



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 08:36 pm BST

PDB ID : 1TT5
Title : Structure of APPBP1-UBA3-Ubc12N26: a unique E1-E2 interaction required for optimal conjugation of the ubiquitin-like protein NEDD8
Authors : Huang, D.T.; Miller, D.W.; Mathew, R.; Cassell, R.; Holton, J.M.; Roussel, M.F.; Schulman, B.A.
Deposited on : 2004-06-21
Resolution : 2.60 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

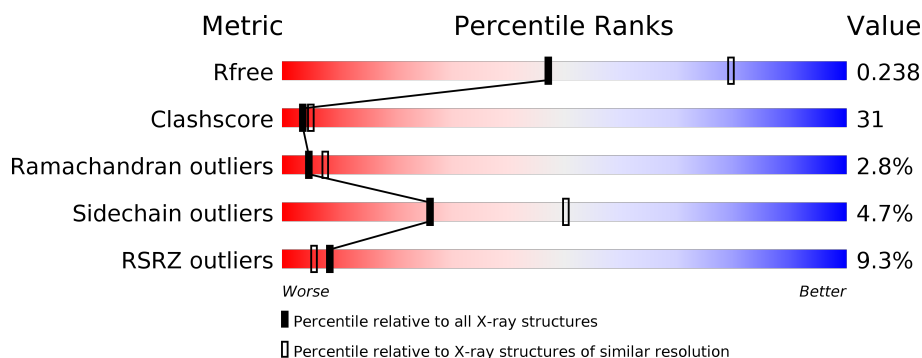
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	531	<div> <div>5%</div> <div> <div>56%</div> <div>38%</div> <div>• • •</div> </div> </div>
1	C	531	<div> <div>8%</div> <div> <div>50%</div> <div>41%</div> <div>5%</div> <div>• •</div> </div> </div>
2	B	434	<div> <div>4%</div> <div> <div>59%</div> <div>33%</div> <div>• 5%</div> </div> </div>
2	D	434	<div> <div>18%</div> <div> <div>48%</div> <div>39%</div> <div>• 9%</div> </div> </div>
3	E	26	<div> <div>8%</div> <div> <div>42%</div> <div>8%</div> <div>50%</div> </div> </div>
3	F	26	<div> <div>38%</div> <div> <div>23%</div> <div>15%</div> <div>62%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14637 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 amyloid protein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	4	0	0
			4108	2600	701	792	15			
1	C	512	Total	C	N	O	S	4	0	0
			4020	2546	684	775	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	GB 4502169
A	0	SER	-	CLONING ARTIFACT	GB 4502169
A	?	-	ASN	DELETION	GB 4502169
A	?	-	GLU	DELETION	GB 4502169
A	?	-	ASN	DELETION	GB 4502169
A	?	-	GLY	DELETION	GB 4502169
A	?	-	ALA	DELETION	GB 4502169
C	-1	GLY	-	CLONING ARTIFACT	GB 4502169
C	0	SER	-	CLONING ARTIFACT	GB 4502169
C	?	-	ASN	DELETION	GB 4502169
C	?	-	GLU	DELETION	GB 4502169
C	?	-	ASN	DELETION	GB 4502169
C	?	-	GLY	DELETION	GB 4502169
C	?	-	ALA	DELETION	GB 4502169

- Molecule 2 is a protein called ubiquitin-activating enzyme E1C isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	0	0
			3152	2010	540	584	18			
2	D	395	Total	C	N	O	S	12	0	0
			2866	1806	503	540	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	CLONING ARTIFACT	GB 38045942
B	10	LYS	-	CLONING ARTIFACT	GB 38045942
B	11	LEU	-	CLONING ARTIFACT	GB 38045942
D	9	MET	-	CLONING ARTIFACT	GB 38045942
D	10	LYS	-	CLONING ARTIFACT	GB 38045942
D	11	LEU	-	CLONING ARTIFACT	GB 38045942

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total 108	C 72	N 19	O 16	S 1	2	0	0
3	F	10	Total 83	C 55	N 15	O 13		9	0	0

