wwPDB X-ray Structure Validation Summary Report (i)

Oct 21, 2024 – 10:27 PM EDT

PDB ID	:	3DQV
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 (i) 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 (1)) were used in the production of this report:

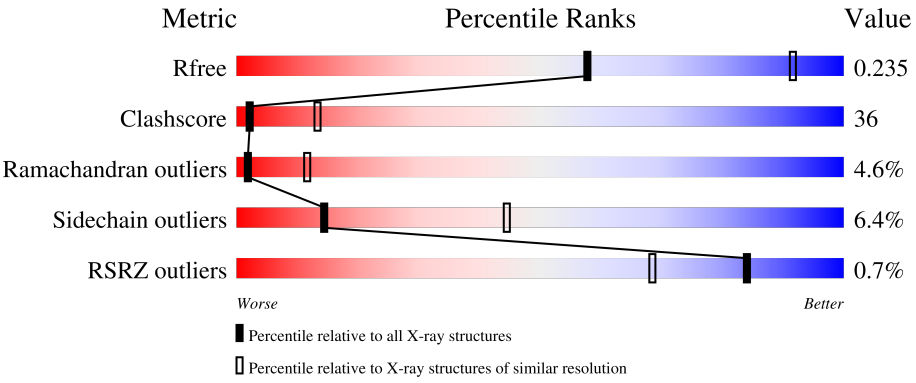
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (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 <=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	38% 53% 5% ·
1	B	81	36% 56% · 5%
2	C	382	42% 49% 7% ·
2	D	382	48% 43% 7% ··
3	R	106	% 35% 41% 6% 19%

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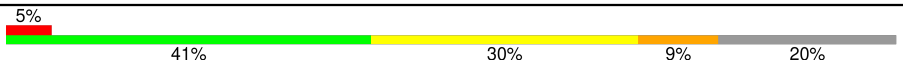
Mol	Chain	Length	Quality of chain
3	Y	106	

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 (three-letter code: ZN) (formula: Zn).

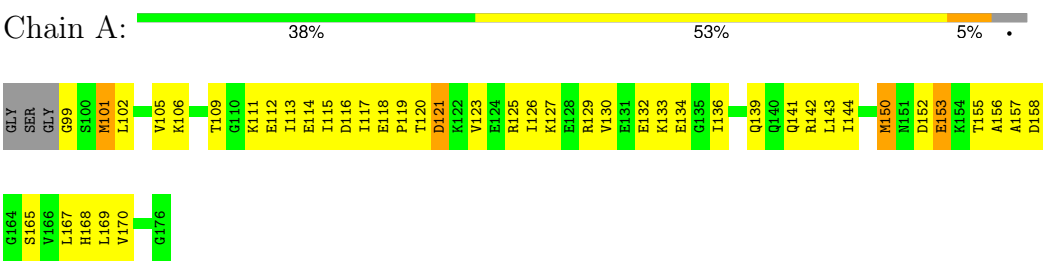
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	3	Total	Zn	0	0
			3	3		
4	Y	3	Total	Zn	0	0
			3	3		

3 Residue-property plots (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.

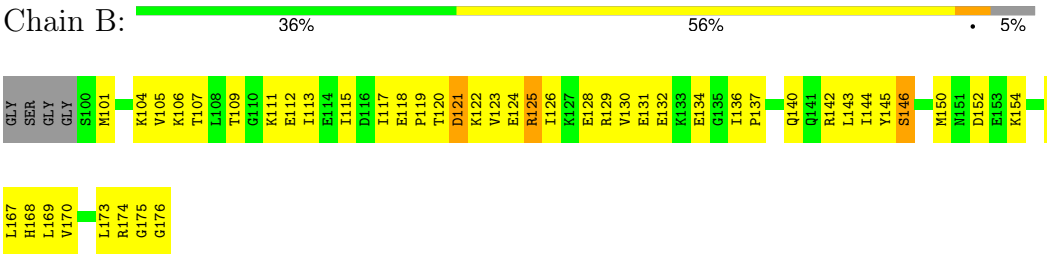
• Molecule 1: NEDD8

Chain A:



