



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 10:08 pm BST

PDB ID : 2HYE
Title : Crystal Structure of the DDB1-Cul4A-Rbx1-SV5V Complex
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Deposited on : 2006-08-05
Resolution : 3.10 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

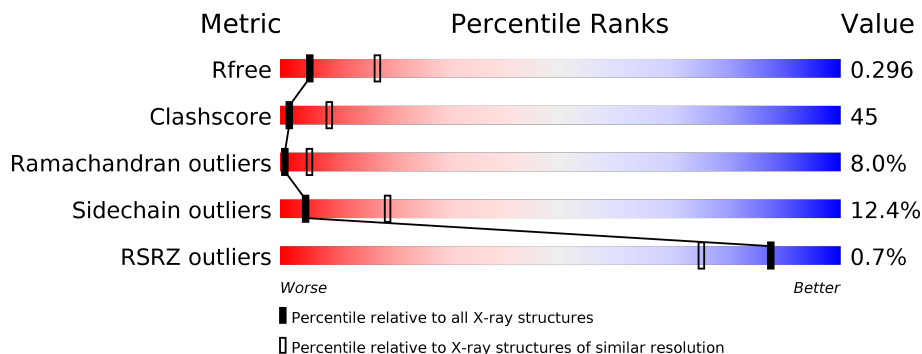
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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	1140	
2	B	222	
3	C	759	
4	D	108	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16943 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1140	8920	5645	1503	1723	49	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	TYR	ASP	CONFLICT	UNP Q16531
A	898	ASP	GLU	CONFLICT	UNP Q16531
A	899	VAL	LEU	CONFLICT	UNP Q16531

- Molecule 2 is a protein called Nonstructural protein V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	180	1373	856	237	272	8	0	0	0

- Molecule 3 is a protein called Cullin-4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	719	5899	3753	1023	1089	34	0	0	0

- Molecule 4 is a protein called RING-box protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	90	746	472	137	128	9	0	0	0

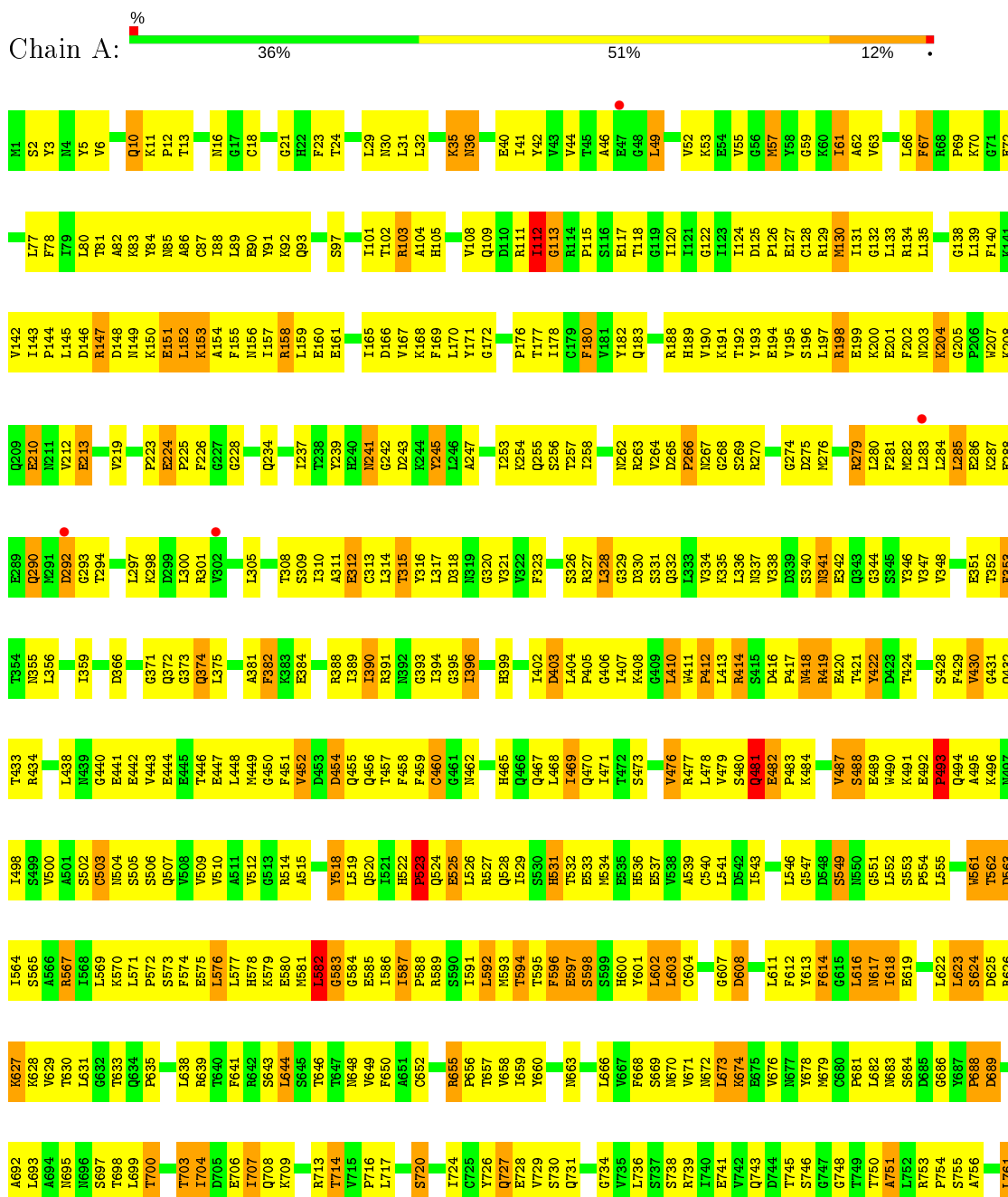
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