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

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

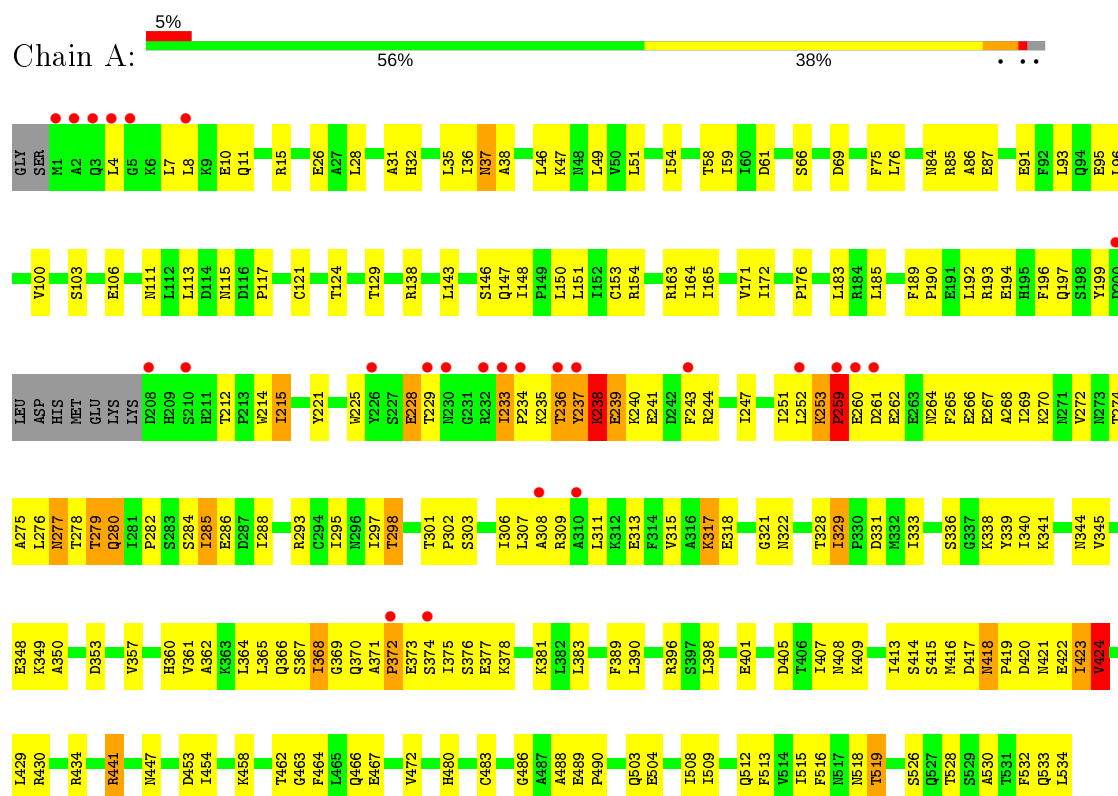
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	114	Total	O	0	0
			114	114		
5	C	45	Total	O	0	0
			45	45		
5	D	29	Total	O	0	0
			29	29		
5	E	5	Total	O	0	0
			5	5		