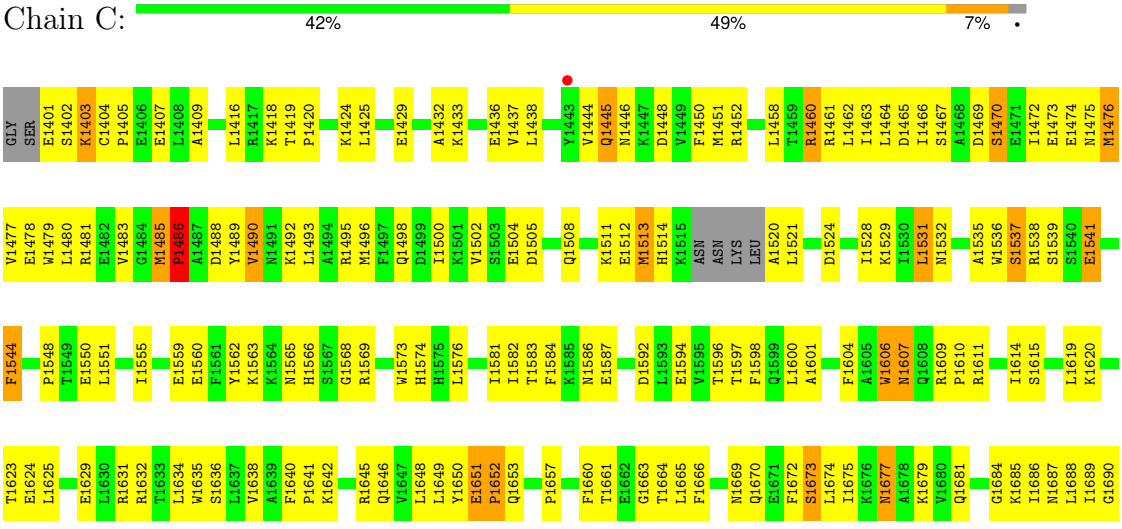
• Molecule 1: NEDD8

Chain B:



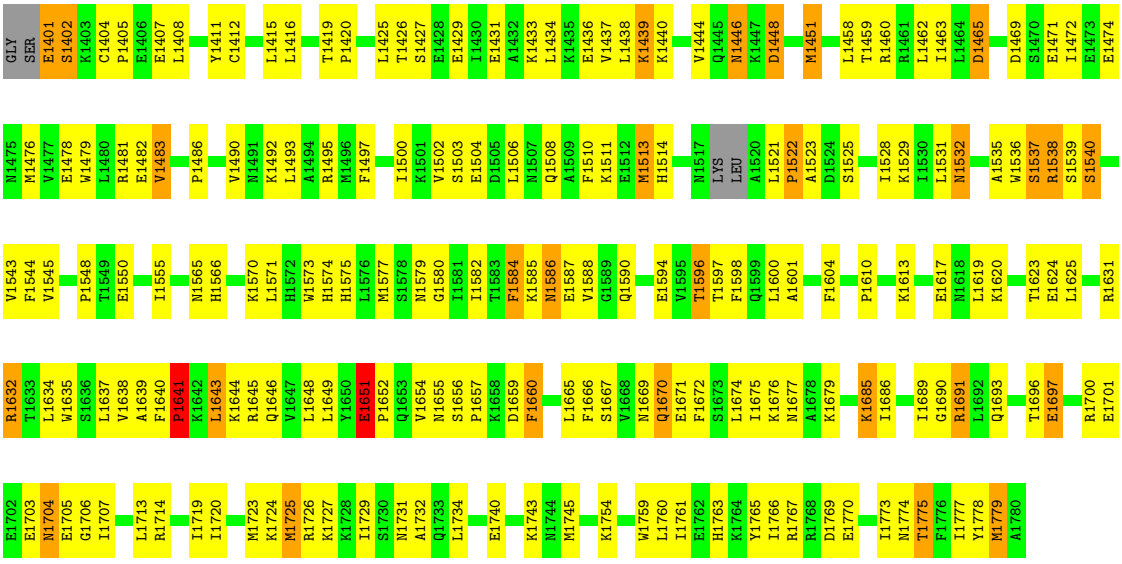
• Molecule 2: Cullin-5

Chain C:



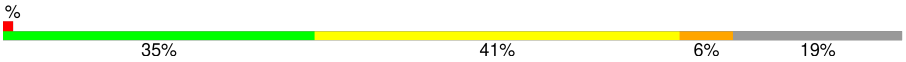
• Molecule 2: Cullin-5

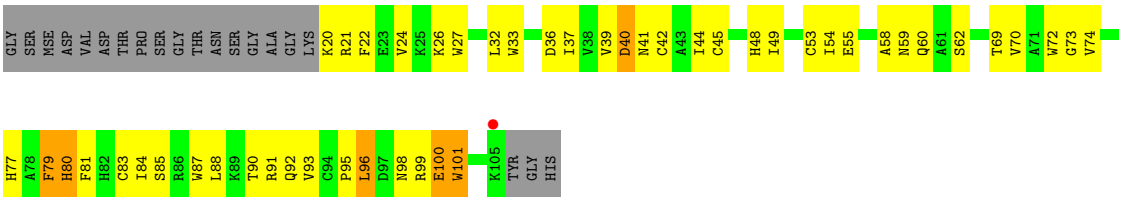
Chain D:



• Molecule 3: Rbx1

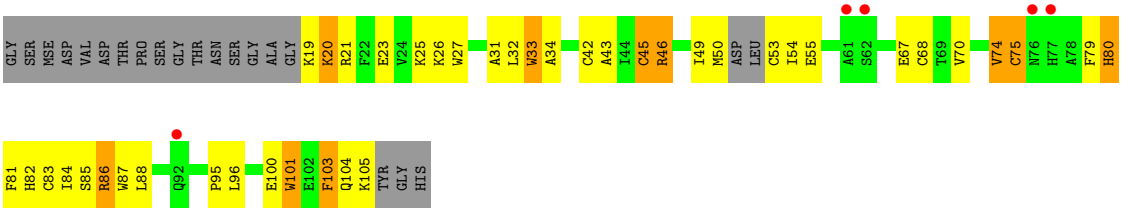
Chain R:





• Molecule 3: Rbx1

Chain Y:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	1440 reflections (5.08%)	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]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[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	0.48	0/611	0.70	0/811
1	B	0.48	0/607	0.74	0/806
2	C	0.47	0/3157	0.69	0/4220
2	D	0.47	1/3173 (0.0%)	0.69	0/4242
3	R	0.54	0/726	0.71	1/984 (0.1%)
3	Y	0.56	1/681 (0.1%)	0.62	0/923
All	All	0.49	2/8955 (0.0%)	0.69	1/11986 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	101	TRP	CZ3-CH2	-6.42	1.29	1.40
2	D	1724	LYS	CE-NZ	-5.14	1.36	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	40	ASP	CB-CG-OD2	5.41	123.16	118.30

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	609	0	641	55	0
1	B	605	0	638	55	0
2	C	3116	0	3205	249	0
2	D	3132	0	3218	198	0
3	R	707	0	659	65	0
3	Y	664	0	605	67	0
4	R	3	0	0	0	0
4	Y	3	0	0	0	0
All	All	8839	0	8966	639	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 36.

The worst 5 of 639 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
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 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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 (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	67/65 (103%)	60 (90%)	7 (10%)	5 23
1	B	67/65 (103%)	66 (98%)	1 (2%)	60 83
2	C	347/339 (102%)	322 (93%)	25 (7%)	12 39
2	D	349/339 (103%)	325 (93%)	24 (7%)	13 42
3	R	74/88 (84%)	71 (96%)	3 (4%)	26 60
3	Y	63/88 (72%)	61 (97%)	2 (3%)	34 67
All	All	967/984 (98%)	905 (94%)	62 (6%)	14 44

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1752	MSE
2	D	1697	GLU
1	B	125	ARG
2	D	1660	PHE
2	D	1779	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	1763	HIS
2	D	1774	ASN
3	Y	80	HIS
2	C	1709	GLN
2	C	1677	ASN

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

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	A	75/81 (92%)	-0.59	0 100 100	38, 61, 75, 85	1 (1%)
1	B	74/81 (91%)	-0.58	0 100 100	35, 64, 81, 91	0
2	C	363/382 (95%)	-0.45	1 (0%) 90 81	32, 71, 112, 132	0
2	D	365/382 (95%)	-0.56	0 100 100	29, 59, 100, 127	0
3	R	83/106 (78%)	-0.04	1 (1%) 76 56	51, 96, 137, 142	0
3	Y	72/106 (67%)	0.39	5 (6%) 24 14	47, 149, 150, 150	0
All	All	1032/1138 (90%)	-0.42	7 (0%) 84 68	29, 68, 141, 150	1 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	77	HIS	2.9
3	R	105	LYS	2.3
2	C	1443	TYR	2.3
3	Y	76	ASN	2.2
3	Y	92	GLN	2.2

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
4	ZN	Y	4001	1/1	0.92	0.06	149,149,149,149	0
4	ZN	Y	4002	1/1	0.92	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	0.96	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

There are no such residues in this entry.