



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 01:38 PM EDT

PDB ID : 6GFI  
Title : Structure of Human Mesotrypsin in complex with APPI variant T11V/M17R/I18F/F34V  
Authors : Shahar, A.; Cohen, I.; Radisky, E.; Papo, N.; Naftaly, S.  
Deposited on : 2018-04-30  
Resolution : 2.30 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

<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>.

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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	:	2.37.1
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)	:	2.37.1

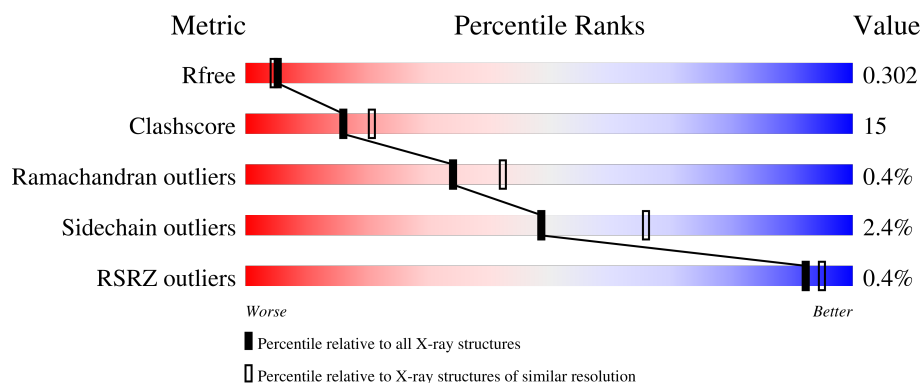
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	224	
1	B	224	
2	C	81	
2	E	81	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4273 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 PRSS3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	1	0
			1706	1073	295	326	12			
1	B	224	Total	C	N	O	S	0	0	0
			1700	1070	294	324	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	SER	conflict	UNP Q8N2U3
B	195	ALA	SER	conflict	UNP Q8N2U3

- Molecule 2 is a protein called Amyloid-beta A4 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	56	Total	C	N	O	S	0	0	0
			425	263	74	81	7			
2	C	56	Total	C	N	O	S	0	0	0
			426	263	74	82	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	TYR	-	expression tag	UNP P05067
E	-8	VAL	-	expression tag	UNP P05067
E	-7	ASP	-	expression tag	UNP P05067
E	-6	TYR	-	expression tag	UNP P05067
E	-5	LYS	-	expression tag	UNP P05067
E	-4	ASP	-	expression tag	UNP P05067
E	-3	ASP	-	expression tag	UNP P05067
E	-2	ASP	-	expression tag	UNP P05067
E	-1	ASP	-	expression tag	UNP P05067
E	0	LYS	-	expression tag	UNP P05067

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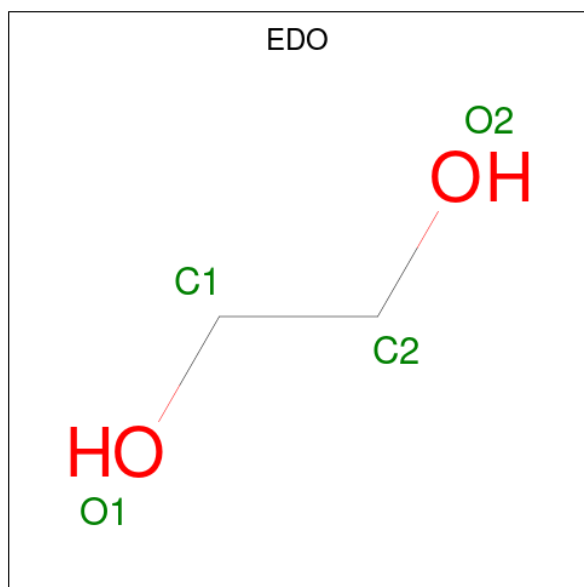
Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLU	-	expression tag	UNP P05067
E	2	VAL	-	expression tag	UNP P05067
E	3	GLU	-	expression tag	UNP P05067
E	4	VAL	-	expression tag	UNP P05067
E	5	CYS	-	expression tag	UNP P05067
E	6	SER	-	expression tag	UNP P05067
E	7	GLU	-	expression tag	UNP P05067
E	11	VAL	THR	engineered mutation	UNP P05067
E	17	ARG	MET	conflict	UNP P05067
E	18	PHE	ILE	conflict	UNP P05067
E	34	VAL	PHE	conflict	UNP P05067
E	61	ARG	-	expression tag	UNP P05067
E	62	HIS	-	expression tag	UNP P05067
E	63	HIS	-	expression tag	UNP P05067
E	64	HIS	-	expression tag	UNP P05067
E	65	HIS	-	expression tag	UNP P05067
E	66	HIS	-	expression tag	UNP P05067
E	67	HIS	-	expression tag	UNP P05067
E	68	ALA	-	expression tag	UNP P05067
E	69	ALA	-	expression tag	UNP P05067
E	70	ALA	-	expression tag	UNP P05067
E	71	ASN	-	expression tag	UNP P05067
C	-9	TYR	-	expression tag	UNP P05067
C	-8	VAL	-	expression tag	UNP P05067
C	-7	ASP	-	expression tag	UNP P05067
C	-6	TYR	-	expression tag	UNP P05067
C	-5	LYS	-	expression tag	UNP P05067
C	-4	ASP	-	expression tag	UNP P05067
C	-3	ASP	-	expression tag	UNP P05067
C	-2	ASP	-	expression tag	UNP P05067
C	-1	ASP	-	expression tag	UNP P05067
C	0	LYS	-	expression tag	UNP P05067
C	1	GLU	-	expression tag	UNP P05067
C	2	VAL	-	expression tag	UNP P05067
C	3	GLU	-	expression tag	UNP P05067
C	4	VAL	-	expression tag	UNP P05067
C	5	CYS	-	expression tag	UNP P05067
C	6	SER	-	expression tag	UNP P05067
C	7	GLU	-	expression tag	UNP P05067
C	11	VAL	THR	engineered mutation	UNP P05067
C	17	ARG	MET	conflict	UNP P05067
C	18	PHE	ILE	conflict	UNP P05067

