



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:06 AM GMT

PDB ID : 1ZM3  
Title : Structure of the apo eEF2-ETA complex  
Authors : Joergensen, R.; Merrill, A.R.; Yates, S.P.; Marquez, V.E.; Schwan, A.L.; Boesen, T.; Andersen, G.R.  
Deposited on : 2005-05-10  
Resolution : 3.07 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
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

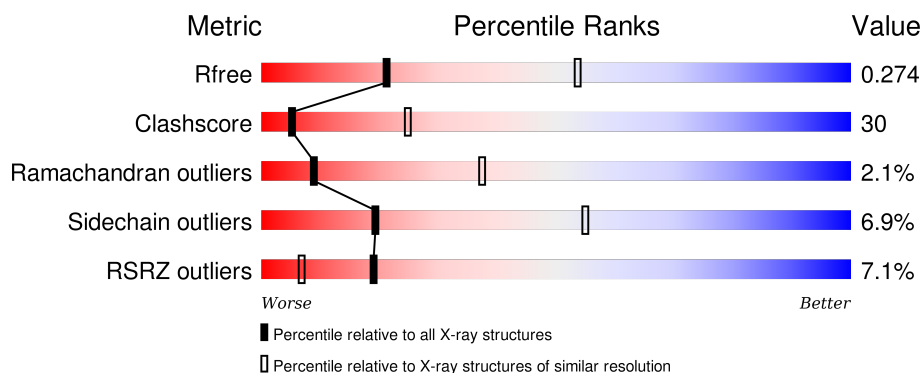
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.07 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	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	842	<div> <div>2%</div> <div>54%</div> <div>40%</div> <div>• •</div> </div>
1	C	842	<div> <div>5%</div> <div>45%</div> <div>48%</div> <div>5%</div> <div>•</div> </div>
1	E	842	<div> <div>19%</div> <div>45%</div> <div>49%</div> <div>• •</div> </div>
2	B	207	<div> <div>%</div> <div>57%</div> <div>35%</div> <div>7%</div> </div>
2	D	207	<div> <div>55%</div> <div>42%</div> <div>•</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	207	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (57%), yellow (36%), and orange (6%). The percentages are labeled below the segments.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23979 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	E	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			

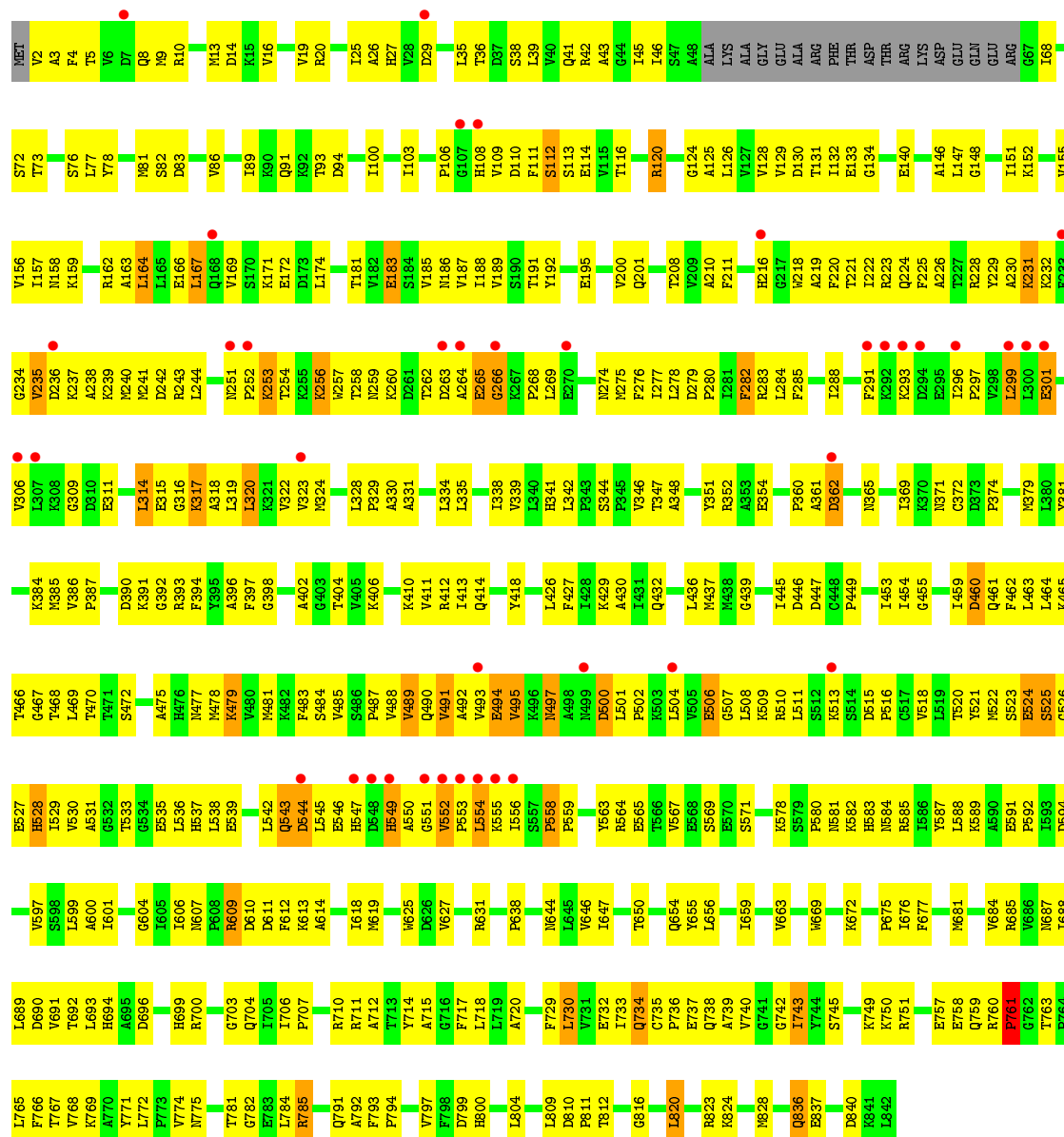
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
C	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
E	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324

