wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 10:40 PM EDT

PDB ID	:	3DBR
Title	:	Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APPBP1-UBA3Arg190Gln-NEDD8Ala72Arg)
Authors	:	Souphron, J.; Schulman, B.A.
Deposited on	:	2008-06-02
Resolution	:	3.05 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:

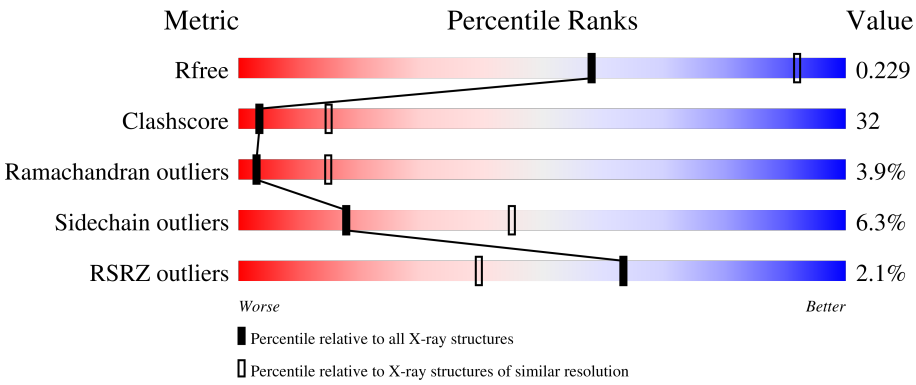
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	531	% 49% 44% 5% •
1	C	531	% 47% 44% 5% • •
1	E	531	2% 55% 36% 5% • •
1	G	531	2% 51% 42% • •
2	B	434	3% 50% 43% 7%

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Mol	Chain	Length	Quality of chain
2	D	434	2% 45% 48% 6%
2	F	434	4% 46% 48% 5%
2	H	434	3% 39% 52% 6%
3	I	88	% 53% 36% 7%
3	J	88	2% 40% 44% 13%
3	K	88	41% 36% 10% 13%
3	L	88	22% 61% 6% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32424 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-activating enzyme E1 regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	4104	2600	699	790	15	0	0	0
1	C	516	4096	2596	698	787	15	0	0	0
1	E	515	4093	2597	696	785	15	0	0	0
1	G	508	4038	2563	686	774	15	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q13564
A	0	SER	-	expression tag	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLU	deletion	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLY	deletion	UNP Q13564
A	?	-	ALA	deletion	UNP Q13564
C	-1	GLY	-	expression tag	UNP Q13564
C	0	SER	-	expression tag	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLU	deletion	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLY	deletion	UNP Q13564
C	?	-	ALA	deletion	UNP Q13564
E	-1	GLY	-	expression tag	UNP Q13564
E	0	SER	-	expression tag	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLU	deletion	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLY	deletion	UNP Q13564
E	?	-	ALA	deletion	UNP Q13564

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q13564
G	0	SER	-	expression tag	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLU	deletion	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLY	deletion	UNP Q13564
G	?	-	ALA	deletion	UNP Q13564

- Molecule 2 is a protein called NEDD8-activating enzyme E1 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	432	3402	2174	575	636	17	0	0	0
			Total	C	N	O	S			
2	D	431	3399	2174	575	633	17	0	0	0
			Total	C	N	O	S			
2	F	431	3395	2171	574	633	17	0	0	0
			Total	C	N	O	S			
2	H	431	3387	2164	573	633	17	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	expression tag	UNP Q8TBC4
B	10	LYS	-	expression tag	UNP Q8TBC4
B	11	LEU	-	expression tag	UNP Q8TBC4
B	190	GLN	ARG	engineered mutation	UNP Q8TBC4
B	216	ALA	CYS	engineered mutation	UNP Q8TBC4
D	9	MET	-	expression tag	UNP Q8TBC4
D	10	LYS	-	expression tag	UNP Q8TBC4
D	11	LEU	-	expression tag	UNP Q8TBC4
D	190	GLN	ARG	engineered mutation	UNP Q8TBC4
D	216	ALA	CYS	engineered mutation	UNP Q8TBC4
F	9	MET	-	expression tag	UNP Q8TBC4
F	10	LYS	-	expression tag	UNP Q8TBC4
F	11	LEU	-	expression tag	UNP Q8TBC4
F	190	GLN	ARG	engineered mutation	UNP Q8TBC4
F	216	ALA	CYS	engineered mutation	UNP Q8TBC4
H	9	MET	-	expression tag	UNP Q8TBC4
H	10	LYS	-	expression tag	UNP Q8TBC4
H	11	LEU	-	expression tag	UNP Q8TBC4
H	190	GLN	ARG	engineered mutation	UNP Q8TBC4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	216	ALA	CYS	engineered mutation	UNP Q8TBC4

