wwPDB X-ray Structure Validation Summary Report (i)

Oct 27, 2023 – 01:09 AM EDT

|		
PDB ID	:	3SIQ
Title	:	Crystal Structure of autoinhibited dIAP1-BIR1 domain
Authors	:	Li, X.; Wang, J.; Shi, Y.
Deposited on	:	2011-06-20
Resolution	:	2.40 Å(reported)

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.214
Clashscore		35
Ramachandran outliers		5.0%
Sidechain outliers		16.3%
RSRZ outliers		0

Worse   *Better*

∎ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
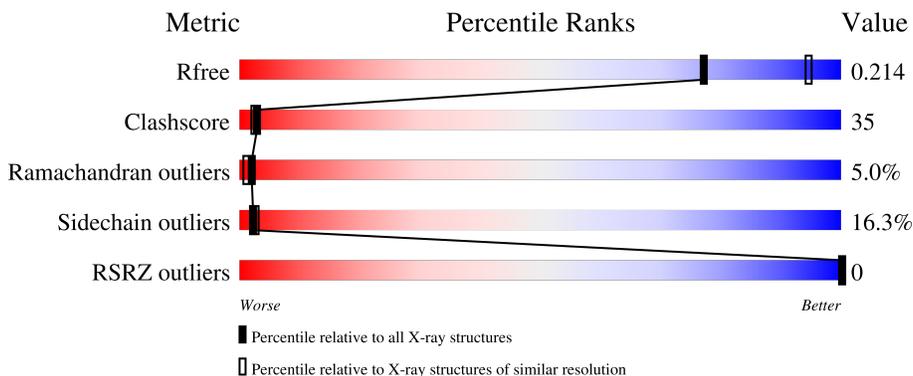
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	136	40% 26% 9% 24%
1	B	136	27% 37% 5% • 30%
1	C	136	37% 29% 5% • 29%
1	D	136	27% 35% 8% • 29%
1	E	136	24% 38% 10% • 27%

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Mol	Chain	Length	Quality of chain
1	F	136	22% 32% 16% 30%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4806 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 Apoptosis 1 inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			834	526	150	153	5			
1	B	95	Total	C	N	O	S	0	0	0
			776	491	140	141	4			
1	C	97	Total	C	N	O	S	0	0	0
			794	501	143	146	4			
1	D	97	Total	C	N	O	S	0	0	0
			796	503	143	146	4			
1	E	99	Total	C	N	O	S	0	1	0
			817	516	147	150	4			
1	F	95	Total	C	N	O	S	0	0	0
			779	494	140	141	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q24306
A	?	-	ASP	deletion	UNP Q24306
A	?	-	LEU	deletion	UNP Q24306
A	?	-	PRO	deletion	UNP Q24306
A	?	-	SER	deletion	UNP Q24306
A	?	-	TYR	deletion	UNP Q24306
A	?	-	GLY	deletion	UNP Q24306
A	89	SER	CYS	engineered mutation	UNP Q24306
A	136	LEU	-	expression tag	UNP Q24306
A	137	GLU	-	expression tag	UNP Q24306
A	138	HIS	-	expression tag	UNP Q24306
A	139	HIS	-	expression tag	UNP Q24306
A	140	HIS	-	expression tag	UNP Q24306
A	141	HIS	-	expression tag	UNP Q24306
A	142	HIS	-	expression tag	UNP Q24306
A	143	HIS	-	expression tag	UNP Q24306
B	?	-	ALA	deletion	UNP Q24306