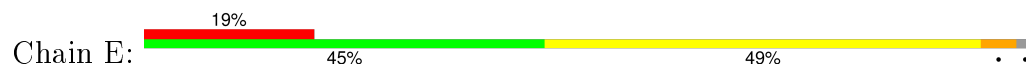
- Molecule 2 is a protein called exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	D	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	F	207	Total	C	N	O	0	0	0
			1588	1001	283	304			

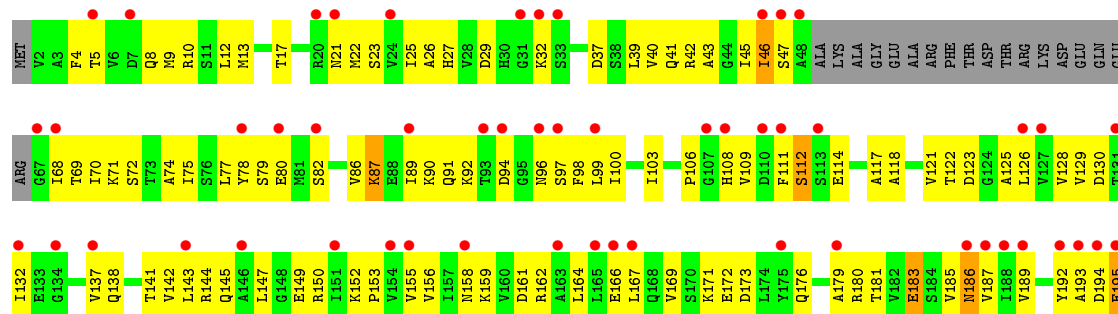


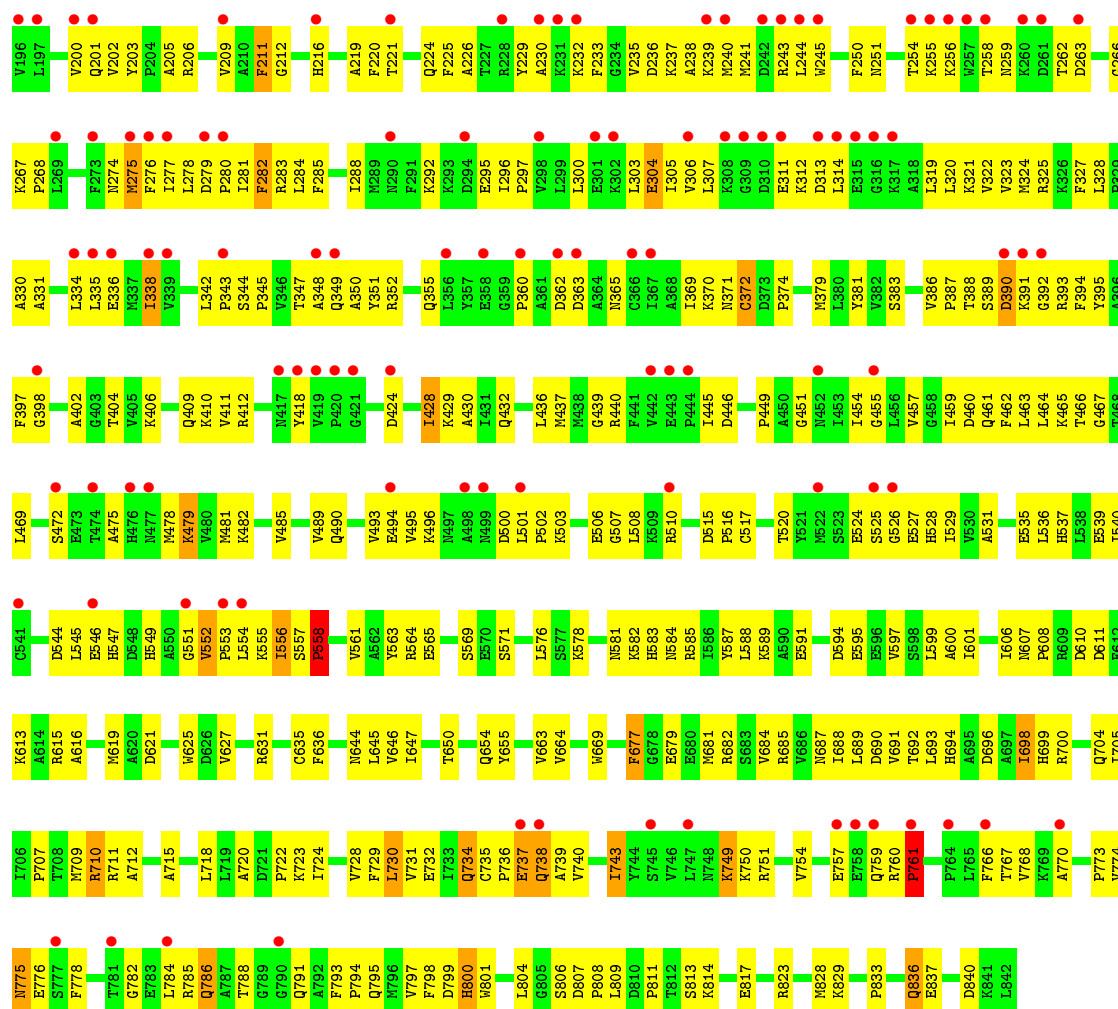


• Molecule 1: Elongation factor 2

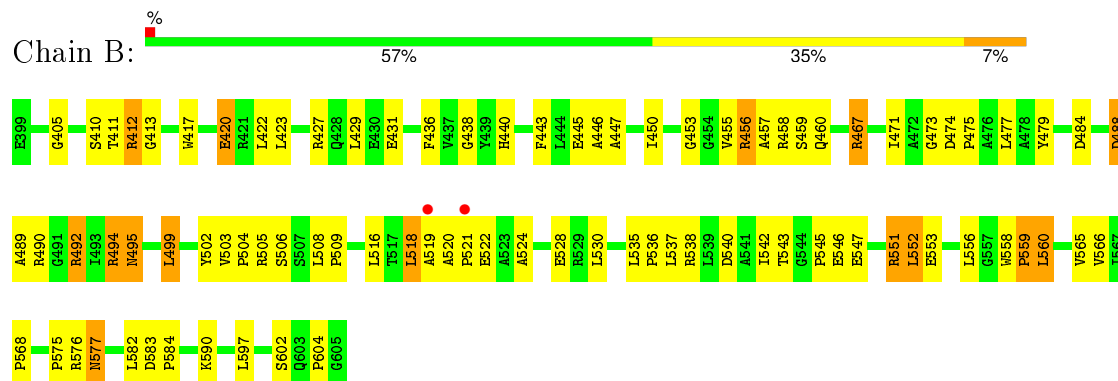


Chain E:

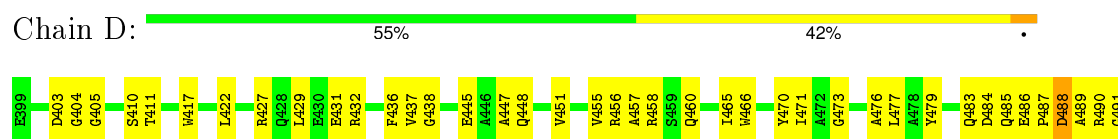


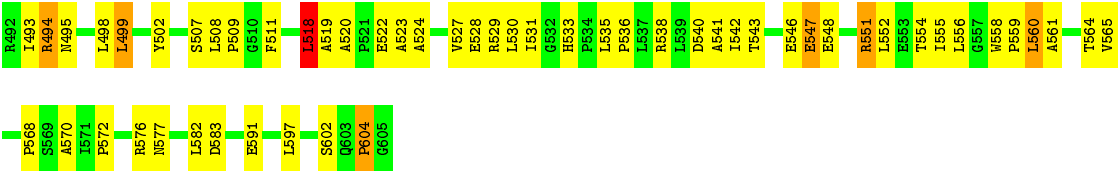


• Molecule 2: exotoxin A

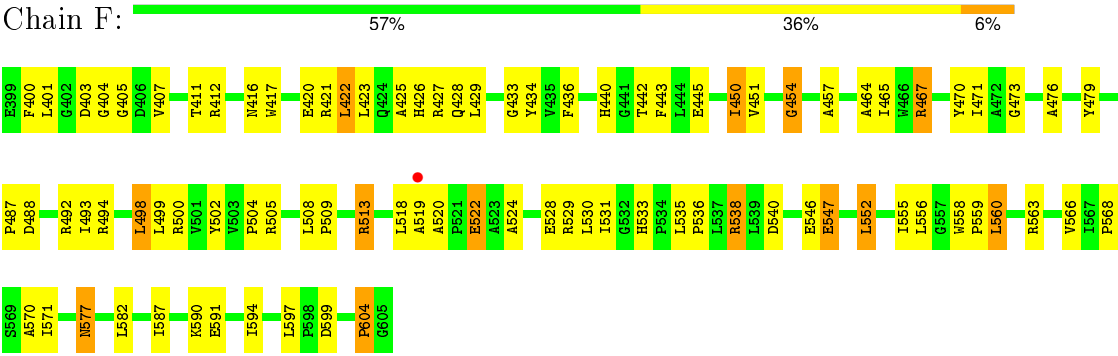


• Molecule 2: exotoxin A





• Molecule 2: exotoxin A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	329.43Å 69.09Å 190.80Å 90.00° 103.46° 90.00°	Depositor
Resolution (Å)	40.00 – 3.07 29.63 – 3.07	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.07) 97.9 (29.63-3.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.282 0.243 , 0.274	Depositor DCC
$R_{free}$ test set	1536 reflections (1.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 78889 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.54 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.7793e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: DDE

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	0.47	0/6517	0.68	1/8823 (0.0%)
1	C	0.49	1/6517 (0.0%)	0.71	1/8823 (0.0%)
1	E	0.44	1/6517 (0.0%)	0.65	1/8823 (0.0%)
2	B	0.64	0/1627	0.85	0/2216
2	D	0.66	0/1627	0.83	1/2216 (0.0%)
2	F	0.58	0/1627	0.83	0/2216
All	All	0.50	2/24432 (0.0%)	0.71	4/33117 (0.0%)

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
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	195	GLU	CD-OE1	6.84	1.33	1.25
1	C	543	GLN	CG-CD	6.52	1.66	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	195	GLU	CG-CD-OE2	-7.76	102.77	118.30
1	A	236	ASP	N-CA-C	-5.55	96.01	111.00
1	C	554	LEU	N-CA-C	5.20	125.04	111.00
2	D	518	LEU	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	195	GLU	Sidechain

## 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	6405	0	6472	345	0
1	C	6405	0	6472	459	0
1	E	6405	0	6472	438	0
2	B	1588	0	1539	84	0
2	D	1588	0	1539	76	0
2	F	1588	0	1539	71	0
All	All	23979	0	24033	1462	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 30.