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	85	666	414	122	128	2	0	0	0
3	J	77	612	384	108	118	2	0	0	0
3	K	77	612	384	108	118	2	0	0	0
3	L	78	616	386	109	119	2	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	89	GLY	-	expression tag	UNP Q15843
I	90	SER	-	expression tag	UNP Q15843
I	91	ARG	-	expression tag	UNP Q15843
I	92	ARG	-	expression tag	UNP Q15843
I	93	ALA	-	expression tag	UNP Q15843
I	94	SER	-	expression tag	UNP Q15843
I	95	VAL	-	expression tag	UNP Q15843
I	96	GLY	-	expression tag	UNP Q15843
I	97	SER	-	expression tag	UNP Q15843
I	98	GLY	-	expression tag	UNP Q15843
I	99	GLY	-	expression tag	UNP Q15843
I	100	SER	-	expression tag	UNP Q15843
I	172	ARG	ALA	engineered mutation	UNP Q15843
J	89	GLY	-	expression tag	UNP Q15843
J	90	SER	-	expression tag	UNP Q15843
J	91	ARG	-	expression tag	UNP Q15843
J	92	ARG	-	expression tag	UNP Q15843
J	93	ALA	-	expression tag	UNP Q15843
J	94	SER	-	expression tag	UNP Q15843
J	95	VAL	-	expression tag	UNP Q15843
J	96	GLY	-	expression tag	UNP Q15843
J	97	SER	-	expression tag	UNP Q15843
J	98	GLY	-	expression tag	UNP Q15843
J	99	GLY	-	expression tag	UNP Q15843
J	100	SER	-	expression tag	UNP Q15843

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Chain	Residue	Modelled	Actual	Comment	Reference
J	172	ARG	ALA	engineered mutation	UNP Q15843
K	89	GLY	-	expression tag	UNP Q15843
K	90	SER	-	expression tag	UNP Q15843
K	91	ARG	-	expression tag	UNP Q15843
K	92	ARG	-	expression tag	UNP Q15843
K	93	ALA	-	expression tag	UNP Q15843
K	94	SER	-	expression tag	UNP Q15843
K	95	VAL	-	expression tag	UNP Q15843
K	96	GLY	-	expression tag	UNP Q15843
K	97	SER	-	expression tag	UNP Q15843
K	98	GLY	-	expression tag	UNP Q15843
K	99	GLY	-	expression tag	UNP Q15843
K	100	SER	-	expression tag	UNP Q15843
K	172	ARG	ALA	engineered mutation	UNP Q15843
L	89	GLY	-	expression tag	UNP Q15843
L	90	SER	-	expression tag	UNP Q15843
L	91	ARG	-	expression tag	UNP Q15843
L	92	ARG	-	expression tag	UNP Q15843
L	93	ALA	-	expression tag	UNP Q15843
L	94	SER	-	expression tag	UNP Q15843
L	95	VAL	-	expression tag	UNP Q15843
L	96	GLY	-	expression tag	UNP Q15843
L	97	SER	-	expression tag	UNP Q15843
L	98	GLY	-	expression tag	UNP Q15843
L	99	GLY	-	expression tag	UNP Q15843
L	100	SER	-	expression tag	UNP Q15843
L	172	ARG	ALA	engineered mutation	UNP Q15843

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

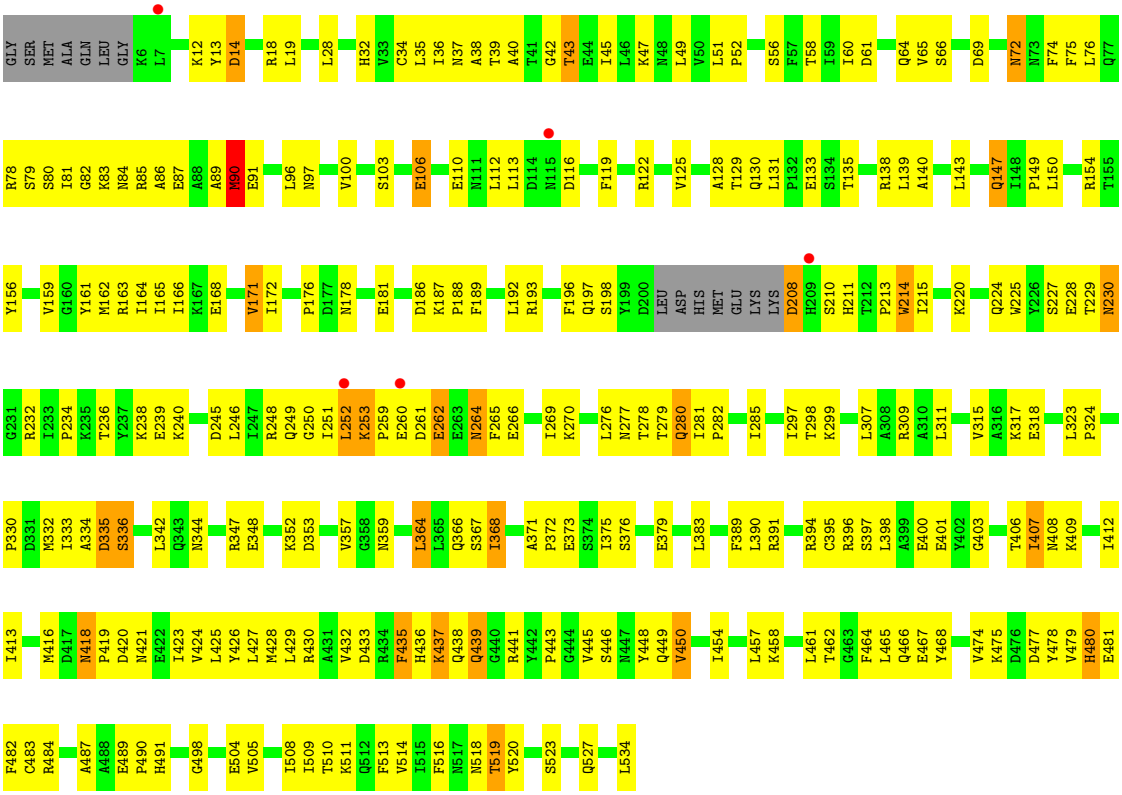
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	B	1	1	1	0	0
4	D	1	1	1	0	0
4	F	1	1	1	0	0
4	H	1	1	1	0	0