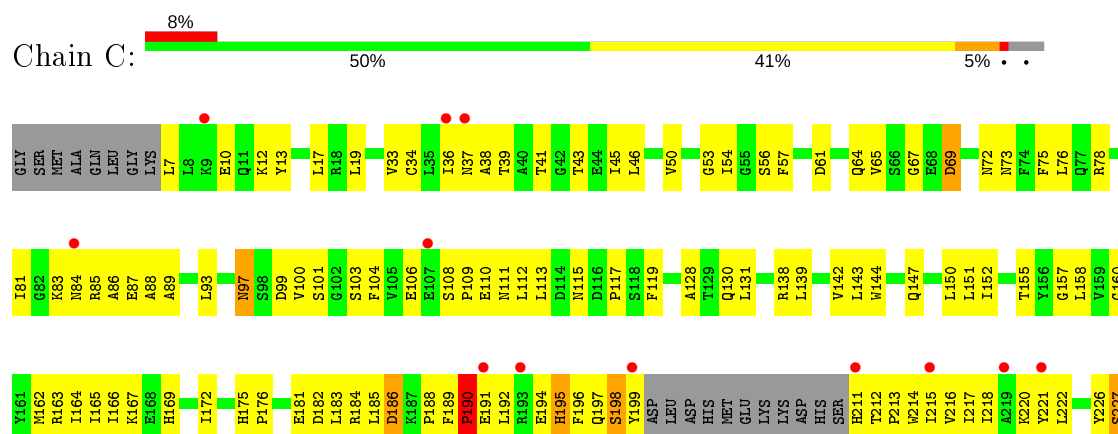
3 Residue-property plots

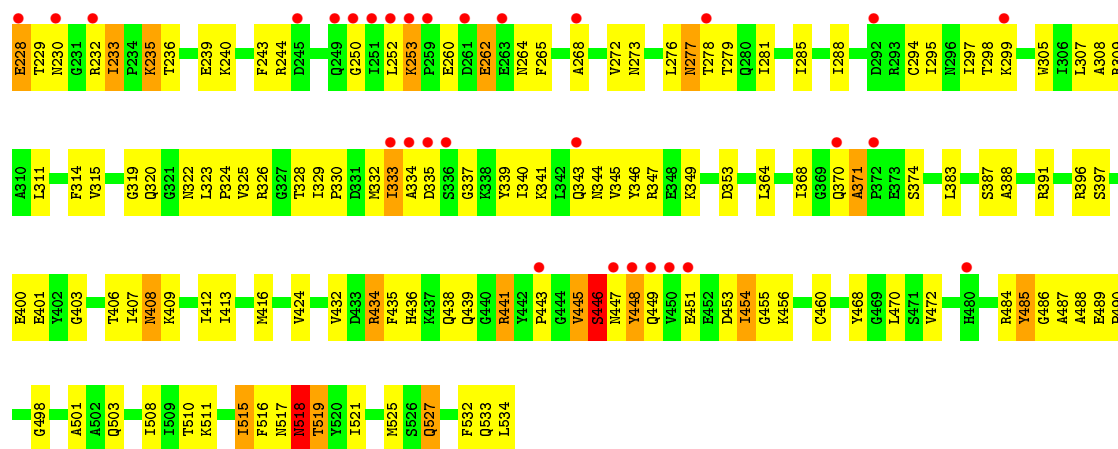
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

