	1.07	1.23
4	D	96	ILE	C-N	6.12	1.44	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	97	GLY	O-C-N	-7.73	110.06	123.20
1	B	769	MET	CB-CA-C	-6.99	96.42	110.40
3	A	262	GLN	CB-CA-C	-6.94	96.52	110.40
4	D	97	GLY	C-N-CA	6.42	135.78	122.30
4	D	97	GLY	CA-C-N	6.18	128.56	116.20

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	B	583	0	620	23	0
2	C	1258	0	1244	41	0
3	A	1487	0	1457	86	0
4	D	633	0	625	19	0
4	E	599	0	594	24	0
5	A	1	0	0	0	0
All	All	4561	0	4540	172	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 19.

The worst 5 of 172 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)
3:A:164:LEU:HD22	3:A:174:GLN:HB2	1.26	1.17
2:C:130:GLN:OE1	2:C:132:PRO:HG2	1.58	1.02
3:A:174:GLN:O	3:A:174:GLN:NE2	2.08	0.86
3:A:167:PRO:HD2	3:A:170:GLU:HB2	1.64	0.80
3:A:167:PRO:HD2	3:A:170:GLU:CB	2.11	0.79

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	B	65/84 (77%)	60 (92%)	5 (8%)	0	100 100
2	C	153/165 (93%)	144 (94%)	8 (5%)	1 (1%)	22 55
3	A	183/214 (86%)	144 (79%)	31 (17%)	8 (4%)	2 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	76/121 (63%)	71 (93%)	5 (7%)	0	100 100
4	E	71/121 (59%)	62 (87%)	8 (11%)	1 (1%)	11 39
All	All	548/705 (78%)	481 (88%)	57 (10%)	10 (2%)	8 35

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	79	ALA
3	A	80	SER
3	A	172	ASP
3	A	177	GLY
3	A	252	GLU

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	B	67/79 (85%)	65 (97%)	2 (3%)	41 69
2	C	136/145 (94%)	129 (95%)	7 (5%)	24 56
3	A	174/196 (89%)	164 (94%)	10 (6%)	20 52
4	D	69/107 (64%)	69 (100%)	0	100 100
4	E	66/107 (62%)	64 (97%)	2 (3%)	41 69
All	All	512/634 (81%)	491 (96%)	21 (4%)	30 62

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	79	GLU
3	A	174	GLN
4	E	60	MET
3	A	175	ILE
3	A	166	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	210	GLN
4	E	23	HIS
4	D	23	HIS
3	A	166	ASN
3	A	47	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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 (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, 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	B	69/84 (82%)	0.08	1 (1%) 75 75	70, 95, 138, 147	0
2	C	155/165 (93%)	0.11	0 100 100	64, 82, 119, 136	0
3	A	187/214 (87%)	0.39	11 (5%) 22 23	69, 103, 169, 188	0
4	D	78/121 (64%)	0.17	0 100 100	68, 95, 113, 146	0
4	E	73/121 (60%)	0.44	0 100 100	66, 101, 120, 125	0
All	All	562/705 (79%)	0.25	12 (2%) 63 62	64, 95, 143, 188	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	261	SER	5.1
3	A	262	GLN	4.2
1	B	363	ARG	3.8
3	A	263	ALA	3.5
3	A	260	SER	3.4

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 monosaccharides 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,

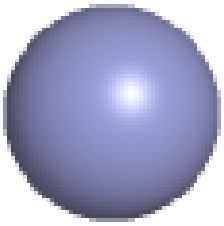
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

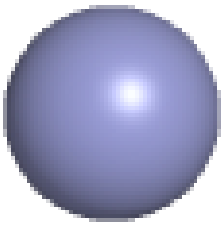
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	A	301	1/1	0.97	0.14	81,81,81,81	0

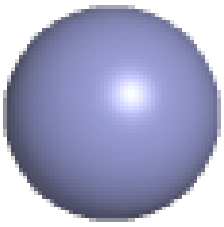
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN A 301:

$2mF_o$-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.