wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:08 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

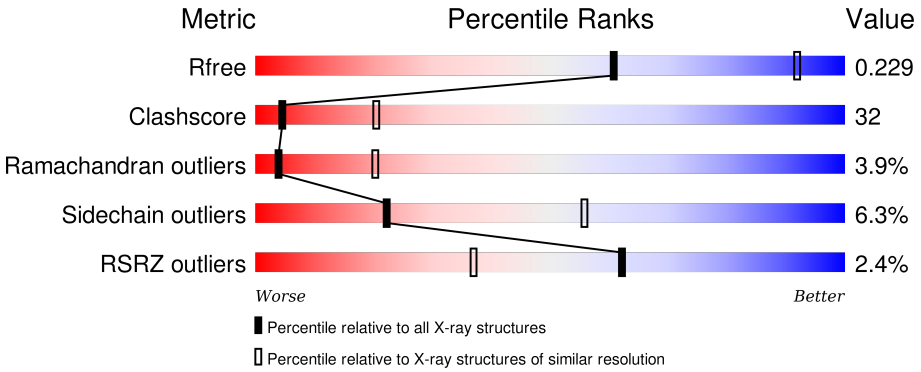
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	55% 36% 5%
1	G	531	51% 42%
2	B	434	4% 50% 43% 7%

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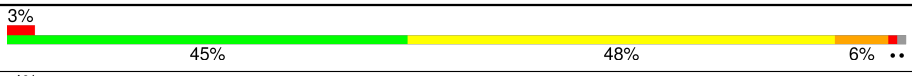
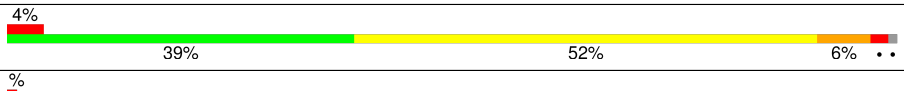
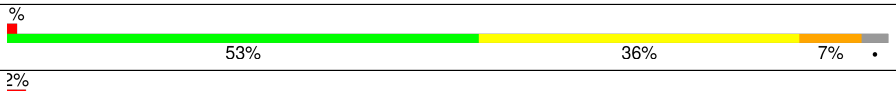
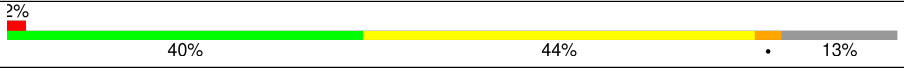
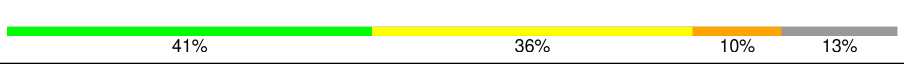
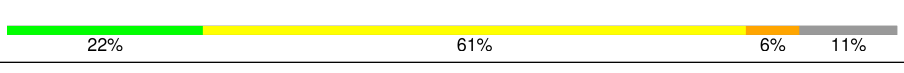
Mol	Chain	Length	Quality of chain
2	D	434	
2	F	434	
2	H	434	
3	I	88	
3	J	88	
3	K	88	
3	L	88	

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

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
2	B	432	Total	C	N	O	S	0	0	0
			3402	2174	575	636	17			
2	D	431	Total	C	N	O	S	0	0	0
			3399	2174	575	633	17			
2	F	431	Total	C	N	O	S	0	0	0
			3395	2171	574	633	17			
2	H	431	Total	C	N	O	S	0	0	0
			3387	2164	573	633	17			

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	UNP Q8TBC4
B	216	ALA	CYS	ENGINEERED	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	UNP Q8TBC4
D	216	ALA	CYS	ENGINEERED	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	UNP Q8TBC4
F	216	ALA	CYS	ENGINEERED	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	UNP Q8TBC4

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

- Molecule 3 is a protein called NEDD8.