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Chain	Residue	Modelled	Actual	Comment	Reference
C	34	VAL	PHE	conflict	UNP P05067
C	61	ARG	-	expression tag	UNP P05067
C	62	HIS	-	expression tag	UNP P05067
C	63	HIS	-	expression tag	UNP P05067
C	64	HIS	-	expression tag	UNP P05067
C	65	HIS	-	expression tag	UNP P05067
C	66	HIS	-	expression tag	UNP P05067
C	67	HIS	-	expression tag	UNP P05067
C	68	ALA	-	expression tag	UNP P05067
C	69	ALA	-	expression tag	UNP P05067
C	70	ALA	-	expression tag	UNP P05067
C	71	ASN	-	expression tag	UNP P05067

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

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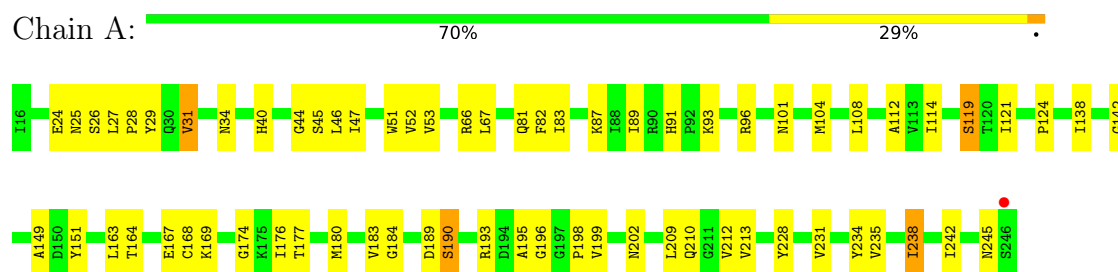
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total	O	0	0
			8	8		
4	C	2	Total	O	0	0
			2	2		

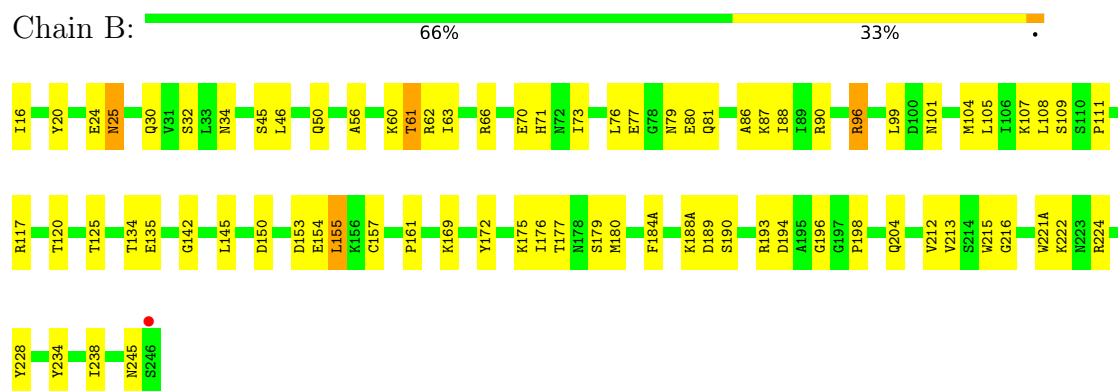
### 3 Residue-property plots [i](#)

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.