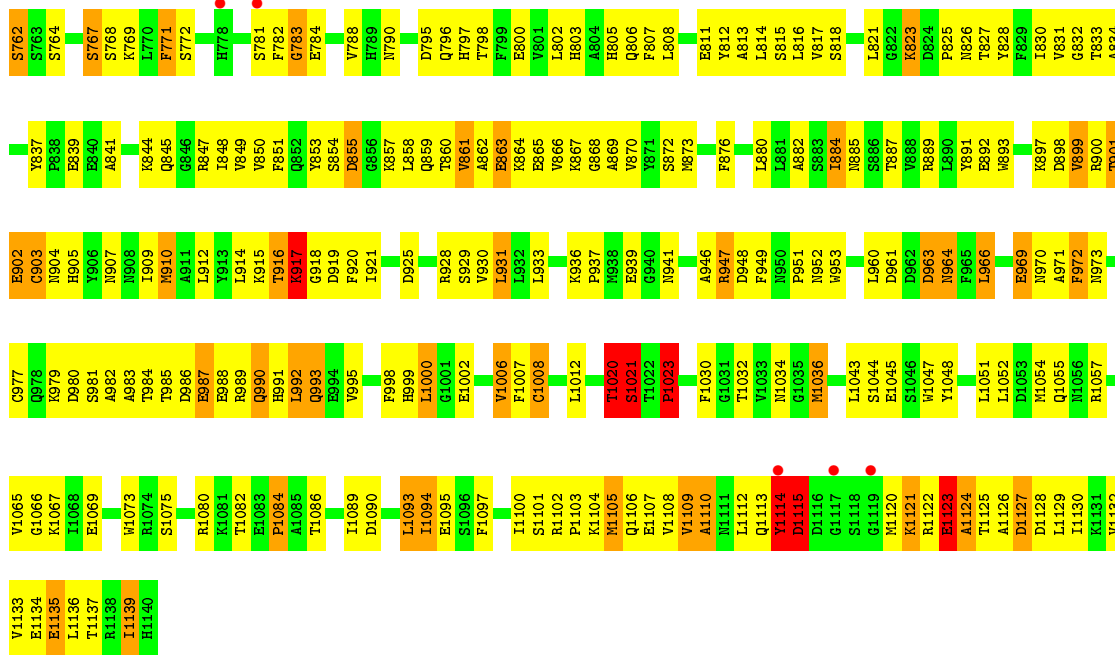
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Zn 2	0	0
5	D	3	Total 3	Zn 3	0	0

