



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 02:01 PM UTC

PDB ID : 3DQV / pdb_00003dqv
Title : Structural Insights into NEDD8 Activation of Cullin-RING Ligases: Conformational Control of Conjugation
Authors : Duda, D.M.; Borg, L.A.; Scott, D.C.; Hunt, H.W.; Hammel, M.; Schulman, B.A.
Deposited on : 2008-07-09
Resolution : 3.00 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 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
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

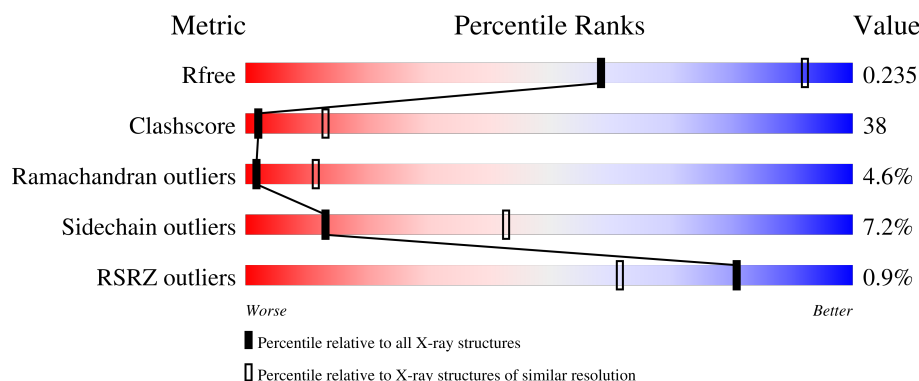
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	81	36% 52% 9% .
1	B	81	31% 59% 5% 5%
2	C	382	42% 48% 8% ..
2	D	382	45% 43% 10% ..
3	R	106	2% 31% 40% 10% 19%

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Mol	Chain	Length	Quality of chain
3	Y	106	6% 39% 30% 10% 20%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8839 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 NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	Se	1	0	0
			609	382	106	118	3			
1	B	77	Total	C	N	O	Se	0	0	0
			605	380	105	117	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	-	insertion	UNP Q15843
A	97	SER	-	insertion	UNP Q15843
A	98	GLY	-	insertion	UNP Q15843
A	99	GLY	-	insertion	UNP Q15843
A	100	SER	-	insertion	UNP Q15843
A	162	MSE	LEU	conflict	UNP Q15843
B	96	GLY	-	insertion	UNP Q15843
B	97	SER	-	insertion	UNP Q15843
B	98	GLY	-	insertion	UNP Q15843
B	99	GLY	-	insertion	UNP Q15843
B	100	SER	-	insertion	UNP Q15843
B	162	MSE	LEU	conflict	UNP Q15843

- Molecule 2 is a protein called Cullin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	376	Total	C	N	O	S Se	0	0	0
			3116	1991	540	570	2 13			
2	D	378	Total	C	N	O	S Se	0	0	0
			3132	1999	544	574	2 13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1399	GLY	-	insertion	UNP Q93034
C	1400	SER	-	insertion	UNP Q93034
C	1407	GLU	LEU	conflict	UNP Q93034
C	1439	LYS	LEU	conflict	UNP Q93034
C	1440	LYS	VAL	conflict	UNP Q93034
D	1399	GLY	-	insertion	UNP Q93034
D	1400	SER	-	insertion	UNP Q93034
D	1407	GLU	LEU	conflict	UNP Q93034
D	1439	LYS	LEU	conflict	UNP Q93034
D	1440	LYS	VAL	conflict	UNP Q93034

- Molecule 3 is a protein called Rbx1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	R	86	Total	C	N	O	S	Se	10	0	0
			707	448	130	120	8	1			
3	Y	85	Total	C	N	O	S	Se	64	0	0
			664	426	121	108	8	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	3	GLY	-	insertion	UNP P62877
R	4	SER	-	insertion	UNP P62877
Y	3	GLY	-	insertion	UNP P62877
Y	4	SER	-	insertion	UNP P62877

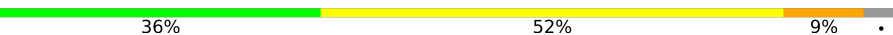
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