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

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	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	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	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	UNP Q15843

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

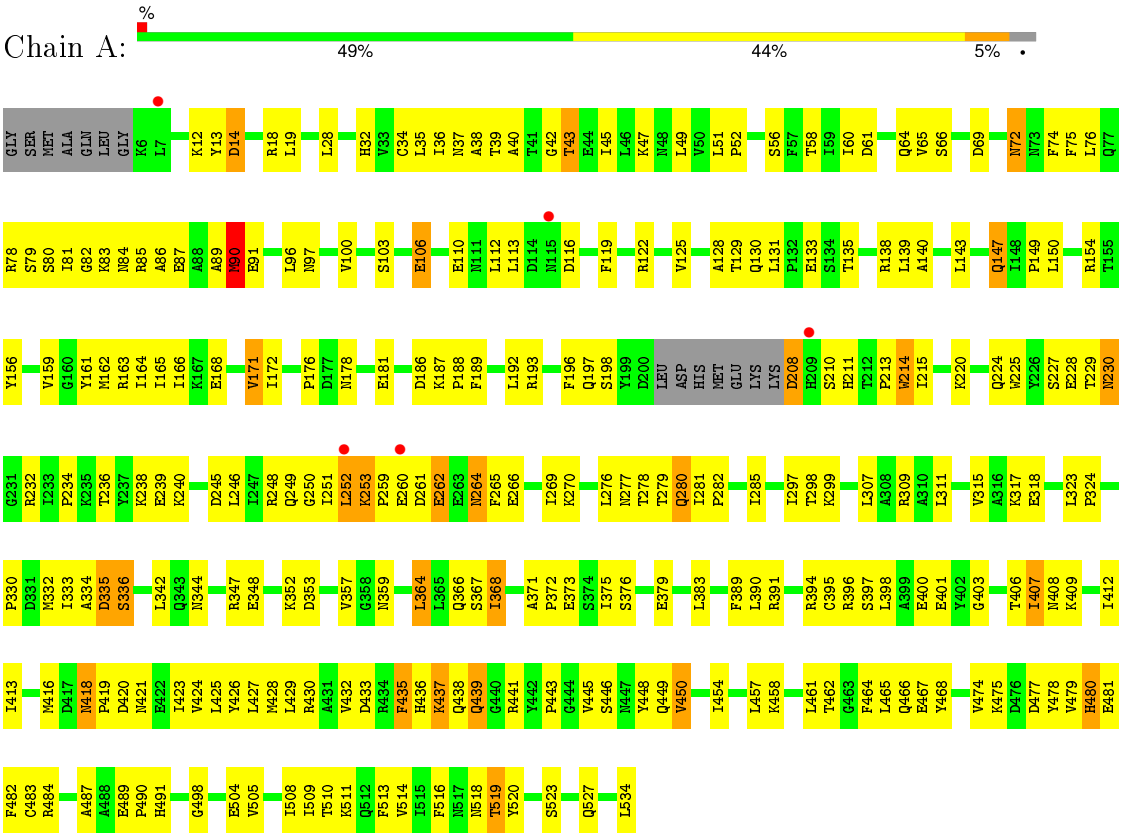
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

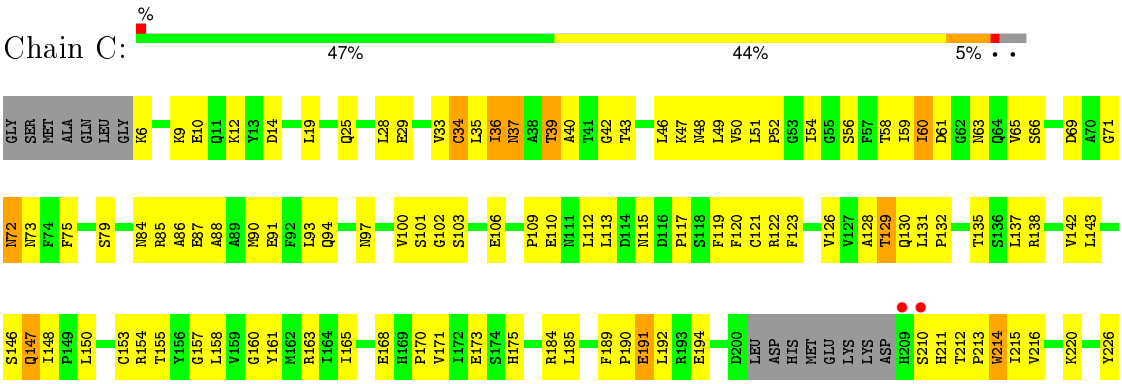
- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