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.

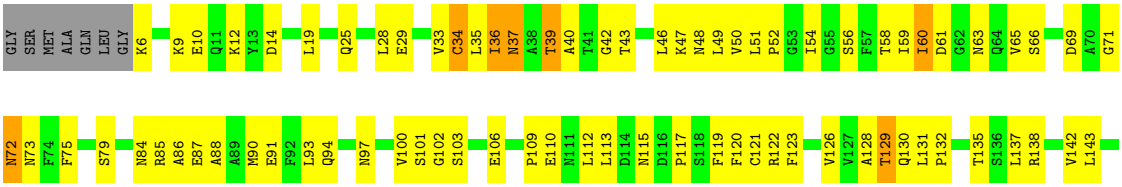
• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

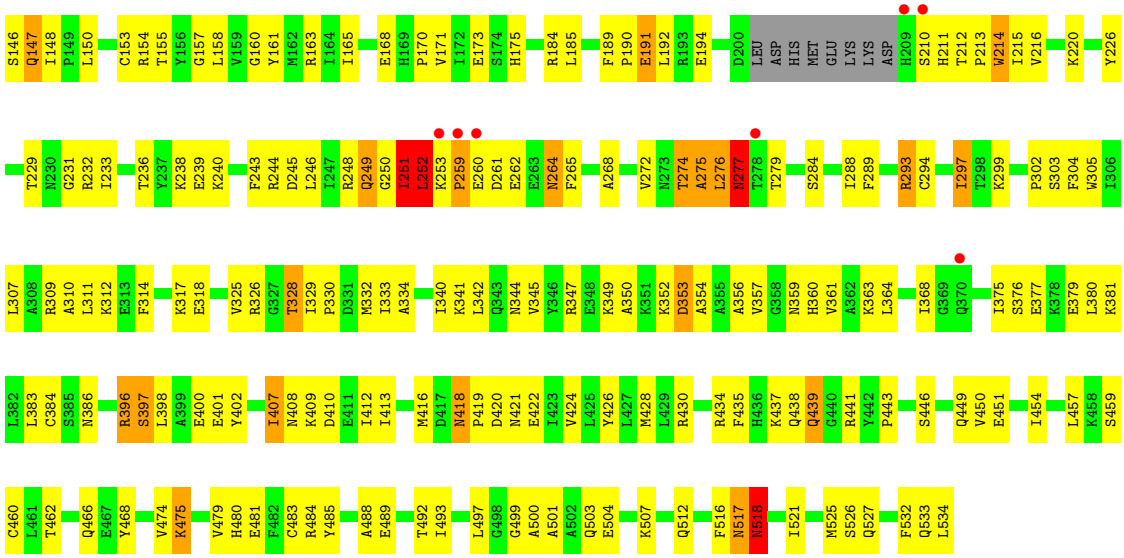
Chain A:



• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

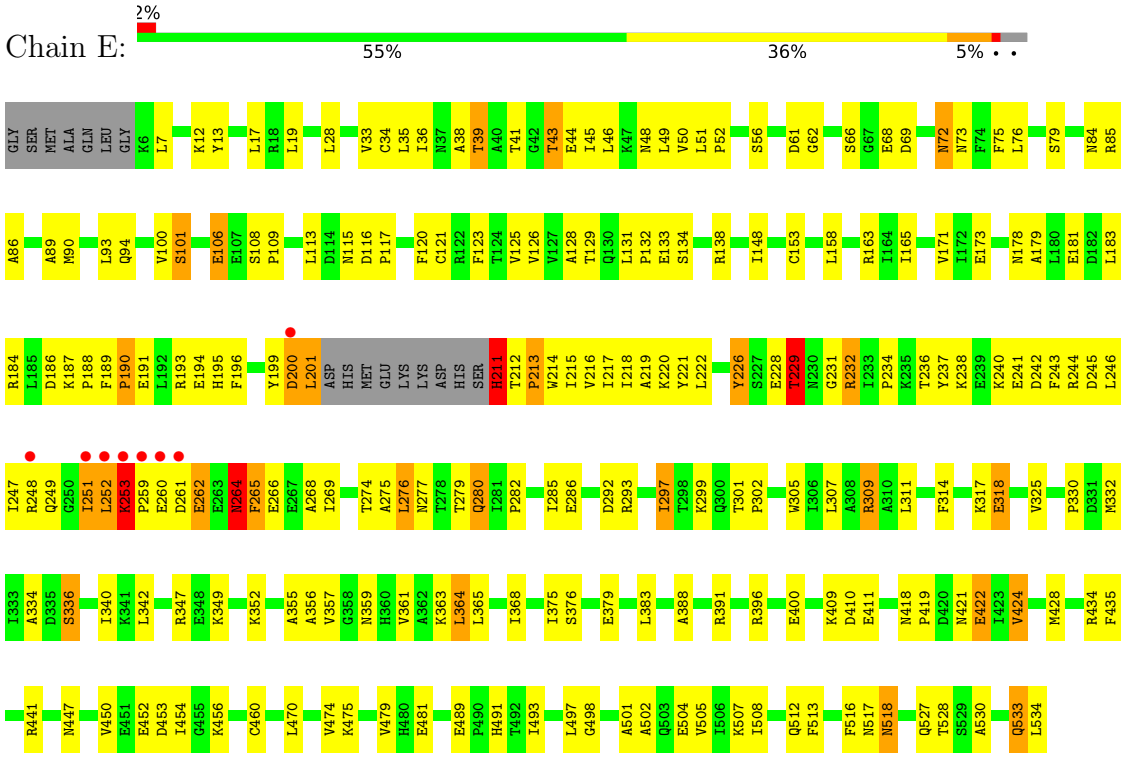
Chain C:





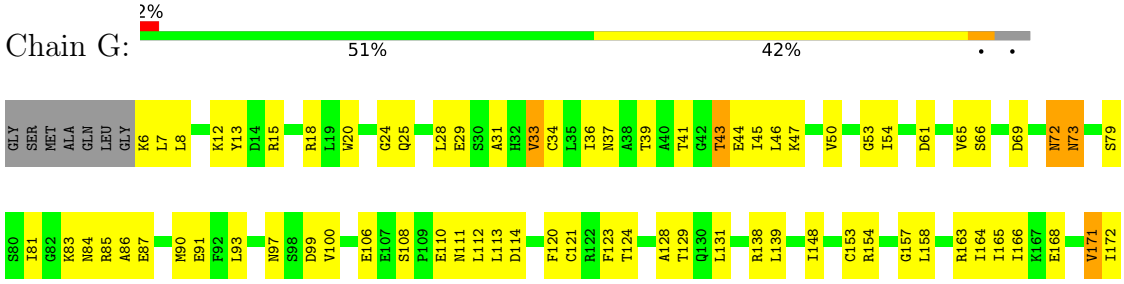
• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain E:



• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain G:



E173 L180 R184 L185 D186 K187 P188 F189 L192 R193 E194 H195 F196 Q197 S198 Y199 ASP LEU ASP HIS MET GLU LYS LYS ASP HIS SER HIS T212 P213 W214 I215 V216 I217 I218 A219 K220 Y221 L222 W225 Y226 T229 N230 G231 R232 I233 P234 K235 T236 Y237 K238 E239 K240 E241 D242

F243 R244 D245 L246 I247 R248 Q249 G250 I251 L252 LYS PRO GLU ASP E262 E263 N264 F265 E266 E267 A268 I269 K270 N271 V272 A275 L276 N277 T278 T279 P282 S283 S284 I285 E286 D287 I288 R293 T298 K299 Q300 W305 I306 L307 L311 F314 E318 G319 Q320 G321 N322 L323

P324 V325 P330 D331 M332 I333 A334 D335 S336 Y339 I340 K341 L342 Q343 N344 V345 Y346 R347 E348 H360 V361 A362 K363 L364 L365 Q366 S367 I368 E377 K381 L382 L383 C384 S385 N386 S387 A388 R391 R394 C395 R396 S397 E400 L404 D405 T406 I407 N408 K409 D410

M416 D417 N418 P419 D420 N421 E422 I423 V424 L425 Y426 L427 M428 V432 D433 R434 F435 H436 K437 Q438 R441 S446 N447 Y448 Q449 Q450 E451 E452 D453 I454 F464 E467 K475 H480 E481 R484 Y485 A488 E489 P490 H491 T492 I493 L497 G498 Q503 E504 K507