3 Residue-property plots

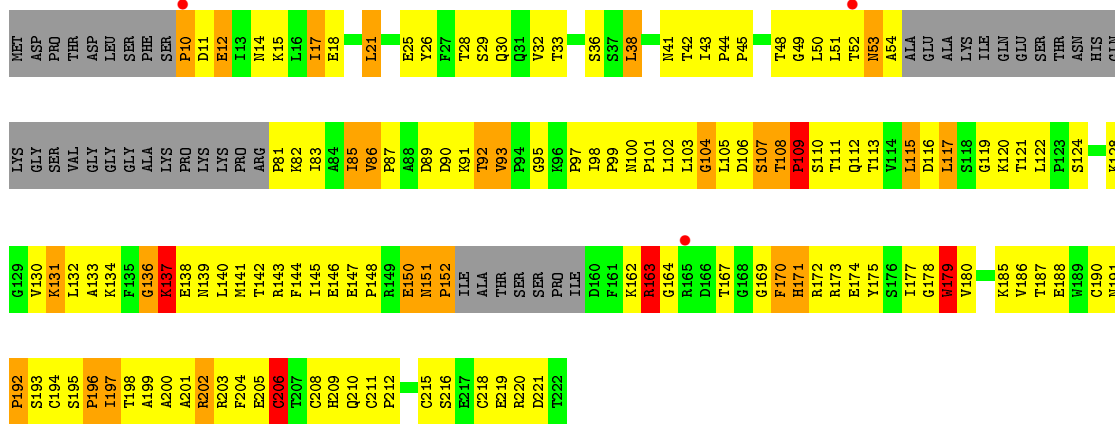
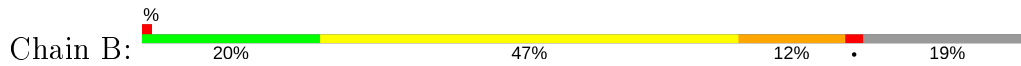
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DNA damage-binding protein 1

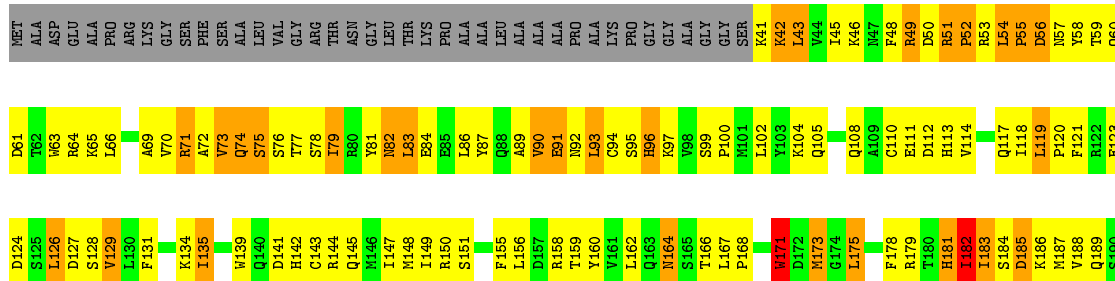
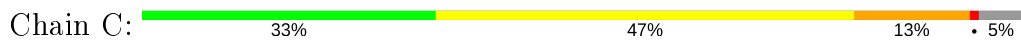