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP Q24306
B	?	-	LEU	deletion	UNP Q24306
B	?	-	PRO	deletion	UNP Q24306
B	?	-	SER	deletion	UNP Q24306
B	?	-	TYR	deletion	UNP Q24306
B	?	-	GLY	deletion	UNP Q24306
B	89	SER	CYS	engineered mutation	UNP Q24306
B	136	LEU	-	expression tag	UNP Q24306
B	137	GLU	-	expression tag	UNP Q24306
B	138	HIS	-	expression tag	UNP Q24306
B	139	HIS	-	expression tag	UNP Q24306
B	140	HIS	-	expression tag	UNP Q24306
B	141	HIS	-	expression tag	UNP Q24306
B	142	HIS	-	expression tag	UNP Q24306
B	143	HIS	-	expression tag	UNP Q24306
C	?	-	ALA	deletion	UNP Q24306
C	?	-	ASP	deletion	UNP Q24306
C	?	-	LEU	deletion	UNP Q24306
C	?	-	PRO	deletion	UNP Q24306
C	?	-	SER	deletion	UNP Q24306
C	?	-	TYR	deletion	UNP Q24306
C	?	-	GLY	deletion	UNP Q24306
C	89	SER	CYS	engineered mutation	UNP Q24306
C	136	LEU	-	expression tag	UNP Q24306
C	137	GLU	-	expression tag	UNP Q24306
C	138	HIS	-	expression tag	UNP Q24306
C	139	HIS	-	expression tag	UNP Q24306
C	140	HIS	-	expression tag	UNP Q24306
C	141	HIS	-	expression tag	UNP Q24306
C	142	HIS	-	expression tag	UNP Q24306
C	143	HIS	-	expression tag	UNP Q24306
D	?	-	ALA	deletion	UNP Q24306
D	?	-	ASP	deletion	UNP Q24306
D	?	-	LEU	deletion	UNP Q24306
D	?	-	PRO	deletion	UNP Q24306
D	?	-	SER	deletion	UNP Q24306
D	?	-	TYR	deletion	UNP Q24306
D	?	-	GLY	deletion	UNP Q24306
D	89	SER	CYS	engineered mutation	UNP Q24306
D	136	LEU	-	expression tag	UNP Q24306
D	137	GLU	-	expression tag	UNP Q24306
D	138	HIS	-	expression tag	UNP Q24306

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Chain	Residue	Modelled	Actual	Comment	Reference
D	139	HIS	-	expression tag	UNP Q24306
D	140	HIS	-	expression tag	UNP Q24306
D	141	HIS	-	expression tag	UNP Q24306
D	142	HIS	-	expression tag	UNP Q24306
D	143	HIS	-	expression tag	UNP Q24306
E	?	-	ALA	deletion	UNP Q24306
E	?	-	ASP	deletion	UNP Q24306
E	?	-	LEU	deletion	UNP Q24306
E	?	-	PRO	deletion	UNP Q24306
E	?	-	SER	deletion	UNP Q24306
E	?	-	TYR	deletion	UNP Q24306
E	?	-	GLY	deletion	UNP Q24306
E	89	SER	CYS	engineered mutation	UNP Q24306
E	136	LEU	-	expression tag	UNP Q24306
E	137	GLU	-	expression tag	UNP Q24306
E	138	HIS	-	expression tag	UNP Q24306
E	139	HIS	-	expression tag	UNP Q24306
E	140	HIS	-	expression tag	UNP Q24306
E	141	HIS	-	expression tag	UNP Q24306
E	142	HIS	-	expression tag	UNP Q24306
E	143	HIS	-	expression tag	UNP Q24306
F	?	-	ALA	deletion	UNP Q24306
F	?	-	ASP	deletion	UNP Q24306
F	?	-	LEU	deletion	UNP Q24306
F	?	-	PRO	deletion	UNP Q24306
F	?	-	SER	deletion	UNP Q24306
F	?	-	TYR	deletion	UNP Q24306
F	?	-	GLY	deletion	UNP Q24306
F	89	SER	CYS	engineered mutation	UNP Q24306
F	136	LEU	-	expression tag	UNP Q24306
F	137	GLU	-	expression tag	UNP Q24306
F	138	HIS	-	expression tag	UNP Q24306
F	139	HIS	-	expression tag	UNP Q24306
F	140	HIS	-	expression tag	UNP Q24306
F	141	HIS	-	expression tag	UNP Q24306
F	142	HIS	-	expression tag	UNP Q24306
F	143	HIS	-	expression tag	UNP Q24306

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	B	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	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: Apoptosis 1 inhibitor
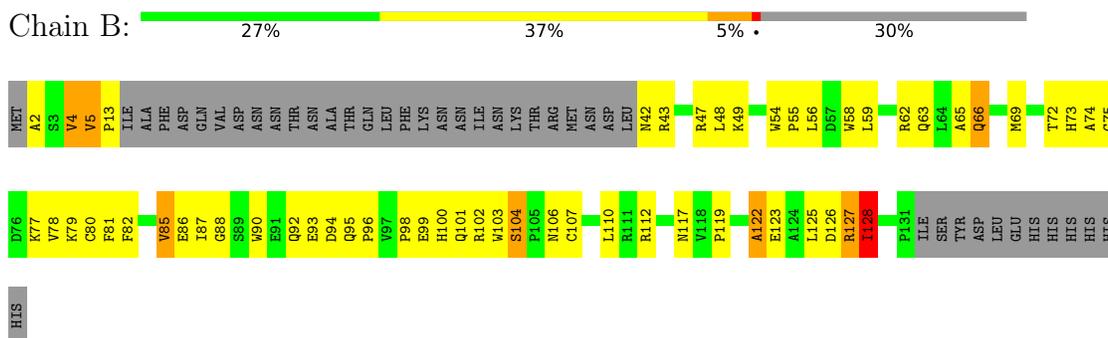
Chain A:

- Molecule 1: Apoptosis 1 inhibitor

Chain B:

- Molecule 1: Apoptosis 1 inhibitor

Chain C:

- Molecule 1: Apoptosis 1 inhibitor

Chain D:

• Molecule 1: Apoptosis 1 inhibitor

Chain E:

• Molecule 1: Apoptosis 1 inhibitor

Chain F:
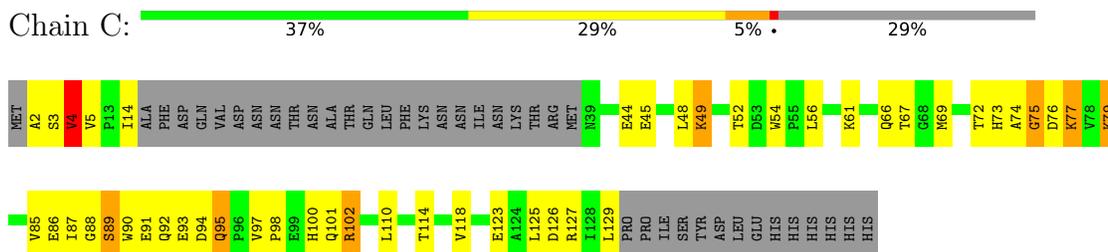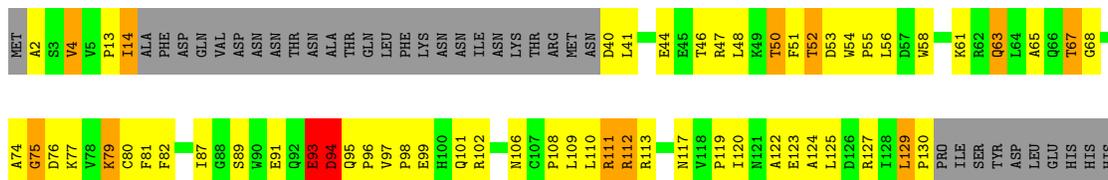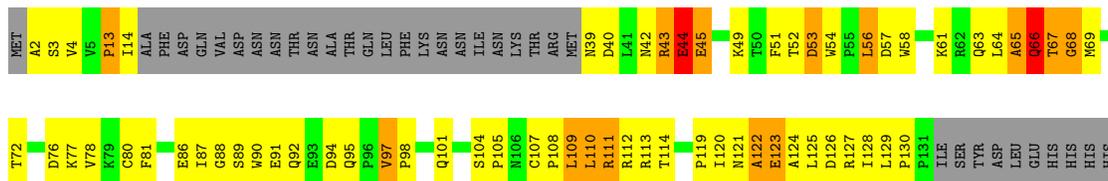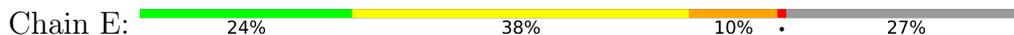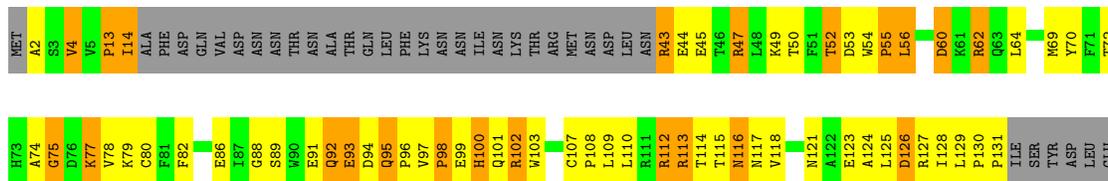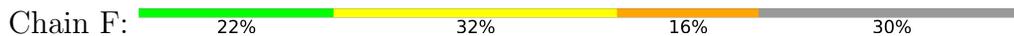
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	99.78Å 99.78Å 71.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.98 – 2.40 32.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (32.98-2.40) 99.5 (32.97-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.146 , 0.217 0.145 , 0.214	Depositor DCC
R_{free} test set	1622 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 11.1	EDS
L-test for twinning[2]	$<|L|>$ = 0.36, $<L^2>$ = 0.18	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l 0.408 for h,-h-k,-l 0.416 for -k,-h,-l	Xtriage
Reported twinning fraction	0.317 for H, K, L 0.182 for -H, H+K, -L 0.305 for -h,-k,l 0.197 for K, H, -L	Depositor
Outliers	0 of 30861 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4806	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/856	0.51	0/1166
1	B	0.28	0/798	0.53	0/1087
1	C	0.29	0/814	0.54	0/1107
1	D	0.27	0/817	0.51	0/1112
1	E	0.30	0/842	0.59	0/1148
1	F	0.28	0/801	0.52	0/1091
All	All	0.29	0/4928	0.54	0/6711

