



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 09:15 AM EDT

PDB ID : 2EWP  
Title : Crystal structure of Estrogen Related Receptor-3 (ERR-gamma) ligand binding domain with tamoxifen analog GSK5182  
Authors : Nolte, R.T.  
Deposited on : unknown  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

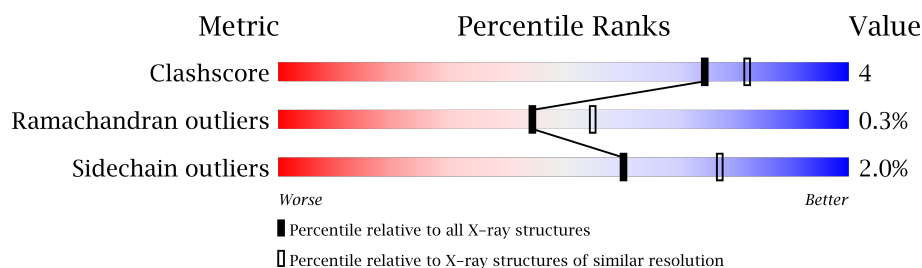
# 1 Overall quality at a glance

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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	226	
1	B	226	
1	C	226	
1	D	226	
1	E	226	

## 2 Entry composition [i](#)

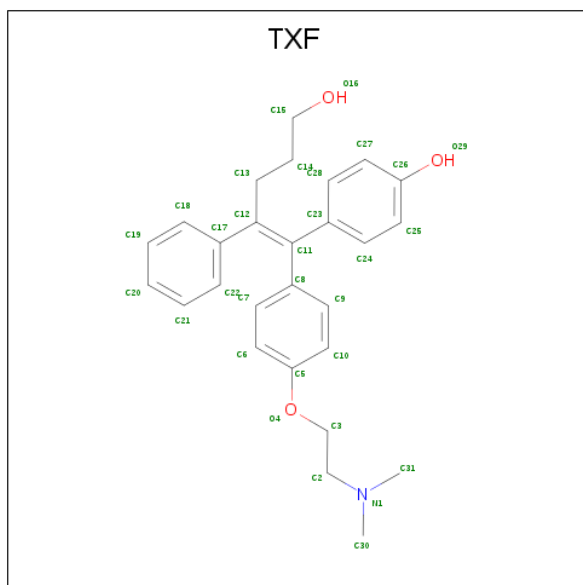
There are 3 unique types of molecules in this entry. The entry contains 9573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Estrogen-related receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	8	0
			1842	1179	296	354	13			
1	B	224	Total	C	N	O	S	0	10	0
			1861	1188	301	359	13			
1	C	223	Total	C	N	O	S	0	4	0
			1804	1155	290	346	13			
1	D	221	Total	C	N	O	S	0	6	0
			1809	1158	293	345	13			
1	E	214	Total	C	N	O	S	0	2	0
			1690	1085	268	326	11			

- Molecule 2 is (Z)-4-(1-{4-[2-(DIMETHYLAMINO)ETHOXY]PHENYL}-5-HYDROXY-2-PHENYLPENT-1-ENYL)PHENOL (three-letter code: TXF) (formula: C<sub>27</sub>H<sub>31</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	27	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			31	27	1	3		
2	C	1	Total	C	N	O	0	0
			31	27	1	3		
2	D	1	Total	C	N	O	0	0
			31	27	1	3		
2	E	1	Total	C	N	O	0	0
			31	27	1	3		

- Molecule 3 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total	O	0	0
			125	125		
3	B	104	Total	O	0	0
			104	104		
3	C	78	Total	O	0	0
			78	78		
3	D	77	Total	O	0	0
			77	77		
3	E	28	Total	O	0	0
			28	28		

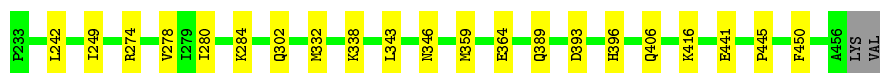
### 3 Residue-property plots [i](#)

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.

Note EDS was not executed.

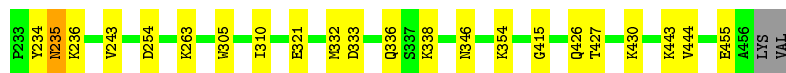
- Molecule 1: Estrogen-related receptor gamma

Chain A: 




- Molecule 1: Estrogen-related receptor gamma

Chain B: 




- Molecule 1: Estrogen-related receptor gamma

Chain C: 




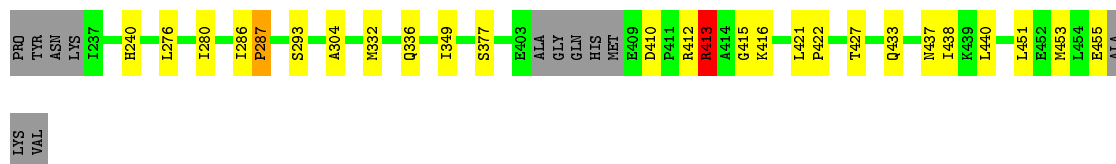
- Molecule 1: Estrogen-related receptor gamma

Chain D: 