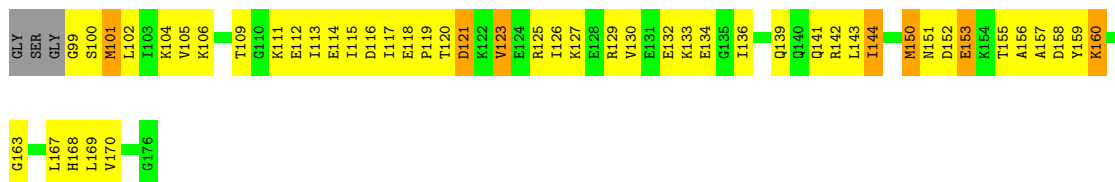
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	3	Total	Zn	0	0
			3	3		
4	Y	3	Total	Zn	0	0
			3	3		

3 Residue-property plots

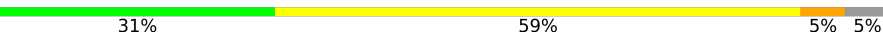
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

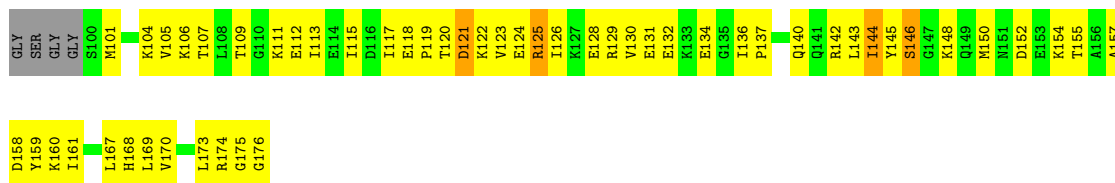
• Molecule 1: NEDD8

Chain A: 

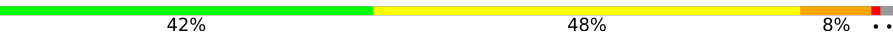


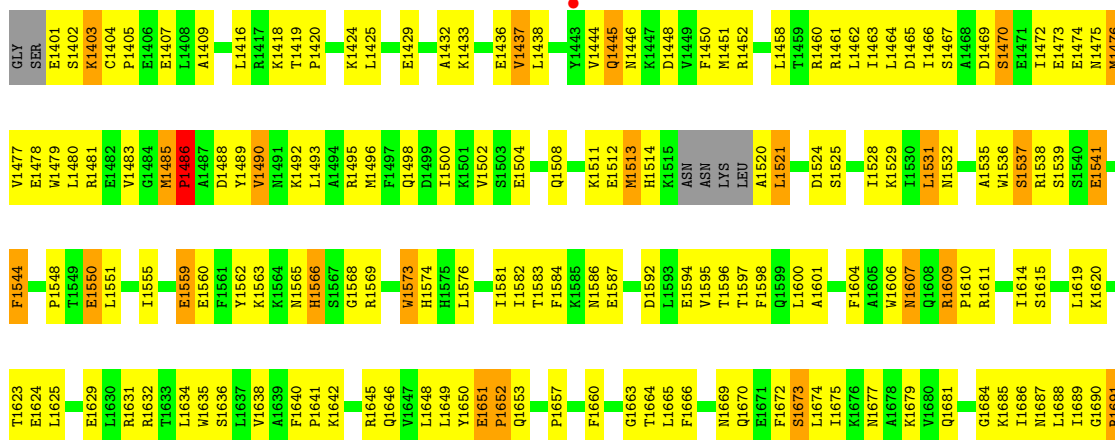
• Molecule 1: NEDD8

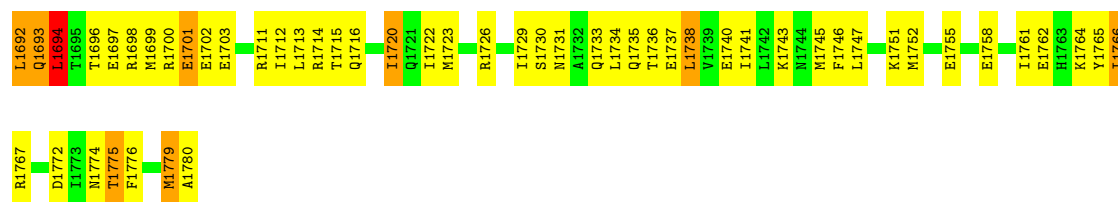
Chain B: 



