



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 07:39 AM UTC

PDB ID : 1JJI / pdb_00001jji
Title : The Crystal Structure of a Hyper-thermophilic Carboxylesterase from the Archaeon *Archaeoglobus fulgidus*
Authors : De Simone, G.; Menchise, V.; Manco, G.; Mandrich, L.; Sorrentino, N.; Lang, D.; Rossi, M.; Pedone, C.
Deposited on : 2001-07-06
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

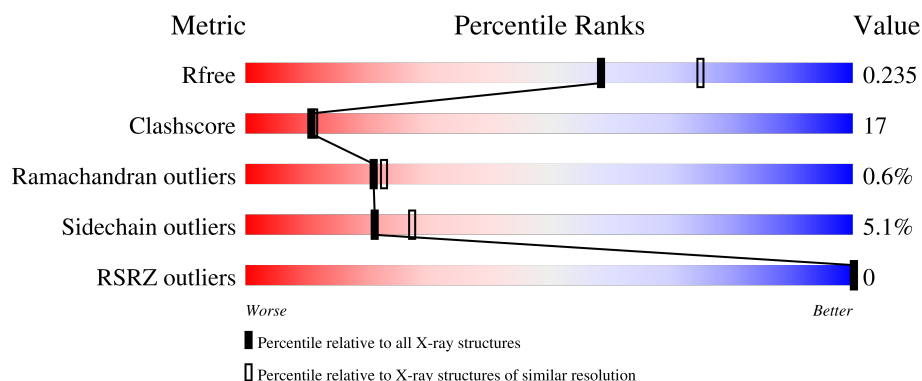
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	311	77% 20% ..
1	B	311	73% 24% .
1	C	311	65% 32% .
1	D	311	65% 31% ..

2 Entry composition [i](#)

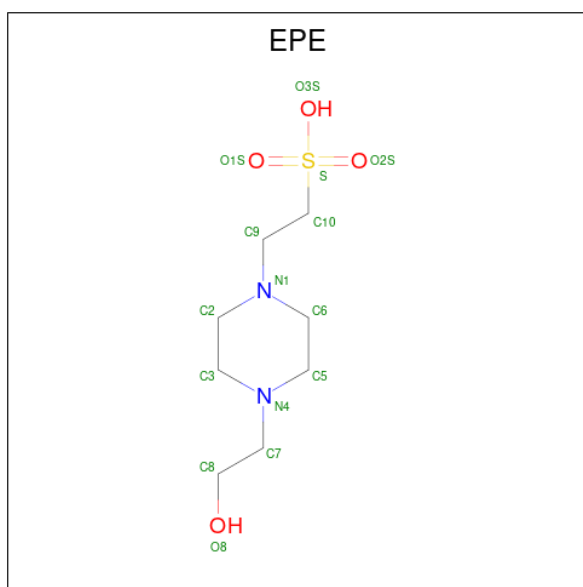
There are 3 unique types of molecules in this entry. The entry contains 10649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carboxylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	53	0	0
			2508	1602	430	468	8			
1	B	311	Total	C	N	O	S	46	0	0
			2508	1602	430	468	8			
1	C	311	Total	C	N	O	S	72	0	0
			2508	1602	430	468	8			
1	D	311	Total	C	N	O	S	54	0	0
			2508	1602	430	468	8			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	3	0
			14	8	2	3	1		
2	B	1	Total	C	N	O	S	3	0
			14	8	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	3	0
			14	8	2	3	1		
2	D	1	Total	C	N	O	S	3	0
			14	8	2	3	1		

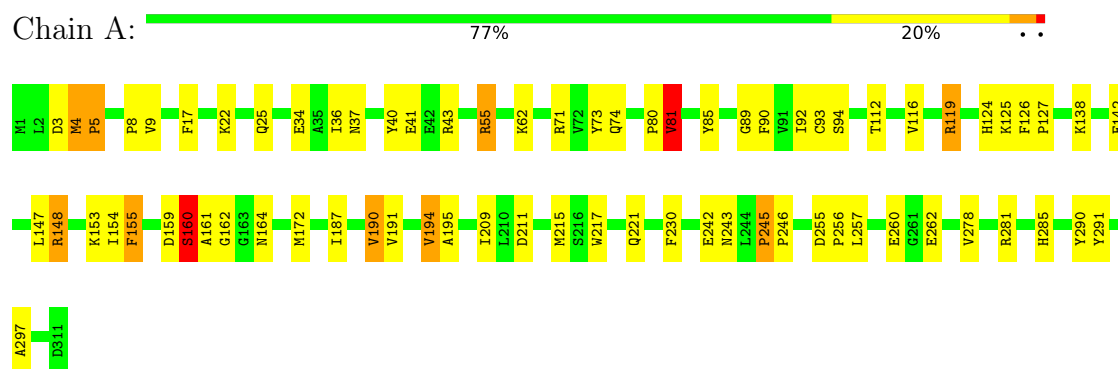
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	165	Total	O	0	0
			165	165		
3	B	180	Total	O	0	0
			180	180		
3	C	108	Total	O	0	0
			108	108		
3	D	108	Total	O	0	0
			108	108		