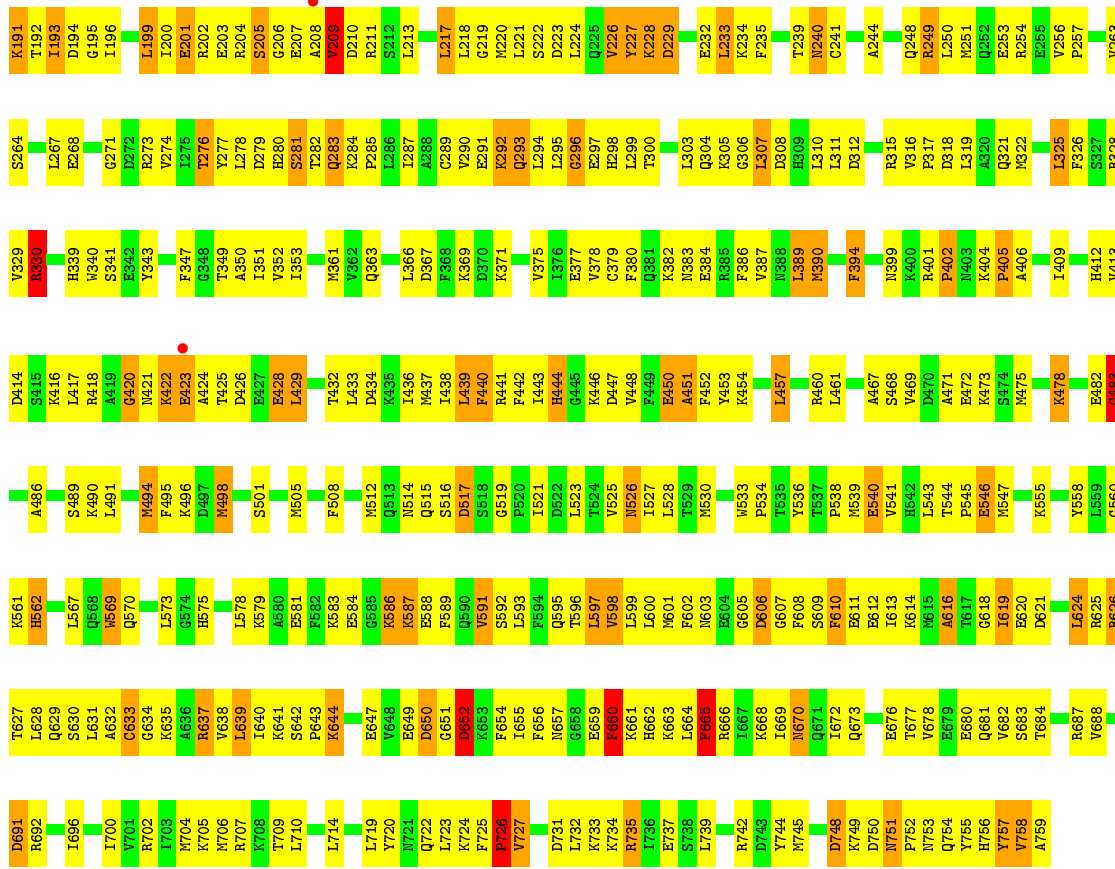


• Molecule 2: Nonstructural protein V

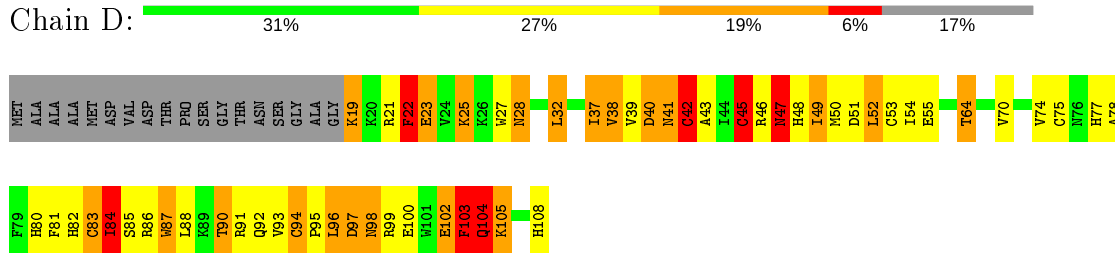


• Molecule 3: Cullin-4A





● Molecule 4: RING-box protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.45Å 203.16Å 424.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.30 – 3.07	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 88.6 (49.30-3.07)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.07Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.316 0.244 , 0.296	Depositor DCC
R_{free} test set	3109 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtrriage
Anisotropy	0.441	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16943	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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:
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	0.48	1/9086 (0.0%)	0.89	30/12311 (0.2%)
2	B	0.54	1/1401 (0.1%)	1.12	10/1899 (0.5%)
3	C	0.47	0/6007	0.80	16/8068 (0.2%)
4	D	0.62	0/768	1.16	11/1040 (1.1%)
All	All	0.49	2/17262 (0.0%)	0.90	67/23318 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	LEU	C-N	6.78	1.45	1.33
2	B	179	TRP	C-N	-5.16	1.22	1.34