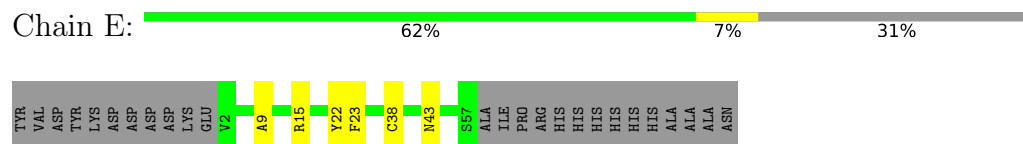
#### • Molecule 1: PRSS3 protein



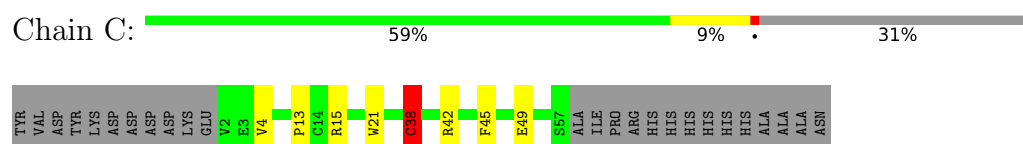
#### • Molecule 1: PRSS3 protein



#### • Molecule 2: Amyloid-beta A4 protein



#### • Molecule 2: Amyloid-beta A4 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.22Å 53.22Å 237.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.09 – 2.30 46.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.09-2.30) 92.5 (46.09-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.07 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.245 , 0.301 0.246 , 0.302	Depositor DCC
$R_{free}$ test set	1978 reflections (5.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.1	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l 0.449 for h,-h-k,-l 0.075 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 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: EDO

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	0/1745	0.73	1/2373 (0.0%)
1	B	0.45	0/1739	0.74	1/2365 (0.0%)
2	C	0.53	1/436 (0.2%)	0.67	0/588
2	E	0.56	0/435	0.67	0/587
All	All	0.48	1/4355 (0.0%)	0.72	2/5913 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	38	CYS	CB-SG	-5.84	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ILE	CG1-CB-CG2	-5.91	98.40	111.40
1	B	155	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	24	GLU	Peptide

## 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	1706	0	1656	59	0
1	B	1700	0	1652	58	0
2	C	426	0	374	8	0
2	E	425	0	373	5	0
3	A	4	0	6	0	0
4	A	1	0	0	0	0
4	B	8	0	0	1	0
4	C	2	0	0	0	0
4	E	1	0	0	0	0
All	All	4273	0	4061	121	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 15.

The worst 5 of 121 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:121:ILE:HD12	1:A:209:LEU:HB2	1.34	1.08
1:A:202:ASN:HD21	1:B:135:GLU:H	1.05	0.93
1:B:224:ARG:NH1	4:B:301:HOH:O	2.03	0.91
2:E:23:PHE:H	2:E:43:ASN:HD21	1.18	0.89
1:B:177:THR:HG23	1:B:179:SER:H	1.46	0.80

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	223/224 (100%)	211 (95%)	12 (5%)	0	100	100
1	B	222/224 (99%)	207 (93%)	13 (6%)	2 (1%)	17	20
2	C	54/81 (67%)	52 (96%)	2 (4%)	0	100	100
2	E	54/81 (67%)	51 (94%)	3 (6%)	0	100	100
All	All	553/610 (91%)	521 (94%)	30 (5%)	2 (0%)	34	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	ASN
1	B	61	THR

### 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	186/185 (100%)	180 (97%)	6 (3%)	39	54
1	B	185/185 (100%)	181 (98%)	4 (2%)	52	69
2	C	44/66 (67%)	43 (98%)	1 (2%)	50	67
2	E	43/66 (65%)	42 (98%)	1 (2%)	50	67
All	All	458/502 (91%)	446 (97%)	12 (3%)	49	63

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	76	LEU
1	B	96	ARG
2	C	38	CYS
1	B	169	LYS
1	A	190[A]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	GLN
1	B	34	ASN
1	B	204	GLN
1	B	40	HIS
2	E	43	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
3	EDO	A	301	-	3,3,3	0.57	0	2,2,2	0.23	0

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
3	EDO	A	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	EDO	O1-C1-C2-O2

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](#)

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, 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	224/224 (100%)	-0.05	1 (0%) 92 95	59, 81, 106, 112	0
1	B	224/224 (100%)	-0.05	1 (0%) 92 95	57, 82, 104, 123	0
2	C	56/81 (69%)	-0.02	0 100 100	56, 75, 102, 126	0
2	E	56/81 (69%)	-0.13	0 100 100	60, 77, 102, 126	0
All	All	560/610 (91%)	-0.05	2 (0%) 92 95	56, 81, 105, 126	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	SER	3.4
1	B	246	SER	3.3

### 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 monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	301	4/4	0.89	0.12	76,78,80,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.