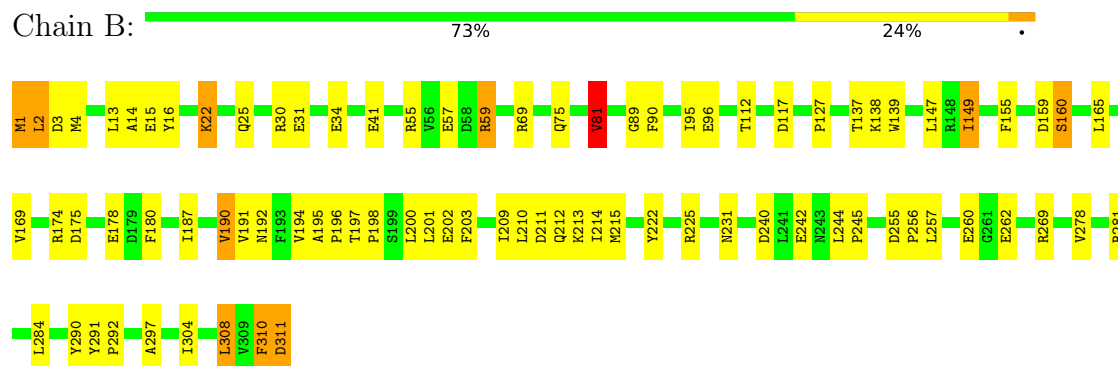
3 Residue-property plots [i](#)

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.

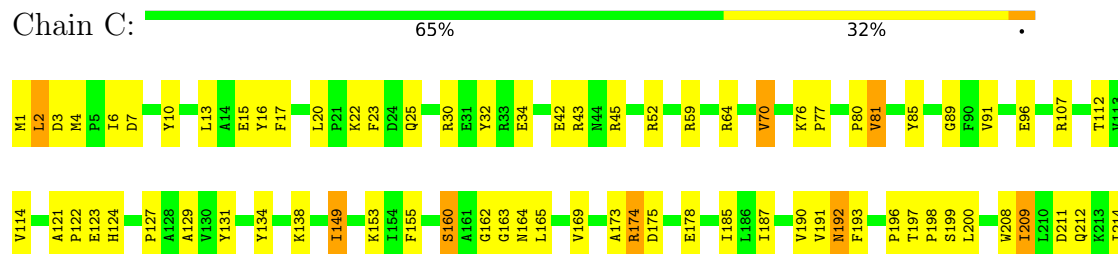
• Molecule 1: Carboxylesterase



• Molecule 1: Carboxylesterase

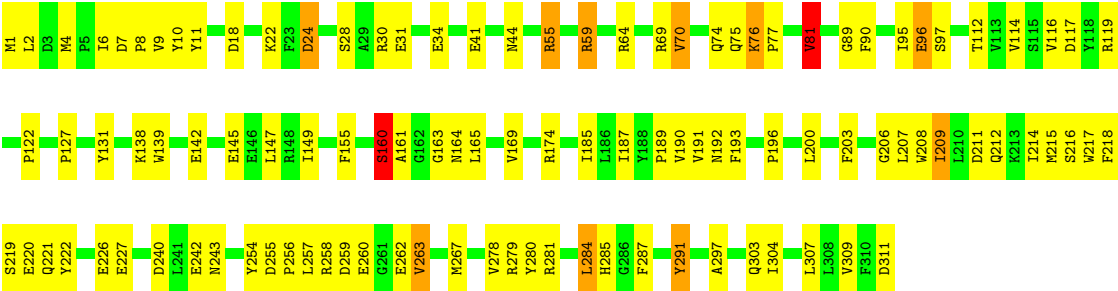


• Molecule 1: Carboxylesterase





● Molecule 1: Carboxylesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	169.05Å 169.05Å 104.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (8.00-2.20) 99.4 (8.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.21Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.235 0.203 , 0.235	Depositor DCC
R_{free} test set	4236 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.104 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10649	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE

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	0.85	0/2568	1.01	11/3482 (0.3%)
1	B	0.84	1/2568 (0.0%)	1.03	10/3482 (0.3%)
1	C	0.77	0/2568	0.96	4/3482 (0.1%)
1	D	0.77	0/2568	0.97	11/3482 (0.3%)
All	All	0.81	1/10272 (0.0%)	0.99	36/13928 (0.3%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	PRO	CA-C	7.93	1.57	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	VAL	CB-CA-C	-8.27	97.76	110.50
1	B	2	LEU	N-CA-C	-7.60	104.51	114.31
1	A	81	VAL	CB-CA-C	-7.57	98.59	110.69
1	B	190	VAL	CB-CA-C	-7.08	101.20	110.84
1	B	160	SER	CB-CA-C	-6.90	107.84	117.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	290	TYR	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	2508	0	2449	54	0
1	B	2508	0	2449	96	0
1	C	2508	0	2449	98	0
1	D	2508	0	2449	99	0
2	A	14	0	17	3	0
2	B	14	0	17	5	0
2	C	14	0	17	6	0
2	D	14	0	17	3	0
3	A	165	0	0	7	0
3	B	180	0	0	2	0
3	C	108	0	0	8	0
3	D	108	0	0	3	0
All	All	10649	0	9864	323	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 17.