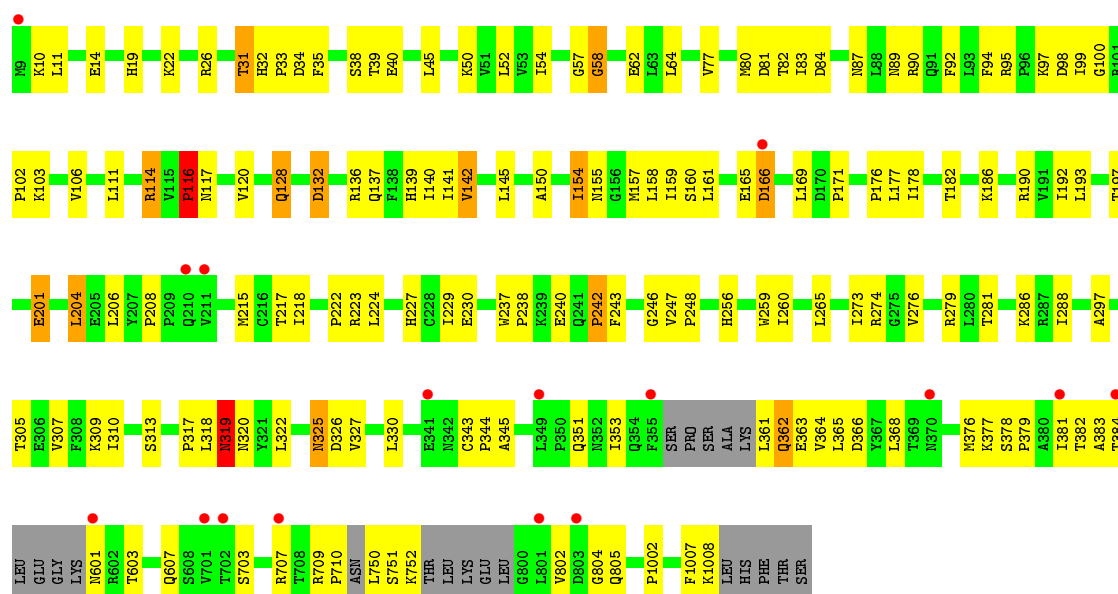


• Molecule 1: amyloid protein-binding protein 1

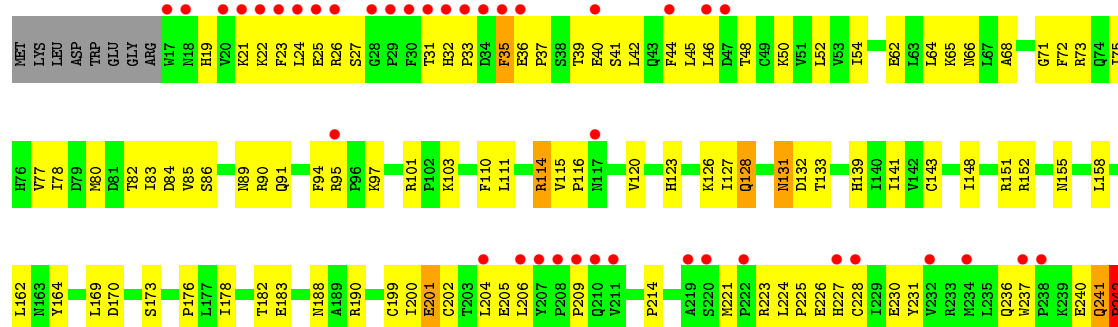


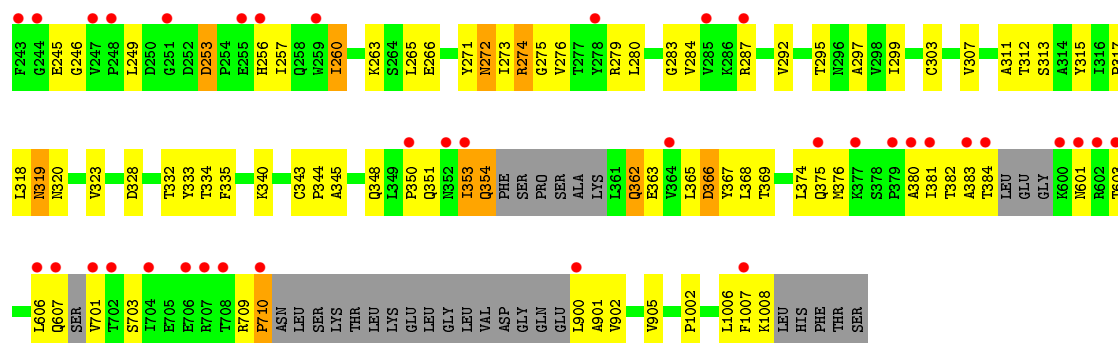


• Molecule 2: ubiquitin-activating enzyme E1C isoform 1

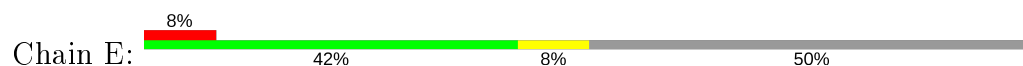


• Molecule 2: ubiquitin-activating enzyme E1C isoform 1





- Molecule 3: Ubiquitin-conjugating enzyme E2 M



- Molecule 3: Ubiquitin-conjugating enzyme E2 M



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.41Å 122.77Å 195.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.60 18.10 – 2.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (18.00-2.60) 98.9 (18.10-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.279 0.238 , 0.238	Depositor DCC
R_{free} test set	3377 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14637	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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	0.44	1/4187 (0.0%)	0.69	9/5664 (0.2%)
1	C	0.34	0/4099	0.59	0/5547
2	B	0.42	0/3219	0.69	3/4380 (0.1%)
2	D	0.41	0/2923	0.74	4/3962 (0.1%)
3	E	0.37	0/108	0.50	0/139
3	F	0.63	0/83	0.83	0/107
All	All	0.40	1/14619 (0.0%)	0.67	16/19799 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	TYR	CB-CG	-5.14	1.44	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	ASP	CB-CG-OD2	-11.96	107.54	118.30
1	A	233	ILE	N-CA-C	8.36	133.57	111.00
1	A	279	THR	N-CA-C	-7.06	91.94	111.00
2	D	710	PRO	N-CA-CB	6.54	111.15	103.30
1	A	239	GLU	N-CA-C	-6.06	94.63	111.00

