



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:44 pm BST

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

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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

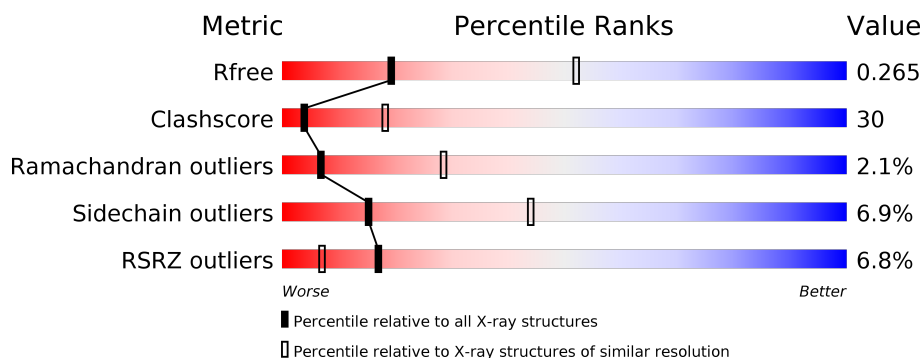
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (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 ≥ 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	842	<div> <div>2%</div> <div> <div>54%</div> <div>40%</div> <div>• •</div> </div> </div>
1	C	842	<div> <div>5%</div> <div> <div>45%</div> <div>48%</div> <div>5%</div> <div>•</div> </div> </div>
1	E	842	<div> <div>18%</div> <div> <div>45%</div> <div>49%</div> <div>• •</div> </div> </div>
2	B	207	<div> <div>57%</div> <div>35%</div> <div>7%</div> </div>
2	D	207	<div> <div>55%</div> <div>42%</div> <div>•</div> </div>
2	F	207	<div> <div>57%</div> <div>36%</div> <div>6%</div> </div>

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

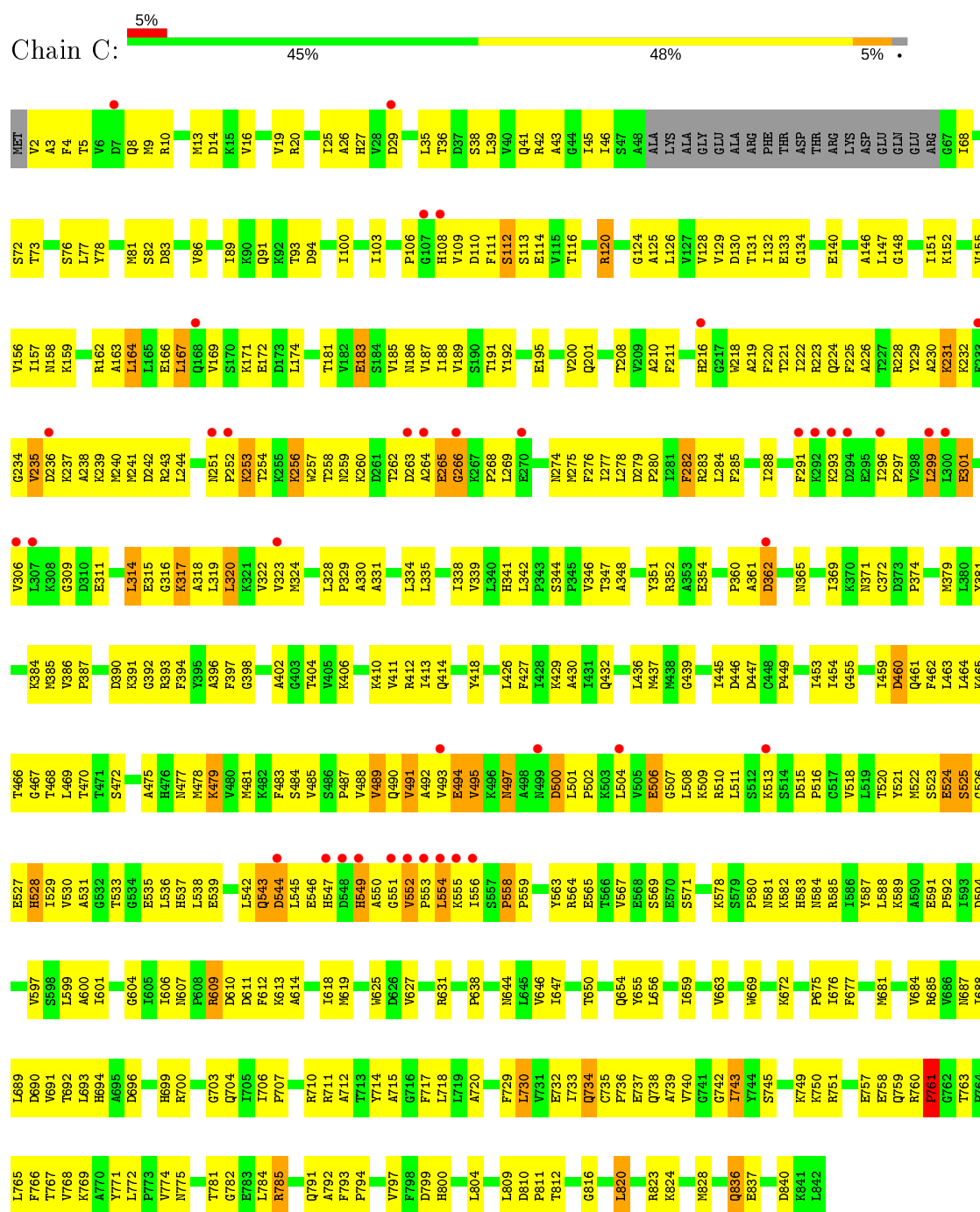
- Molecule 2 is a protein called exotoxin A.