I508 I509 T510 K511 Q512 F513 V514 I515 F516 N517 N518 Q527 F532 Q533 L534

- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain B: 3% 50% 43% 7%

MET LYS L11 D12 W13 E14 G15 R16 W17 N18 H19 K22 F23 L24 E25 R26 S27 G28 T31 H32 P33 D34 P37 S38 L46 C49 K50 V51 L52 E62 L63 L64 K65 N66 L67 A68 L69 R73 Q74 I78 D81 T82 I83 D84 V85 S86 N87 F92 L93 F94

R95 P96 K97 D98 I99 P102 K103 A104 E105 L111 R114 V115 P116 N117 C118 N119 H123 K126 I127 Q128 D129 F130 N131 D132 T133 F134 Q137 F138 H139 I149 A150 R151 R152 W153 I154 N155 G156 M157 L158 D166 G167 V168 L177 I178 T182 F185 K186 G187 N188

A189 Q190 V191 G195 M196 T197 A198 C199 I200 T203 V207 P208 V211 P214 T217 I218 A219 S220 M221 P222 R223 E226 I229 E230 Y231 V232 R233 Q236 W237 P238 K239 E240 Q241 P242 F243 G246 L249 D250 G251 D252 D253 P254 E255 H256 I257 I260 K263

S264 L265 R274 Y278 R279 L280 T281 V284 V285 K286 R287 I288 I289 P290 A291 V292 N296 A300 A301 V302 E306 K309 I310 A311 T312 S313 A314 Y315 I316 P317 L318 N319 N320 Y321 L322 N325 D326 W327 D328 Y331 T334 F335 E336 A337 E338 R339 N342 C343

C346 S347 Q348 L349 P350 Q351 N352 I353 Q354 F355 S356 P357 S358 A359 K360 L361 Q362 E363 V364 Y367 L368 L374 Q375 M376 A380 I381 T382 L385 E386 G387 K388 N389 R390 T391 L392 Y393 L394 S399 I400 E401 E402 R403 T404 R405 P406 N407 L408 T411 L412 K413 E414 L415 G416 L417

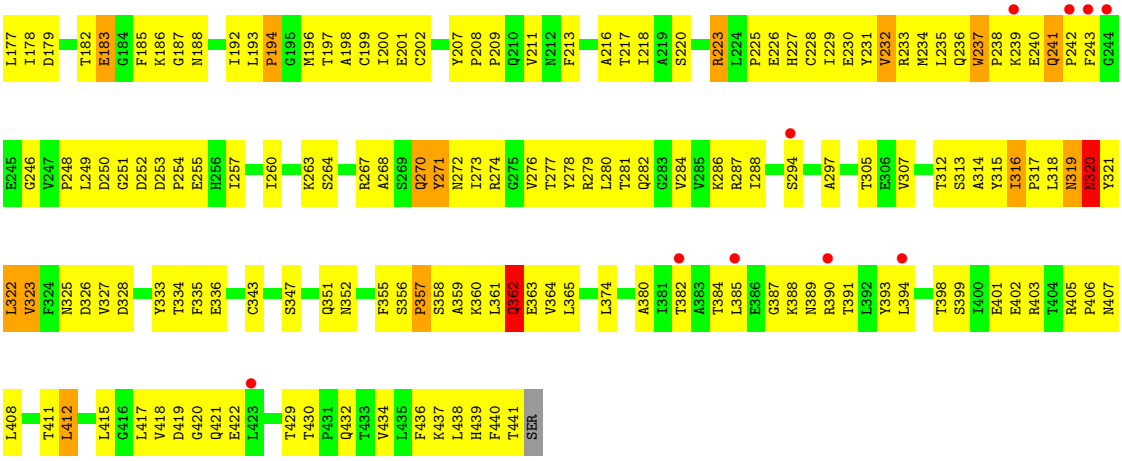
V418 D419 G420 Q421 E422 L423 A424 V425 A426 D427 V428 T429 T430 P431 V434 L435 F436 K437 L438 H439 F440 T441 S442

- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain D: 2% 45% 48% 6%

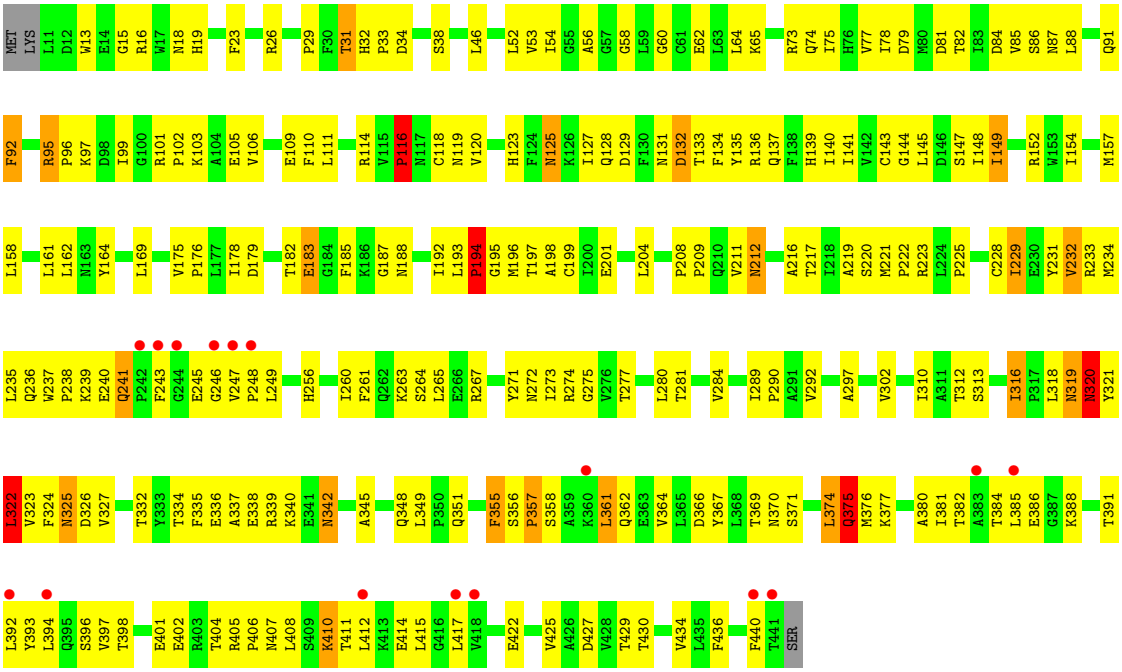
MET LYS L11 D12 W13 E14 G15 R16 W17 N18 H19 V20 K21 K22 F23 L24 E25 R26 S27 G28 P29 F30 T31 H32 P33 D34 P37 S41 L46 I54 G57 G58 E62 L63 L64 K65 N66 L67 F72 R73 Q74 I75 H76 V77 T82 I83 N87 R90 Q91 F92

L93 F94 K97 D98 I99 K103 V106 E109 F110 L111 N112 D113 R114 V115 P116 N119 F124 N125 Q128 N131 D132 R136 Q137 F138 H139 I140 I141 V142 L145 I148 I149 A150 R151 R152 W153 I154 M157 L158 L162 L169 D170 P171 S172 V175 P176



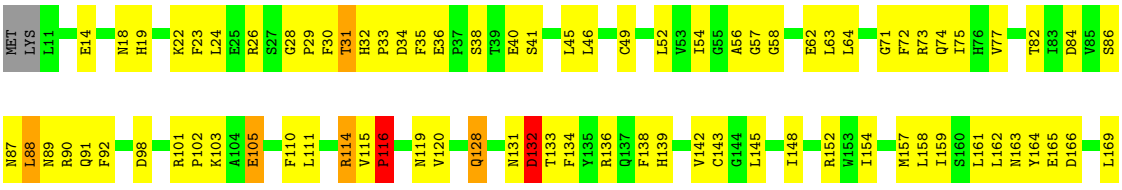
- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

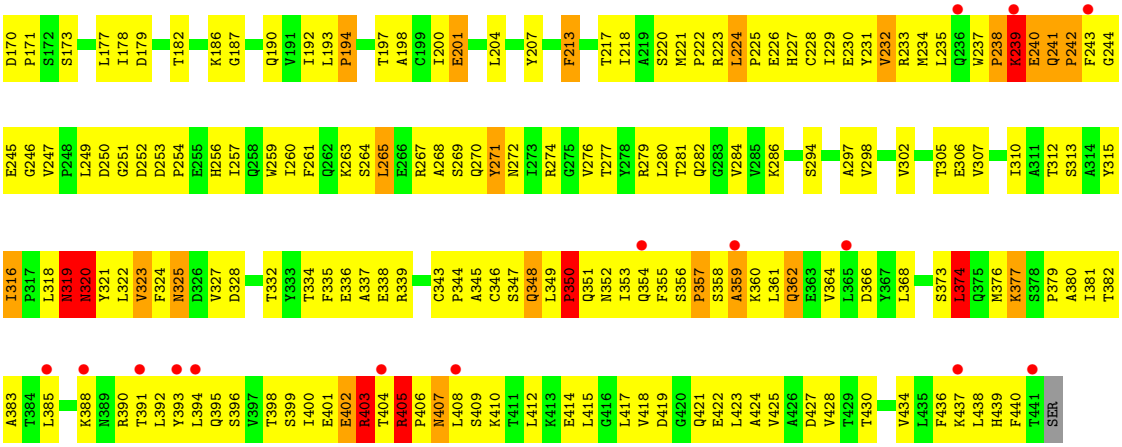
Chain F:



- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

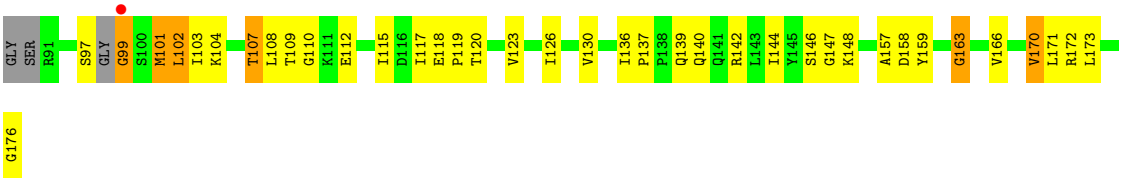
Chain H:





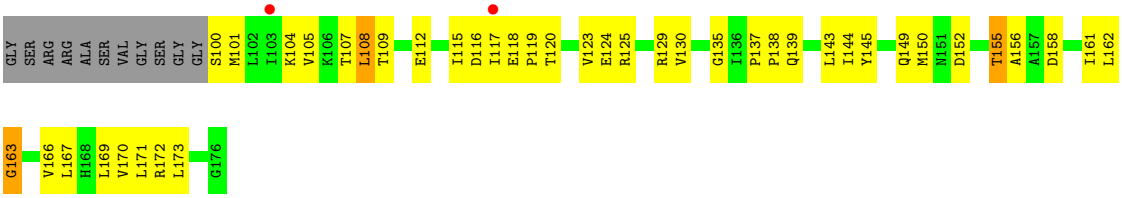
- Molecule 3: NEDD8

Chain I:



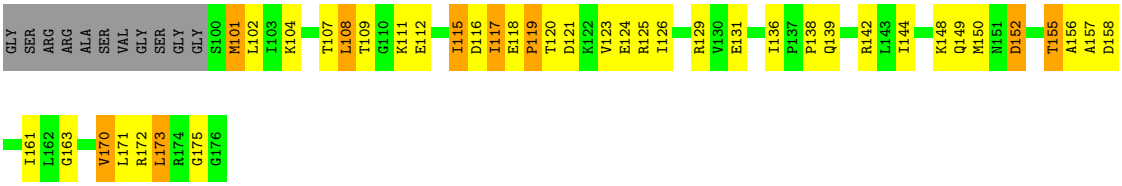
- Molecule 3: NEDD8

Chain J:



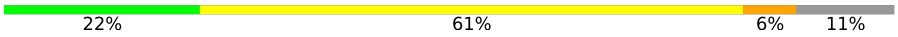
- Molecule 3: NEDD8

Chain K:



- Molecule 3: NEDD8

Chain L:



E153
K154
T155
A156
A157
D158
Y159
K160
I161
L162
G163
G164
S165
V166
L167
H168
L169
V170
L171
R172
L173
R174
G175
G176

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	134.32Å 198.53Å 208.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.05 48.29 – 3.07	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-3.05) 95.3 (48.29-3.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 3.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.280 0.232 , 0.229	Depositor DCC
R_{free} test set	4982 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32424	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% 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 (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	0.43	0/4184	0.68	1/5660 (0.0%)
1	C	0.45	0/4176	0.73	9/5649 (0.2%)
1	E	0.48	1/4172 (0.0%)	0.71	2/5643 (0.0%)
1	G	0.41	0/4114	0.67	1/5563 (0.0%)
2	B	0.50	1/3480 (0.0%)	0.75	4/4736 (0.1%)
2	D	0.44	0/3477	0.72	2/4732 (0.0%)
2	F	0.46	0/3473	0.73	3/4728 (0.1%)
2	H	0.50	0/3465	0.85	10/4718 (0.2%)
3	I	0.55	2/670 (0.3%)	0.77	0/891
3	J	0.43	0/617	0.82	1/823 (0.1%)
3	K	0.46	0/617	0.78	0/823
3	L	0.61	1/621 (0.2%)	0.98	5/828 (0.6%)
All	All	0.46	5/33066 (0.0%)	0.74	38/44794 (0.1%)

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
2	F	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	442	SER	C-O	8.06	1.38	1.23
1	E	211	HIS	CG-CD2	-6.33	1.25	1.35
3	I	99	GLY	C-O	-5.79	1.14	1.23
3	I	99	GLY	CA-C	5.25	1.60	1.51
3	L	99	GLY	N-CA	5.09	1.53	1.46

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	320	ASN	N-CA-C	12.33	144.30	111.00
2	B	442	SER	N-CA-C	-9.77	84.61	111.00
2	D	320	ASN	N-CA-C	9.75	137.32	111.00
3	L	100	SER	N-CA-C	9.41	136.40	111.00
2	H	271	TYR	N-CA-C	-8.89	86.99	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	319	ASN	Mainchain

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	4104	0	4052	264	0
1	C	4096	0	4048	255	0
1	E	4093	0	4059	220	0
1	G	4038	0	4009	220	0
2	B	3402	0	3380	253	0
2	D	3399	0	3386	241	0
2	F	3395	0	3375	269	0
2	H	3387	0	3354	311	0
3	I	666	0	703	49	0
3	J	612	0	648	46	0
3	K	612	0	648	47	0
3	L	616	0	651	74	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
All	All	32424	0	32313	2093	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 32.