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	4108	0	4038	288	0
1	C	4020	0	3937	264	0
2	B	3152	0	2998	165	0
2	D	2866	0	2608	212	0
3	E	108	0	128	3	0
3	F	83	0	92	6	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	105	0	0	12	0
5	B	114	0	0	9	0
5	C	45	0	0	4	0
5	D	29	0	0	3	0
5	E	5	0	0	0	0
All	All	14637	0	13801	882	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 31.

The worst 5 of 882 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:518:ASN:ND2	1:A:534:LEU:H	1.07	1.41
1:A:518:ASN:ND2	1:A:534:LEU:N	1.76	1.31
1:A:225:TRP:NE1	1:A:233:ILE:HD11	1.58	1.19
1:A:282:PRO:HB2	1:A:285:ILE:HD13	1.19	1.18
1:A:235:LYS:HB2	1:A:239:GLU:HG3	1.22	1.17

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	518/531 (98%)	477 (92%)	30 (6%)	11 (2%)	7	13
1	C	508/531 (96%)	435 (86%)	56 (11%)	17 (3%)	4	6
2	B	404/434 (93%)	362 (90%)	33 (8%)	9 (2%)	6	12
2	D	385/434 (89%)	330 (86%)	41 (11%)	14 (4%)	3	4
3	E	11/26 (42%)	11 (100%)	0	0	100	100
3	F	8/26 (31%)	7 (88%)	1 (12%)	0	100	100
All	All	1834/1982 (92%)	1622 (88%)	161 (9%)	51 (3%)	5	7

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	THR
2	B	384	THR
1	C	38	ALA
1	C	227	SER
1	C	228	GLU

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	445/462 (96%)	427 (96%)	18 (4%)	31	57
1	C	435/462 (94%)	415 (95%)	20 (5%)	27	51
2	B	325/383 (85%)	308 (95%)	17 (5%)	23	46
2	D	278/383 (73%)	263 (95%)	15 (5%)	22	44
3	E	12/22 (54%)	12 (100%)	0	100	100
3	F	9/22 (41%)	9 (100%)	0	100	100
All	All	1504/1734 (87%)	1434 (95%)	70 (5%)	26	50

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

Mol	Chain	Res	Type
2	B	201	GLU

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Mol	Chain	Res	Type
1	C	103	SER
2	D	260	ILE
2	B	204	LEU
1	C	69	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	351	GLN
1	C	147	GLN
2	D	256	HIS
1	C	111	ASN
1	C	195	HIS

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 2 ligands modelled in this entry, 2 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	608:SER	C	701:VAL	N	6.15

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	521/531 (98%)	-0.05	26 (4%) 28 23	25, 52, 111, 130	0
1	C	511/531 (96%)	0.28	42 (8%) 11 8	38, 74, 122, 143	0
2	B	414/434 (95%)	-0.16	16 (3%) 39 32	25, 44, 107, 125	0
2	D	392/434 (90%)	0.79	77 (19%) 1 0	34, 82, 141, 160	0
3	E	13/26 (50%)	0.58	2 (15%) 2 1	58, 69, 83, 88	1 (7%)
3	F	10/26 (38%)	4.06	10 (100%) 0 0	105, 108, 110, 112	3 (30%)
All	All	1861/1982 (93%)	0.22	173 (9%) 8 6	25, 61, 126, 160	4 (0%)

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	33	PRO	10.1
1	A	236	THR	8.3
2	D	707	ARG	7.7
2	D	259	TRP	7.0
2	D	31	THR	6.8

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
4	ZN	D	1014	1/1	0.98	0.09	62,62,62,62	0
4	ZN	B	1014	1/1	0.99	0.08	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.