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			

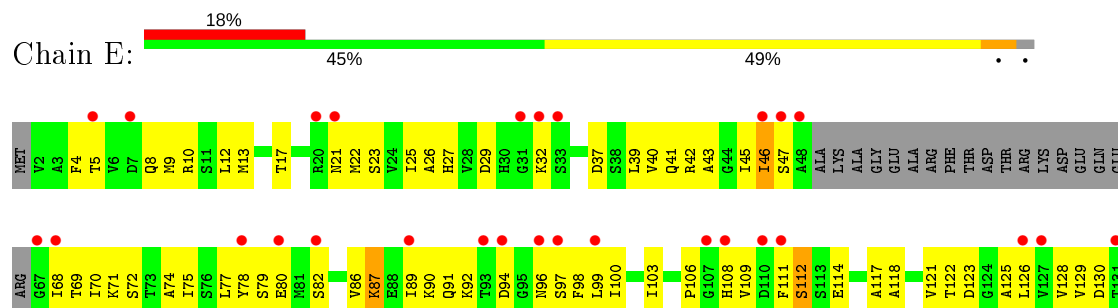
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

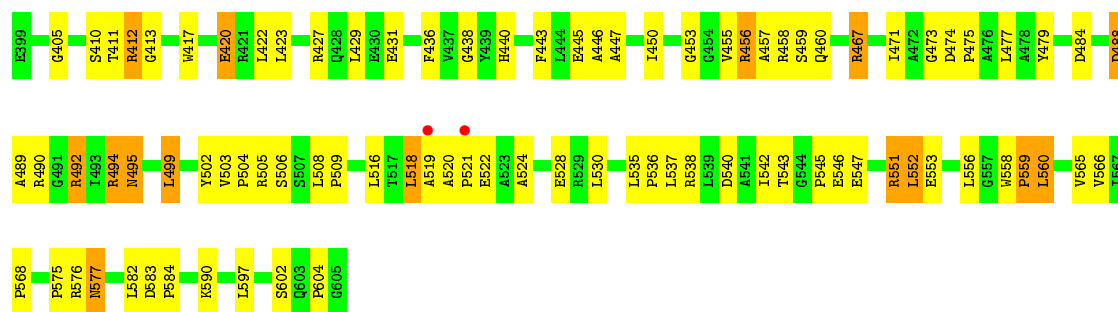
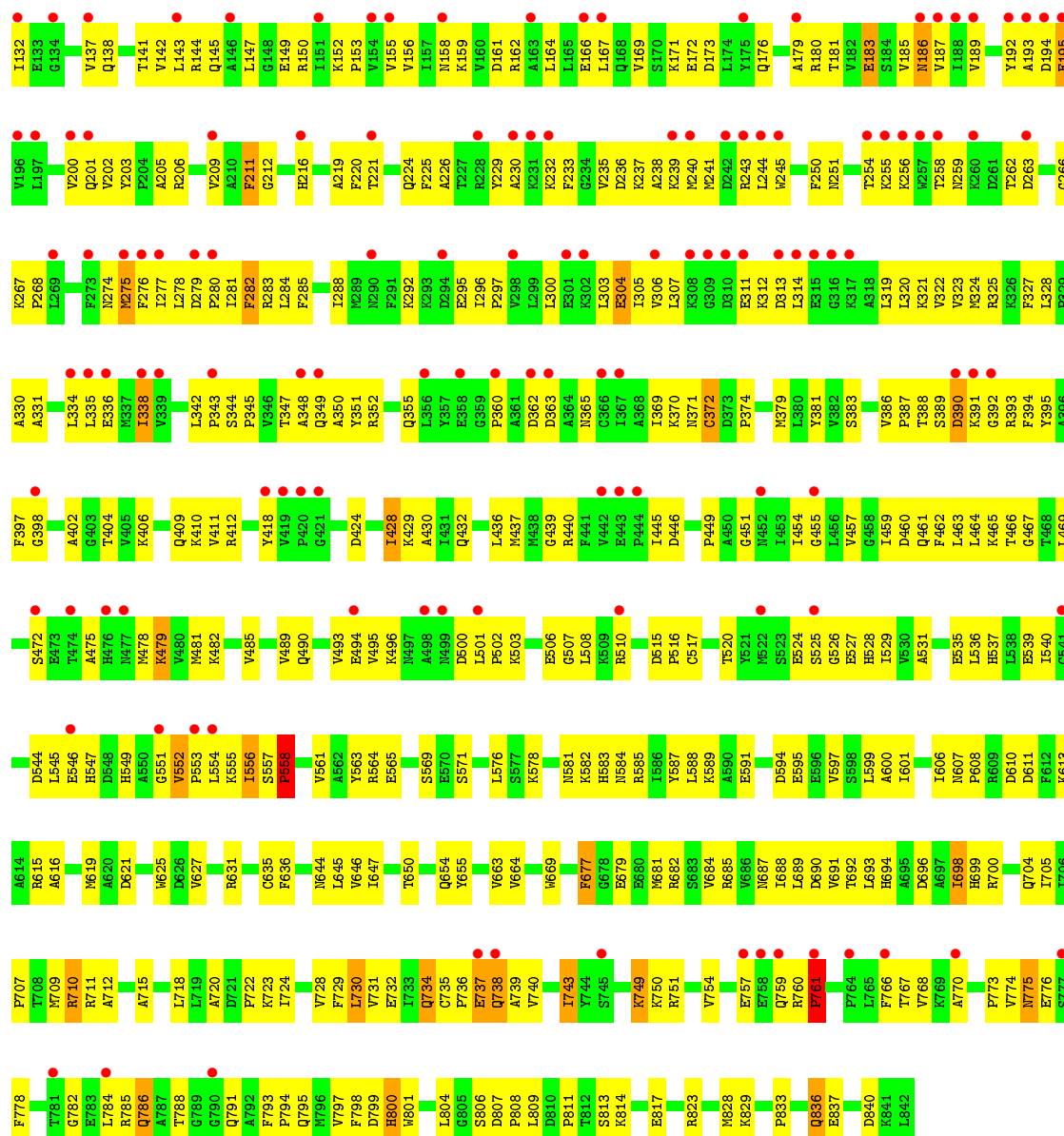
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- WORLD WIDE
PDB
PROTEIN DATA BANK