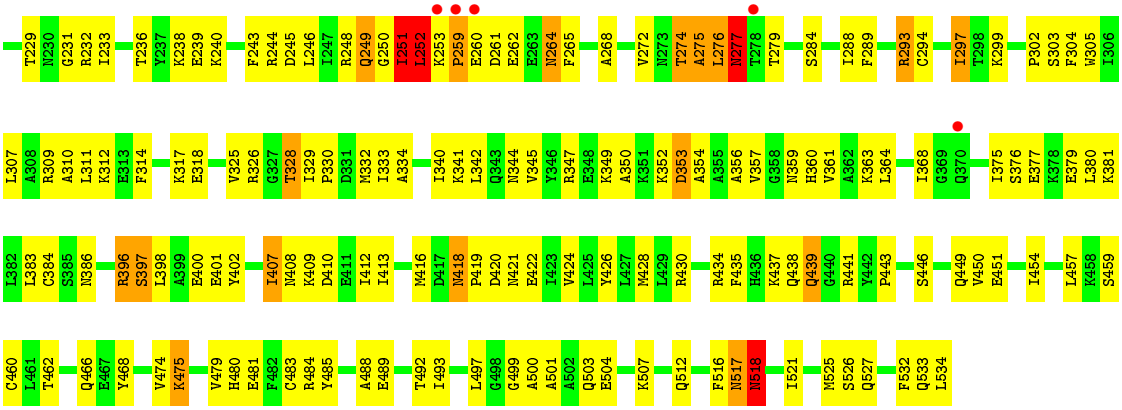
Chain A:



- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

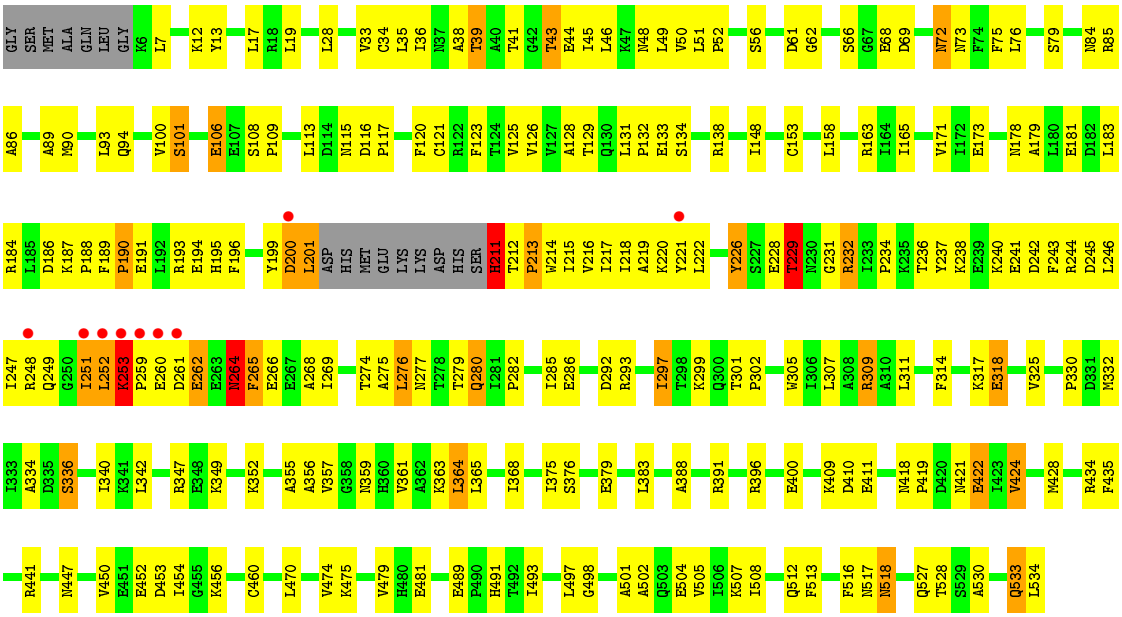
Chain C:





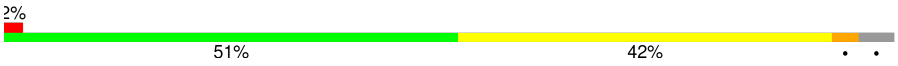
• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

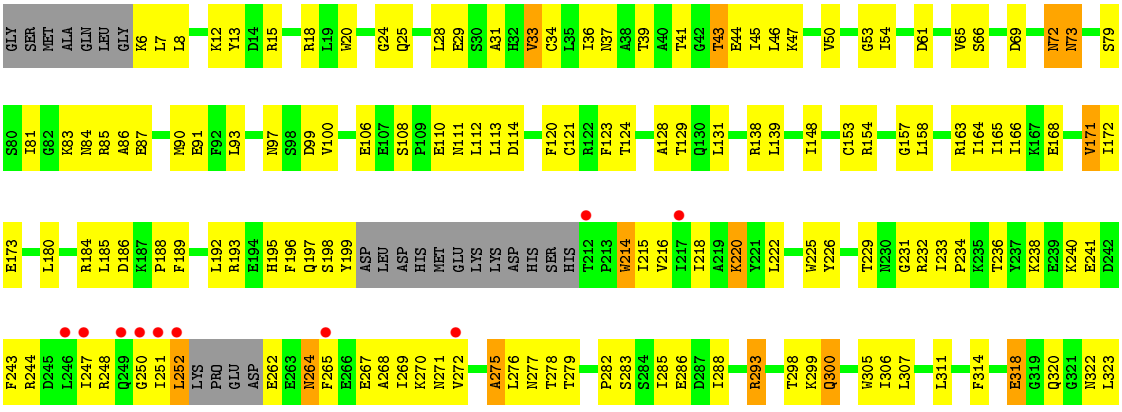
Chain E:

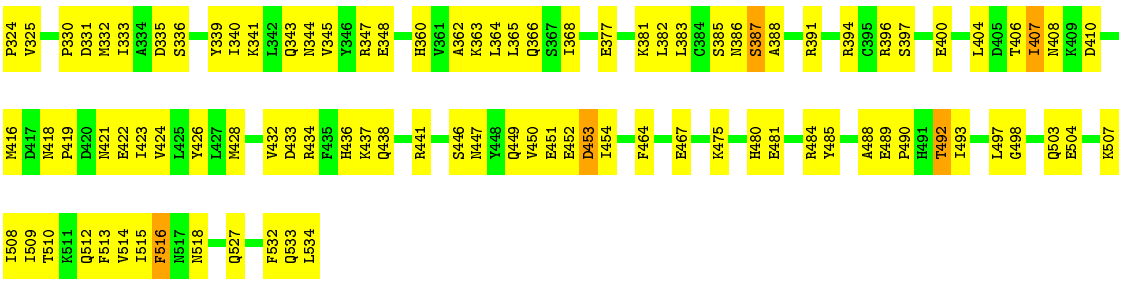


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

Chain G:

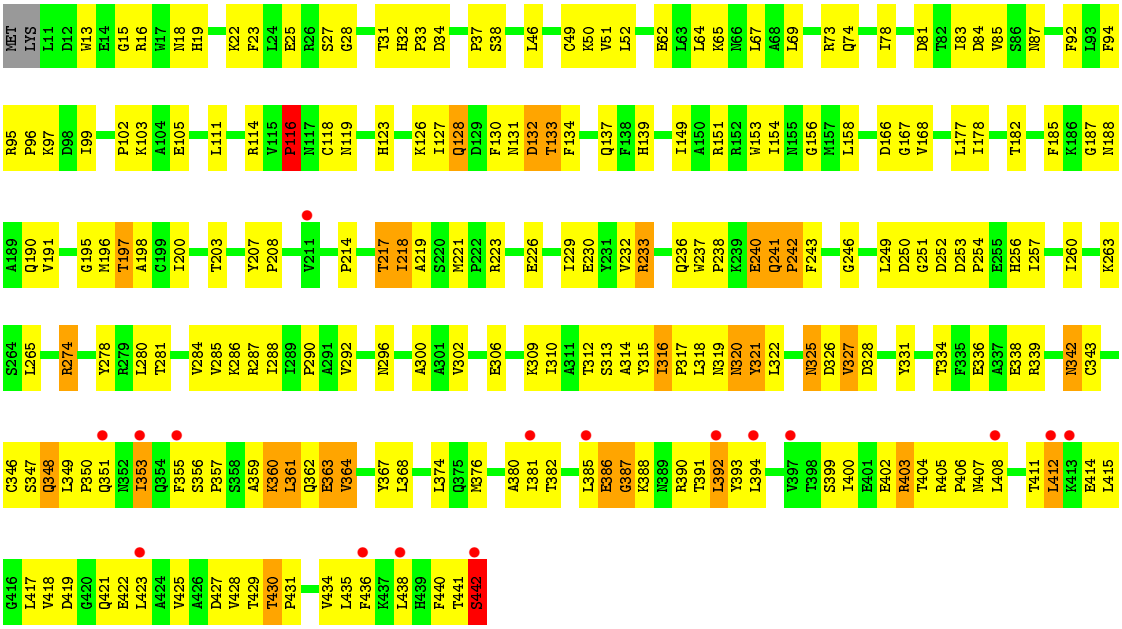






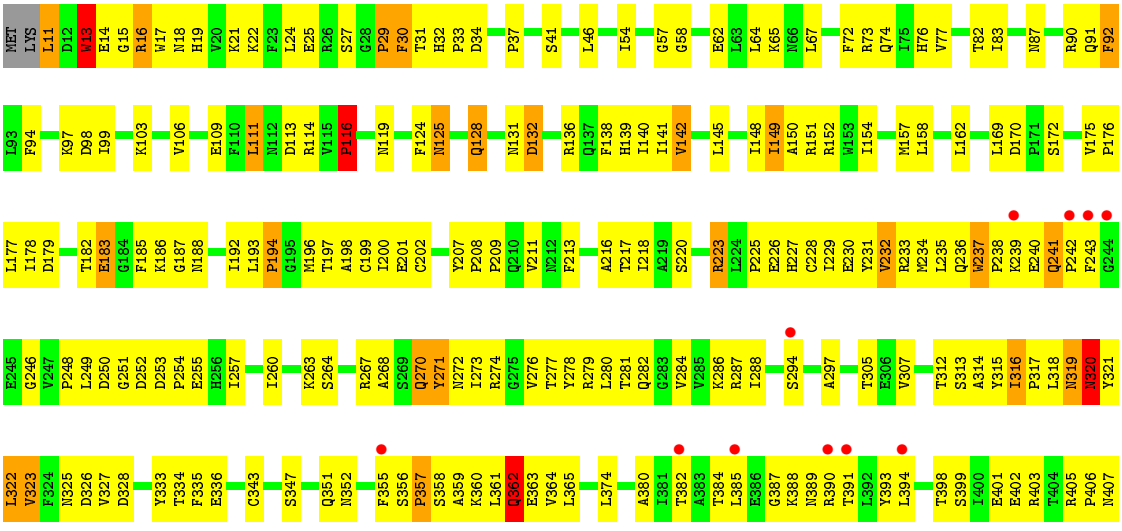
• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

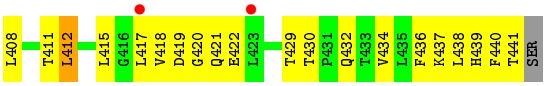
Chain B:



• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

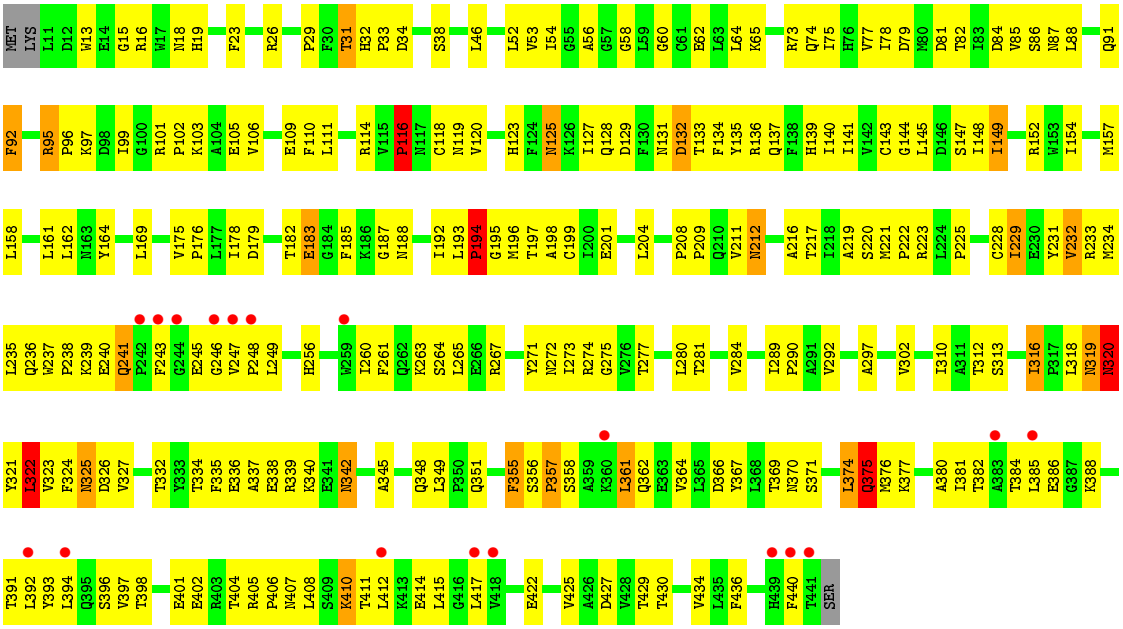
Chain D:





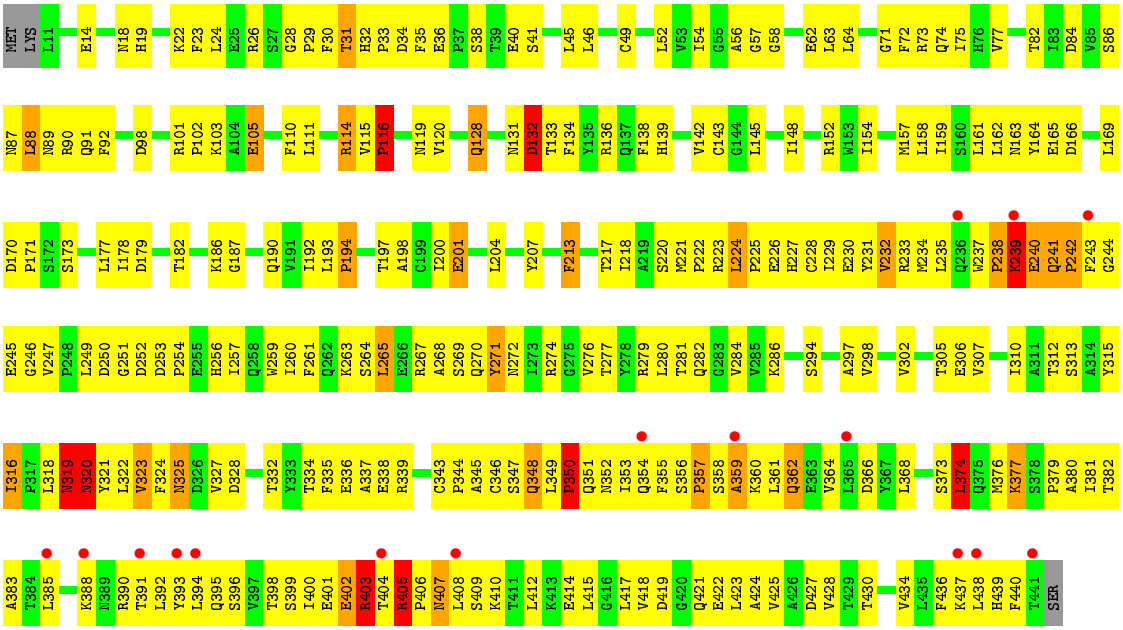
- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain F:



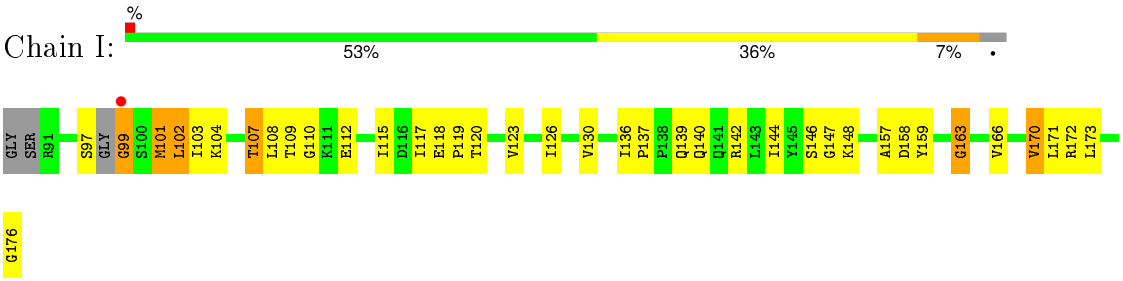
- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

Chain H:



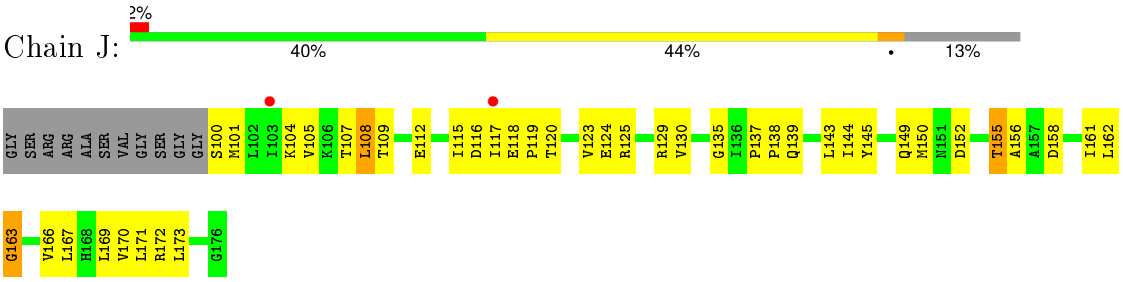
- Molecule 3: NEDD8

Chain I:



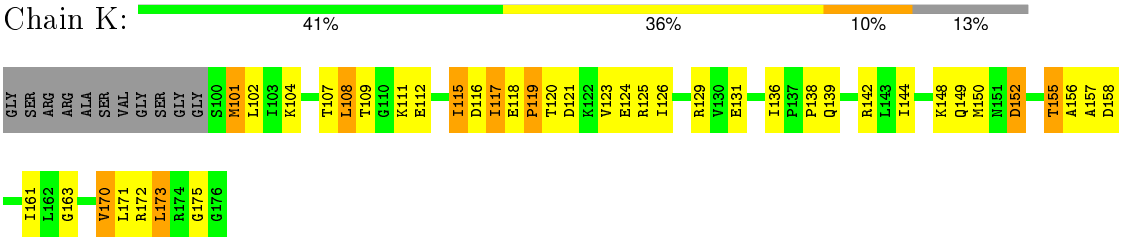
- Molecule 3: NEDD8

Chain J:



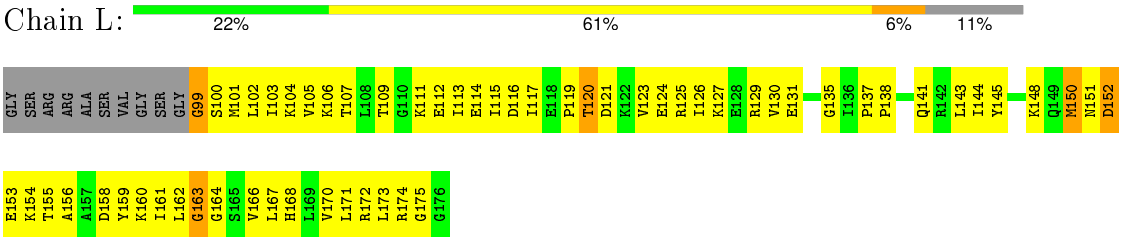
- Molecule 3: NEDD8

Chain K:



- Molecule 3: NEDD8

Chain L:



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%)	DCC
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
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 100052 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.43	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%)	5	25
1	C	512/531 (96%)	432 (84%)	59 (12%)	21 (4%)	3	19
1	E	511/531 (96%)	447 (88%)	46 (9%)	18 (4%)	4	23
1	G	502/531 (94%)	434 (86%)	54 (11%)	14 (3%)	6	28
2	B	430/434 (99%)	362 (84%)	56 (13%)	12 (3%)	6	28
2	D	429/434 (99%)	347 (81%)	62 (14%)	20 (5%)	3	16
2	F	429/434 (99%)	362 (84%)	51 (12%)	16 (4%)	4	22
2	H	429/434 (99%)	344 (80%)	60 (14%)	25 (6%)	2	11
3	I	81/88 (92%)	71 (88%)	5 (6%)	5 (6%)	2	10
3	J	75/88 (85%)	66 (88%)	7 (9%)	2 (3%)	6	28
3	K	75/88 (85%)	63 (84%)	8 (11%)	4 (5%)	2	14
3	L	76/88 (86%)	60 (79%)	12 (16%)	4 (5%)	2	14
All	All	4062/4212 (96%)	3421 (84%)	484 (12%)	157 (4%)	4	20

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%)	26	61
1	C	448/462 (97%)	425 (95%)	23 (5%)	29	65
1	E	448/462 (97%)	417 (93%)	31 (7%)	19	52
1	G	442/462 (96%)	419 (95%)	23 (5%)	29	64
2	B	378/382 (99%)	349 (92%)	29 (8%)	16	48
2	D	378/382 (99%)	352 (93%)	26 (7%)	19	52
2	F	377/382 (99%)	350 (93%)	27 (7%)	18	51
2	H	375/382 (98%)	348 (93%)	27 (7%)	18	51
3	I	73/74 (99%)	67 (92%)	6 (8%)	14	44
3	J	68/74 (92%)	66 (97%)	2 (3%)	50	81
3	K	68/74 (92%)	62 (91%)	6 (9%)	12	41
3	L	68/74 (92%)	67 (98%)	1 (2%)	72	90
All	All	3572/3672 (97%)	3346 (94%)	226 (6%)	22	56

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

Mol	Chain	Res	Type
2	D	322	LEU
1	E	277	ASN
2	H	154	ILE
2	D	388	LYS
1	E	79	SER

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

Mol	Chain	Res	Type
2	D	432	GLN
1	E	466	GLN
2	H	236	GLN
1	E	115	ASN
1	E	277	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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

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	517/531 (97%)	-0.08	5 (0%) 84 66	46, 76, 107, 130	0
1	C	516/531 (97%)	-0.00	7 (1%) 78 57	53, 82, 116, 140	0
1	E	515/531 (96%)	-0.04	9 (1%) 73 49	36, 62, 128, 141	0
1	G	508/531 (95%)	-0.02	10 (1%) 68 44	44, 71, 135, 147	0
2	B	432/434 (99%)	0.01	16 (3%) 45 21	46, 68, 122, 131	0
2	D	431/434 (99%)	0.19	13 (3%) 54 27	47, 85, 118, 131	0
2	F	431/434 (99%)	0.11	18 (4%) 40 18	41, 70, 121, 134	0
2	H	431/434 (99%)	0.09	16 (3%) 45 21	45, 79, 127, 140	0
3	I	85/88 (96%)	0.06	1 (1%) 81 61	54, 77, 99, 110	0
3	J	77/88 (87%)	0.32	2 (2%) 59 33	59, 90, 106, 116	0
3	K	77/88 (87%)	-0.00	0 100 100	56, 81, 99, 104	0
3	L	78/88 (88%)	0.24	0 100 100	70, 105, 125, 129	0
All	All	4098/4212 (97%)	0.04	97 (2%) 62 37	36, 76, 122, 147	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	HIS	5.2
1	G	252	LEU	4.7
2	D	243	PHE	4.3
2	B	392	LEU	3.8
1	E	260	GLU	3.8

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 (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	D	3	1/1	1.00	0.13	-0.72	67,67,67,67	0
4	ZN	F	4	1/1	0.99	0.14	-0.75	67,67,67,67	0
4	ZN	H	2	1/1	0.99	0.15	-0.76	84,84,84,84	0
4	ZN	B	1	1/1	0.99	0.14	-0.86	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.