The worst 5 of 323 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:D:41:GLU:HG2	1:D:96:GLU:HB2	1.23	1.16
1:C:174:ARG:HG2	1:C:174:ARG:HH11	1.14	1.10
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.22	1.02
1:D:263:VAL:HG12	1:D:267:MET:HE3	1.42	1.00
1:D:122:PRO:HG3	1:D:221:GLN:HE21	1.23	1.00

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	309/311 (99%)	293 (95%)	15 (5%)	1 (0%)	36	42
1	B	309/311 (99%)	293 (95%)	15 (5%)	1 (0%)	36	42
1	C	309/311 (99%)	288 (93%)	18 (6%)	3 (1%)	12	11
1	D	309/311 (99%)	283 (92%)	24 (8%)	2 (1%)	21	23
All	All	1236/1244 (99%)	1157 (94%)	72 (6%)	7 (1%)	21	23

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	209	ILE
1	B	209	ILE
1	D	209	ILE
1	A	5	PRO
1	C	3	ASP

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	266/266 (100%)	257 (97%)	9 (3%)	32	44
1	B	266/266 (100%)	253 (95%)	13 (5%)	22	29
1	C	266/266 (100%)	251 (94%)	15 (6%)	19	24
1	D	266/266 (100%)	249 (94%)	17 (6%)	16	19
All	All	1064/1064 (100%)	1010 (95%)	54 (5%)	21	27

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	149	ILE
1	C	219	SER
1	D	212	GLN
1	C	160	SER
1	C	208	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	221	GLN
1	D	303	GLN
1	D	266	GLN
1	B	289	ASN
1	D	212	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
2	EPE	D	455	1	11,14,15	1.72	2 (18%)	15,17,20	1.22	1 (6%)
2	EPE	B	455	1	11,14,15	1.36	1 (9%)	15,17,20	1.58	1 (6%)
2	EPE	A	455	1	11,14,15	1.32	1 (9%)	15,17,20	1.56	1 (6%)
2	EPE	C	455	1	11,14,15	1.14	1 (9%)	15,17,20	1.61	2 (13%)

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
2	EPE	D	455	1	-	2/8/18/19	0/1/1/1
2	EPE	B	455	1	-	2/8/18/19	0/1/1/1
2	EPE	A	455	1	-	3/8/18/19	0/1/1/1
2	EPE	C	455	1	-	2/8/18/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	455	EPE	C7-N4	3.62	1.55	1.47
2	B	455	EPE	C7-N4	3.17	1.54	1.47
2	D	455	EPE	C9-N1	3.01	1.54	1.47
2	A	455	EPE	C7-N4	2.89	1.54	1.47
2	C	455	EPE	C7-N4	2.63	1.53	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	455	EPE	O1S-S-C10	5.33	115.29	105.54
2	B	455	EPE	O1S-S-C10	5.05	114.79	105.54
2	C	455	EPE	O1S-S-C10	4.45	113.69	105.54
2	D	455	EPE	O1S-S-C10	3.41	111.77	105.54
2	C	455	EPE	C10-C9-N1	-3.09	106.04	113.17

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	455	EPE	C9-C10-S-O1S

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Mol	Chain	Res	Type	Atoms
2	A	455	EPE	C9-C10-S-O2S
2	B	455	EPE	C9-C10-S-O1S
2	B	455	EPE	C9-C10-S-O2S
2	C	455	EPE	C9-C10-S-O1S

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	455	EPE	3	0
2	B	455	EPE	5	0
2	A	455	EPE	3	0
2	C	455	EPE	6	0

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	309/311 (99%)	-1.52	0 100 100	16, 34, 53, 60	9 (2%)
1	B	308/311 (99%)	-1.45	0 100 100	22, 36, 57, 74	5 (1%)
1	C	307/311 (98%)	-1.34	0 100 100	26, 44, 63, 82	11 (3%)
1	D	311/311 (100%)	-1.31	0 100 100	19, 46, 65, 80	13 (4%)
All	All	1235/1244 (99%)	-1.40	0 100 100	16, 40, 61, 82	38 (3%)

There are no RSRZ outliers to report.

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 oligosaccharides 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
2	EPE	D	455	14/15	0.98	0.04	60,67,67,67	3
2	EPE	B	455	14/15	0.99	0.05	55,60,61,61	3
2	EPE	C	455	14/15	0.99	0.05	60,65,65,65	3
2	EPE	A	455	14/15	0.99	0.04	54,56,58,58	3

6.5 Other polymers [i](#)

There are no such residues in this entry.