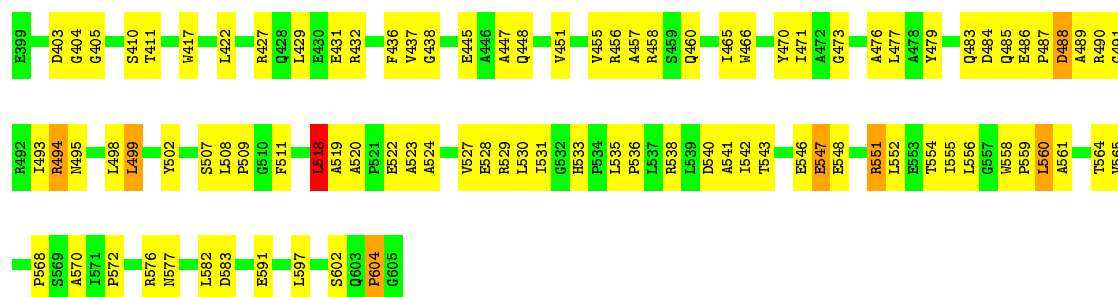


• Molecule 1: Elongation factor 2





Chain D:  55% 42%



• Molecule 2: exotoxin A

Chain F:  57% 36% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.282 0.240 , 0.265	Depositor DCC
R_{free} test set	1571 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23979	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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:HE3	1:C:253:LYS:HA	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%)	9	34
1	C	818/842 (97%)	716 (88%)	80 (10%)	22 (3%)	5	23
1	E	818/842 (97%)	712 (87%)	90 (11%)	16 (2%)	7	29
2	B	205/207 (99%)	181 (88%)	22 (11%)	2 (1%)	15	47
2	D	205/207 (99%)	182 (89%)	17 (8%)	6 (3%)	4	22
2	F	205/207 (99%)	179 (87%)	21 (10%)	5 (2%)	6	25
All	All	3069/3147 (98%)	2699 (88%)	305 (10%)	65 (2%)	7	28

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%)	22	53
1	C	699/714 (98%)	649 (93%)	50 (7%)	14	42
1	E	699/714 (98%)	659 (94%)	40 (6%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	161/162 (99%)	142 (88%)	19 (12%)	5	20
2	D	161/162 (99%)	146 (91%)	15 (9%)	9	31
2	F	161/162 (99%)	144 (89%)	17 (11%)	6	24
All	All	2580/2628 (98%)	2402 (93%)	178 (7%)	15	44

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	0.63	0	3,12,30	1.51	1 (33%)
1	DDE	C	699	1	5,10,21	0.52	0	3,12,30	1.53	1 (33%)
1	DDE	E	699	1	5,10,21	0.58	0	3,12,30	1.37	1 (33%)

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	-	0/5/6/23	0/1/1/1
1	DDE	C	699	1	-	0/5/6/23	0/1/1/1
1	DDE	E	699	1	-	0/5/6/23	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	DDE	CD2-NE2-CE1	2.13	109.11	105.78
1	A	699	DDE	CD2-NE2-CE1	2.10	109.05	105.78
1	E	699	DDE	CD2-NE2-CE1	2.06	109.00	105.78

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 [i](#)

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 [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	822/842 (97%)	-0.22	14 (1%) 70 48	8, 57, 85, 104	0
1	C	822/842 (97%)	0.10	39 (4%) 31 14	10, 69, 123, 135	0
1	E	822/842 (97%)	0.78	154 (18%) 1 0	6, 105, 128, 146	0
2	B	207/207 (100%)	-0.59	2 (0%) 82 66	5, 24, 57, 74	0
2	D	207/207 (100%)	-0.60	0 100 100	5, 23, 61, 76	0
2	F	207/207 (100%)	-0.54	0 100 100	10, 31, 63, 82	0
All	All	3087/3147 (98%)	0.06	209 (6%) 17 7	5, 60, 123, 146	0

The worst 5 of 209 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	GLY	8.6
1	E	189	VAL	7.2
1	C	551	GLY	6.5
1	C	251	ASN	6.2
1	E	759	GLN	6.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	DDE	E	699	10/21	0.93	0.16	44,48,49,50	0
1	DDE	C	699	10/21	0.95	0.14	43,47,48,50	0
1	DDE	A	699	10/21	0.96	0.12	40,42,44,45	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.