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	PRO	CA-N-CD	-17.53	86.95	111.50
1	A	151	GLU	N-CA-C	-16.61	66.15	111.00
1	A	561	TRP	N-CA-C	15.57	153.04	111.00
1	A	561	TRP	CB-CA-C	-15.48	79.43	110.40
2	B	109	PRO	CA-N-CD	-15.47	89.85	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8920	0	8880	812	0
2	B	1373	0	1356	176	0
3	C	5899	0	5977	489	1
4	D	746	0	699	82	0
5	B	2	0	0	0	0
5	D	3	0	0	0	0
All	All	16943	0	16912	1515	1

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 45.

The worst 5 of 1515 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:TYR:CD1	1:A:1114:TYR:O	1.68	1.47
1:A:381:ALA:O	1:A:720:SER:HB3	1.35	1.23
3:C:422:LYS:NZ	3:C:422:LYS:HB3	1.30	1.22
1:A:381:ALA:O	1:A:720:SER:CB	1.90	1.18
1:A:889:ARG:HD3	1:A:904:ASN:HD21	1.16	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:GLN:NE2	3:C:60:GLN:NE2[3_554]	2.09	0.11

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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1138/1140 (100%)	869 (76%)	201 (18%)	68 (6%)	1	9
2	B	174/222 (78%)	119 (68%)	37 (21%)	18 (10%)	0	3
3	C	717/759 (94%)	516 (72%)	132 (18%)	69 (10%)	0	3
4	D	88/108 (82%)	47 (53%)	27 (31%)	14 (16%)	0	0
All	All	2117/2229 (95%)	1551 (73%)	397 (19%)	169 (8%)	1	5

5 of 169 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ILE
1	A	290	GLN
1	A	292	ASP
1	A	430	VAL
1	A	583	GLY

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	999/999 (100%)	871 (87%)	128 (13%)	4	18
2	B	157/191 (82%)	137 (87%)	20 (13%)	4	18
3	C	656/679 (97%)	586 (89%)	70 (11%)	6	26
4	D	79/90 (88%)	62 (78%)	17 (22%)	1	4
All	All	1891/1959 (96%)	1656 (88%)	235 (12%)	4	19

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	964	ASN
2	B	85	ILE
3	C	751	ASN

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Mol	Chain	Res	Type
1	A	987	GLU
1	A	1069	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	859	GLN
1	A	1056	ASN
3	C	756	HIS
1	A	904	ASN
1	A	990	GLN

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 5 ligands modelled in this entry, 5 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1140/1140 (100%)	-0.30	9 (0%) 86 72	22, 68, 125, 202	0
2	B	180/222 (81%)	-0.05	3 (1%) 70 49	32, 86, 135, 167	0
3	C	719/759 (94%)	-0.42	2 (0%) 94 88	23, 71, 126, 173	0
4	D	90/108 (83%)	-0.37	0 100 100	44, 75, 117, 140	0
All	All	2129/2229 (95%)	-0.32	14 (0%) 87 75	22, 71, 126, 202	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1117	GLY	4.7
1	A	778	HIS	4.1
2	B	10	PRO	3.2
3	C	423	GLU	3.0
2	B	165	ARG	2.8

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 carbohydrates in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
5	ZN	D	4003	1/1	0.96	0.20	84,84,84,84	0
5	ZN	B	3001	1/1	0.96	0.09	114,114,114,114	0
5	ZN	D	4001	1/1	0.97	0.16	77,77,77,77	0
5	ZN	D	4002	1/1	0.98	0.16	99,99,99,99	0
5	ZN	B	3002	1/1	0.99	0.10	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.