• Molecule 2: Cullin-5

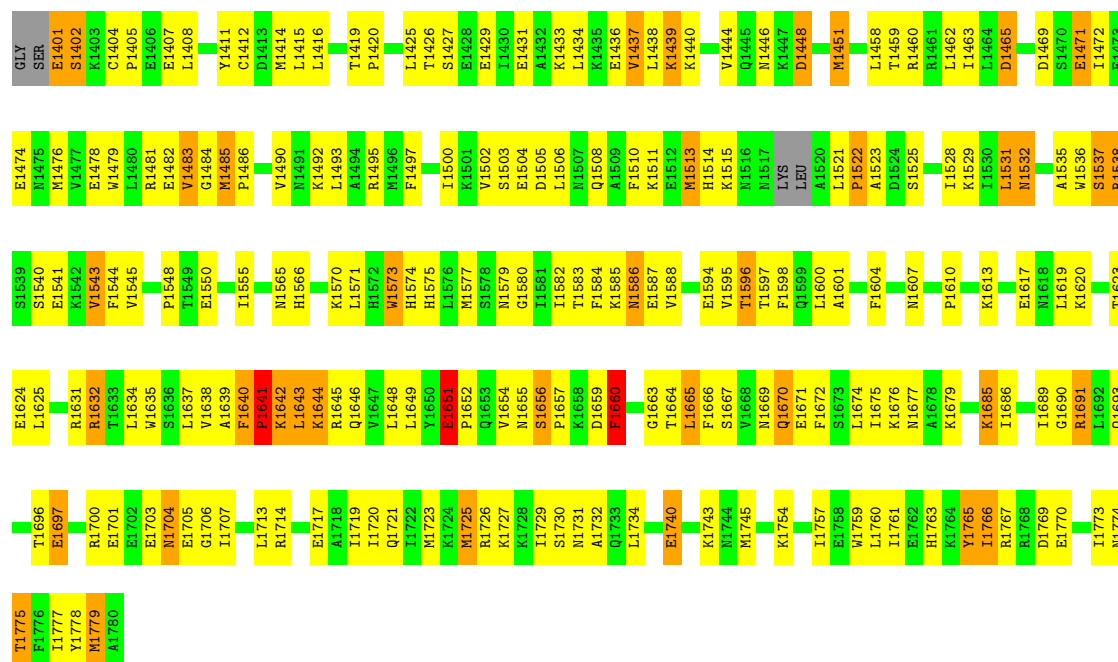
Chain C: 





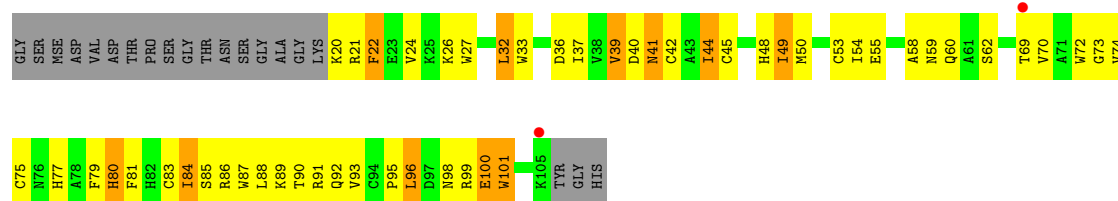
• Molecule 2: Cullin-5

Chain D: 45% 43% 10% ..



• Molecule 3: Rbx1

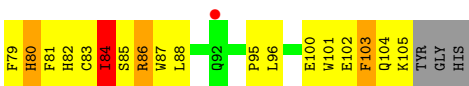
Chain R: 2% 31% 40% 10% 19%



• Molecule 3: Rbx1

Chain Y: 6% 39% 30% 10% 20%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.31Å 122.44Å 128.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.00) 99.1 (50.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.299 0.246 , 0.235	Depositor DCC
R_{free} test set	1449 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8839	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: 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	0.58	0/611	1.03	1/811 (0.1%)
1	B	0.58	0/607	1.07	2/806 (0.2%)
2	C	0.56	0/3157	1.04	12/4220 (0.3%)
2	D	0.59	0/3173	1.04	21/4242 (0.5%)
3	R	0.62	1/726 (0.1%)	1.06	7/984 (0.7%)
3	Y	0.56	0/681	0.95	1/923 (0.1%)
All	All	0.58	1/8955 (0.0%)	1.03	44/11986 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	39	VAL	CA-CB	5.05	1.61	1.54