The worst 5 of 2093 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:C:252:LEU:O	1:C:259:PRO:HD2	1.17	1.33
1:A:252:LEU:O	1:A:259:PRO:HD2	1.25	1.30
1:C:517:ASN:ND2	1:C:518:ASN:H	1.31	1.28
2:F:371:SER:CB	2:F:374:LEU:HD11	1.64	1.26
1:C:517:ASN:HD22	1:C:518:ASN:N	1.35	1.24

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	513/531 (97%)	433 (84%)	64 (12%)	16 (3%)	4 19
1	C	512/531 (96%)	432 (84%)	59 (12%)	21 (4%)	3 14
1	E	511/531 (96%)	447 (88%)	46 (9%)	18 (4%)	3 17
1	G	502/531 (94%)	434 (86%)	54 (11%)	14 (3%)	5 21
2	B	430/434 (99%)	362 (84%)	56 (13%)	12 (3%)	5 21
2	D	429/434 (99%)	347 (81%)	62 (14%)	20 (5%)	2 12
2	F	429/434 (99%)	362 (84%)	51 (12%)	16 (4%)	3 16
2	H	429/434 (99%)	344 (80%)	60 (14%)	25 (6%)	1 8
3	I	81/88 (92%)	71 (88%)	5 (6%)	5 (6%)	1 7
3	J	75/88 (85%)	66 (88%)	7 (9%)	2 (3%)	5 21
3	K	75/88 (85%)	63 (84%)	8 (11%)	4 (5%)	2 10
3	L	76/88 (86%)	60 (79%)	12 (16%)	4 (5%)	2 10
All	All	4062/4212 (96%)	3421 (84%)	484 (12%)	157 (4%)	3 15

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	LYS
2	B	116	PRO
2	B	127	ILE
2	B	241	GLN
2	B	387	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	449/462 (97%)	424 (94%)	25 (6%)	21	49
1	C	448/462 (97%)	425 (95%)	23 (5%)	24	53
1	E	448/462 (97%)	417 (93%)	31 (7%)	15	42
1	G	442/462 (96%)	419 (95%)	23 (5%)	23	52
2	B	378/382 (99%)	349 (92%)	29 (8%)	13	38
2	D	378/382 (99%)	352 (93%)	26 (7%)	15	42
2	F	377/382 (99%)	350 (93%)	27 (7%)	14	40
2	H	375/382 (98%)	348 (93%)	27 (7%)	14	40
3	I	73/74 (99%)	67 (92%)	6 (8%)	11	35
3	J	68/74 (92%)	66 (97%)	2 (3%)	42	70
3	K	68/74 (92%)	62 (91%)	6 (9%)	10	32
3	L	68/74 (92%)	67 (98%)	1 (2%)	65	83
All	All	3572/3672 (97%)	3346 (94%)	226 (6%)	18	45

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	101	SER
2	H	402	GLU
2	F	38	SER
2	H	366	ASP
2	H	49	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	447	ASN
2	H	19	HIS
2	H	348	GLN
1	C	517	ASN
1	C	512	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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	517/531 (97%)	-0.10	5 (0%)	82	63	46, 76, 107, 130	0
1	C	516/531 (97%)	-0.03	7 (1%)	75	53	53, 82, 116, 140	0
1	E	515/531 (96%)	-0.06	8 (1%)	72	49	36, 62, 128, 141	0
1	G	508/531 (95%)	-0.05	10 (1%)	65	41	44, 71, 135, 147	0
2	B	432/434 (99%)	-0.02	13 (3%)	50	25	46, 68, 122, 131	0
2	D	431/434 (99%)	0.17	10 (2%)	60	36	47, 85, 118, 131	0
2	F	431/434 (99%)	0.09	16 (3%)	41	20	41, 70, 121, 134	0
2	H	431/434 (99%)	0.07	15 (3%)	44	22	45, 79, 127, 140	0
3	I	85/88 (96%)	0.03	1 (1%)	79	58	54, 77, 99, 110	0
3	J	77/88 (87%)	0.29	2 (2%)	56	30	58, 90, 106, 116	0
3	K	77/88 (87%)	-0.03	0	100	100	56, 81, 99, 104	0
3	L	78/88 (88%)	0.21	0	100	100	70, 105, 125, 129	0
All	All	4098/4212 (97%)	0.01	87 (2%)	63	39	36, 76, 122, 147	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	HIS	5.1
1	G	252	LEU	4.6
2	D	243	PHE	4.2
1	E	260	GLU	3.7
2	B	392	LEU	3.7

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 monosaccharides 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(Å^2)	Q<0.9
4	ZN	B	1	1/1	0.99	0.14	70,70,70,70	0
4	ZN	F	4	1/1	0.99	0.14	67,67,67,67	0
4	ZN	H	2	1/1	0.99	0.15	84,84,84,84	0
4	ZN	D	3	1/1	1.00	0.13	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.