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
1	E	0	4
1	F	0	1
All	All	0	11

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	128	ILE	Peptide
1	B	5	VAL	Peptide
1	C	127	ARG	Peptide
1	C	4	VAL	Peptide

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	834	0	796	32	0
1	B	776	0	745	59	0
1	C	794	0	763	44	0
1	D	796	0	768	71	0
1	E	817	0	789	64	0
1	F	779	0	754	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	F	1	0	0	0	0
All	All	4806	0	4615	330	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 35.

The worst 5 of 330 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:D:47:ARG:O	1:D:50:THR:HG22	1.08	1.25
1:C:77:LYS:HE2	1:C:86:GLU:OE2	1.35	1.23
1:C:77:LYS:CE	1:C:86:GLU:OE2	1.91	1.19
1:D:47:ARG:O	1:D:50:THR:CG2	1.92	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:PRO:O	1:E:14:ILE:HD12	1.42	1.15

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	99/136 (73%)	85 (86%)	11 (11%)	3 (3%)	4	3
1	B	91/136 (67%)	75 (82%)	12 (13%)	4 (4%)	2	2
1	C	93/136 (68%)	85 (91%)	6 (6%)	2 (2%)	6	7
1	D	93/136 (68%)	76 (82%)	14 (15%)	3 (3%)	4	3
1	E	96/136 (71%)	69 (72%)	19 (20%)	8 (8%)	1	0
1	F	91/136 (67%)	72 (79%)	11 (12%)	8 (9%)	1	0
All	All	563/816 (69%)	462 (82%)	73 (13%)	28 (5%)	2	1

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	B	123	GLU
1	C	4	VAL
1	D	93	GLU
1	D	94	ASP

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	91/125 (73%)	76 (84%)	15 (16%)		2	2
1	B	85/125 (68%)	76 (89%)	9 (11%)		6	9
1	C	87/125 (70%)	72 (83%)	15 (17%)		2	2
1	D	88/125 (70%)	71 (81%)	17 (19%)		1	1
1	E	91/125 (73%)	78 (86%)	13 (14%)		3	4
1	F	86/125 (69%)	69 (80%)	17 (20%)		1	1
All	All	528/750 (70%)	442 (84%)	86 (16%)		2	3

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	VAL
1	F	43	ARG
1	E	53	ASP
1	E	97	VAL
1	F	56	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	63	GLN
1	D	121	ASN
1	F	116	ASN
1	F	92	GLN
1	F	101	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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(Å²)	Q<0.9
1	A	103/136 (75%)	-0.60	0	100	100	12, 25, 41, 52	0
1	B	95/136 (69%)	-0.61	0	100	100	19, 31, 42, 50	0
1	C	97/136 (71%)	-0.61	0	100	100	14, 26, 38, 44	0
1	D	97/136 (71%)	-0.65	0	100	100	21, 31, 41, 48	0
1	E	99/136 (72%)	-0.60	0	100	100	11, 27, 42, 53	0
1	F	95/136 (69%)	-0.59	0	100	100	21, 33, 43, 48	0
All	All	586/816 (71%)	-0.61	0	100	100	11, 30, 42, 53	0

There are no RSRZ outliers to report.

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, 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(Å²)	Q<0.9
2	ZN	B	200	1/1	0.99	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	200	1/1	1.00	0.14	28,28,28,28	0
2	ZN	C	200	1/1	1.00	0.13	29,29,29,29	0
2	ZN	D	200	1/1	1.00	0.12	40,40,40,40	0
2	ZN	E	200	1/1	1.00	0.13	28,28,28,28	0
2	ZN	F	200	1/1	1.00	0.11	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.