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1691	ARG	N-CA-C	8.66	121.71	110.53
2	D	1595	VAL	N-CA-C	8.56	121.07	108.65
1	B	148	LYS	N-CA-C	8.00	123.03	110.32
3	R	89	LYS	N-CA-C	-7.81	103.90	113.19
2	C	1595	VAL	N-CA-C	7.32	118.70	108.23

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	609	0	641	57	0
1	B	605	0	638	57	0
2	C	3116	0	3205	255	0
2	D	3132	0	3218	207	0
3	R	707	0	659	69	0
3	Y	664	0	605	71	0
4	R	3	0	0	0	0
4	Y	3	0	0	0	0
All	All	8839	0	8966	665	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 38.

The worst 5 of 665 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:Y:84:ILE:HD13	3:Y:103:PHE:CZ	1.87	1.08
3:Y:49:ILE:HG23	3:Y:70:VAL:HG21	1.35	1.07
2:C:1481:ARG:HB2	2:C:1490:VAL:HG11	1.37	1.06
1:A:152:ASP:H	2:D:1774:ASN:HD21	1.06	1.01
2:C:1689:ILE:HG22	2:C:1690:GLY:H	1.28	0.97

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	76/81 (94%)	66 (87%)	8 (10%)	2 (3%)	4	23
1	B	75/81 (93%)	67 (89%)	5 (7%)	3 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	372/382 (97%)	305 (82%)	54 (14%)	13 (4%)	3	16
2	D	374/382 (98%)	315 (84%)	43 (12%)	16 (4%)	2	12
3	R	84/106 (79%)	61 (73%)	17 (20%)	6 (7%)	1	4
3	Y	81/106 (76%)	50 (62%)	22 (27%)	9 (11%)	0	1
All	All	1062/1138 (93%)	864 (81%)	149 (14%)	49 (5%)	2	11

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	LYS
1	A	163	GLY
2	C	1445	GLN
2	C	1536	TRP
2	C	1537	SER

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	67/65 (103%)	58 (87%)	9 (13%)	4	18
1	B	67/65 (103%)	66 (98%)	1 (2%)	57	80
2	C	347/339 (102%)	323 (93%)	24 (7%)	14	45
2	D	349/339 (103%)	320 (92%)	29 (8%)	10	37
3	R	74/88 (84%)	70 (95%)	4 (5%)	20	53
3	Y	63/88 (72%)	60 (95%)	3 (5%)	23	57
All	All	967/984 (98%)	897 (93%)	70 (7%)	13	43

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	1651	GLU
2	D	1697	GLU

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Mol	Chain	Res	Type
2	D	1775	THR
2	C	1694	LEU
2	C	1681	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	1655	ASN
3	Y	57	GLN
2	D	1693	GLN
2	D	1749	GLN
3	Y	82	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [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	75/81 (92%)	-0.45	0	100 100	38, 61, 75, 85	1 (1%)
1	B	74/81 (91%)	-0.43	0	100 100	35, 64, 81, 91	0
2	C	363/382 (95%)	-0.31	1 (0%)	90 79	32, 71, 112, 132	0
2	D	365/382 (95%)	-0.41	0	100 100	29, 59, 100, 127	0
3	R	83/106 (78%)	0.11	2 (2%)	59 36	51, 96, 137, 142	0
3	Y	72/106 (67%)	0.54	6 (8%)	17 9	47, 149, 150, 150	0
All	All	1032/1138 (90%)	-0.27	9 (0%)	81 61	29, 68, 141, 150	1 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	77	HIS	3.0
3	R	105	LYS	2.4
2	C	1443	TYR	2.4
3	Y	76	ASN	2.4
3	Y	92	GLN	2.4

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 [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($\text{\AA}^2$)	Q<0.9
4	ZN	Y	4001	1/1	0.92	0.06	149,149,149,149	0
4	ZN	Y	4002	1/1	0.93	0.05	149,149,149,149	0
4	ZN	Y	4003	1/1	0.93	0.05	149,149,149,149	0
4	ZN	R	4006	1/1	0.97	0.04	105,105,105,105	0
4	ZN	R	4004	1/1	0.99	0.04	79,79,79,79	0
4	ZN	R	4005	1/1	1.00	0.03	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.