The worst 5 of 1462 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:391:LYS:HG2	1:C:392:GLY:H	1.13	1.11
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.32	1.11
1:E:556:ILE:HG22	1:E:557:SER:H	1.10	1.10
1:A:16:VAL:HG13	1:A:345:PRO:HG2	1.33	1.09
1:C:253:LYS:HA	1:C:253:LYS:HE3	1.35	1.06

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	818/842 (97%)	729 (89%)	75 (9%)	14 (2%)	11	43
1	C	818/842 (97%)	716 (88%)	80 (10%)	22 (3%)	6	31
1	E	818/842 (97%)	712 (87%)	90 (11%)	16 (2%)	9	38
2	B	205/207 (99%)	181 (88%)	22 (11%)	2 (1%)	19	58
2	D	205/207 (99%)	182 (89%)	17 (8%)	6 (3%)	6	29
2	F	205/207 (99%)	179 (87%)	21 (10%)	5 (2%)	7	33
All	All	3069/3147 (98%)	2699 (88%)	305 (10%)	65 (2%)	9	37

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	761	PRO
2	B	518	LEU
2	B	519	ALA
1	C	235	VAL

### 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	699/714 (98%)	662 (95%)	37 (5%)	28	64
1	C	699/714 (98%)	649 (93%)	50 (7%)	18	53
1	E	699/714 (98%)	659 (94%)	40 (6%)	25	62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	161/162 (99%)	142 (88%)	19 (12%)	6	25
2	D	161/162 (99%)	146 (91%)	15 (9%)	11	39
2	F	161/162 (99%)	144 (89%)	17 (11%)	8	32
All	All	2580/2628 (98%)	2402 (93%)	178 (7%)	19	55

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	461	GLN
1	C	738	GLN
2	F	467	ARG
1	C	494	GLU
1	C	552	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	414	GLN
1	C	583	HIS
1	E	753	GLN
1	C	452	ASN
1	C	537	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DDE	A	699	1	5,10,21	0.57	0	3,12,30	1.88	2 (66%)
1	DDE	C	699	1	5,10,21	0.49	0	3,12,30	1.84	2 (66%)
1	DDE	E	699	1	5,10,21	0.53	0	3,12,30	1.74	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	A	699	1	-	0/4/6/23	0/1/1/1
1	DDE	C	699	1	-	0/4/6/23	0/1/1/1
1	DDE	E	699	1	-	0/4/6/23	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	DDE	O-C-CA	-2.33	119.43	125.49
1	C	699	DDE	O-C-CA	-2.19	119.79	125.49
1	E	699	DDE	O-C-CA	-2.01	120.26	125.49
1	E	699	DDE	CD2-NE2-CE1	2.09	109.00	105.71
1	A	699	DDE	CD2-NE2-CE1	2.12	109.05	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	699	DDE	1	0
1	C	699	DDE	1	0
1	E	699	DDE	4	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	822/842 (97%)	-0.20	14 (1%) 73 51	8, 57, 85, 104	0
1	C	822/842 (97%)	0.12	40 (4%) 33 14	10, 69, 123, 135	0
1	E	822/842 (97%)	0.82	162 (19%) 1 0	6, 105, 128, 146	0
2	B	207/207 (100%)	-0.58	2 (0%) 84 68	5, 24, 57, 74	0
2	D	207/207 (100%)	-0.59	0 100 100	5, 23, 61, 76	0
2	F	207/207 (100%)	-0.52	1 (0%) 91 82	10, 31, 63, 82	0
All	All	3087/3147 (98%)	0.08	219 (7%) 19 7	5, 60, 123, 146	0

The worst 5 of 219 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	GLY	8.8
1	E	189	VAL	7.3
1	C	551	GLY	6.7
1	C	251	ASN	6.3
1	E	759	GLN	6.1

### 6.2 Non-standard residues in protein, DNA, RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	DDE	A	699	10/21	0.96	0.12	-	40,42,44,45	0
1	DDE	C	699	10/21	0.95	0.14	-	43,47,48,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DDE	E	699	10/21	0.93	0.16	-	44,48,49,50	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.