- Molecule 1: Estrogen-related receptor gamma

Chain E: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.88Å 75.78Å 185.09Å 90.00° 104.84° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30	Depositor
% Data completeness (in resolution range)	87.5 (19.94-2.30)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.187 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.50	0/1874	0.60	1/2534 (0.0%)
1	B	0.50	0/1894	0.60	1/2561 (0.0%)
1	C	0.50	0/1835	0.60	0/2482
1	D	0.48	0/1839	0.57	0/2483
1	E	0.40	0/1718	0.55	1/2330 (0.0%)
All	All	0.48	0/9160	0.58	3/12390 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	ASN	N-CA-C	8.18	133.08	111.00
1	A	274	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	E	413	ARG	NE-CZ-NH1	6.13	123.36	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	234	TYR	Peptide

## 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	1842	0	1857	18	0
1	B	1861	0	1863	9	1
1	C	1804	0	1820	14	0
1	D	1809	0	1841	10	0
1	E	1690	0	1684	19	0
2	A	31	0	31	1	0
2	B	31	0	30	1	0
2	C	31	0	31	0	0
2	D	31	0	30	0	0
2	E	31	0	30	2	0
3	A	125	0	0	4	0
3	B	104	0	0	1	0
3	C	78	0	0	3	0
3	D	77	0	0	0	1
3	E	28	0	0	1	0
All	All	9573	0	9217	68	1

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 4.

All (68) 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:332:MET:CE	1:A:346:ASN:ND2	2.52	0.72
1:E:413:ARG:HG3	1:E:413:ARG:HH11	1.57	0.69
1:C:249:ILE:HD11	1:C:278:VAL:HG21	1.77	0.66
1:A:332:MET:HE1	1:A:346:ASN:HD21	1.63	0.64
1:C:333:ASP:H	1:C:336:GLN:HE21	1.47	0.62
1:D:310:ILE:HD13	1:D:427:THR:HG22	1.82	0.62
1:A:389[B]:GLN:NE2	1:A:393[B]:ASP:OD1	2.31	0.62
1:B:332:MET:CE	1:B:346:ASN:HD21	2.14	0.61
1:E:332:MET:HA	1:E:336:GLN:NE2	2.18	0.58
1:C:333:ASP:H	1:C:336:GLN:NE2	2.01	0.58
1:E:440:LEU:O	2:E:505:TXF:H313	2.05	0.57
1:E:332:MET:HA	1:E:336:GLN:HE21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ASP:H	1:B:336:GLN:HE21	1.54	0.56
1:D:333:ASP:H	1:D:336:GLN:HE21	1.52	0.56
1:D:352:LEU:HD22	1:D:356:TYR:CE2	2.41	0.55
1:B:332:MET:CE	1:B:346:ASN:ND2	2.70	0.55
1:A:332:MET:CE	1:A:346:ASN:HD21	2.18	0.52
1:C:298[B]:MET:HG3	3:C:581:HOH:O	2.09	0.52
1:E:413:ARG:HH11	1:E:413:ARG:CG	2.24	0.50
1:E:240:HIS:ND1	1:E:240:HIS:O	2.44	0.50
1:A:441:GLU:HA	2:A:501:TXF:H302	1.94	0.49
1:A:389[B]:GLN:HE21	1:A:393[B]:ASP:CG	2.17	0.47
1:A:359:MET:HE3	1:A:416:LYS:HB3	1.96	0.47
1:D:261:ASP:OD1	1:D:261:ASP:N	2.46	0.47
1:B:426:GLN:HE21	1:B:430:LYS:NZ	2.13	0.47
1:E:349:ILE:HG12	1:E:427:THR:HG21	1.96	0.47
1:A:280:ILE:HD11	1:A:450:PHE:CD1	2.50	0.47
1:A:445:PRO:HA	3:A:597:HOH:O	2.15	0.46
1:A:332:MET:CE	1:A:346:ASN:HD22	2.26	0.46
1:A:406:GLN:HB3	3:A:612:HOH:O	2.15	0.46
1:C:433:GLN:NE2	3:C:530:HOH:O	2.47	0.46
1:A:332:MET:HE1	1:A:346:ASN:ND2	2.23	0.46
1:B:254:ASP:O	1:B:263:LYS:NZ	2.49	0.46
1:C:389:GLN:OE1	1:D:355:LYS:NZ	2.49	0.46
1:B:310:ILE:HD13	1:B:427:THR:HG22	1.98	0.46
1:C:429:THR:HG23	1:D:430[A]:LYS:HE3	1.97	0.46
1:E:412:ARG:O	1:E:415:GLY:N	2.37	0.46
1:C:298[B]:MET:HG2	1:C:454:LEU:CD1	2.46	0.45
1:A:242:LEU:HD11	1:A:364:GLU:HG3	1.99	0.45
1:E:438:ILE:HG13	1:E:440:LEU:HG	1.98	0.44
1:A:338:LYS:HG2	1:A:343:LEU:HD22	2.00	0.44
1:C:254:ASP:CG	1:C:256:THR:HG1	2.21	0.44
1:C:332:MET:HA	1:C:336:GLN:NE2	2.33	0.44
1:E:304:ALA:HB2	1:E:377:SER:HB3	2.00	0.43
1:A:249:ILE:HD11	1:A:278:VAL:HG21	1.99	0.43
1:B:321[A]:GLU:HG2	3:B:601:HOH:O	2.17	0.43
1:E:286:ILE:HG23	1:E:287:PRO:HD2	2.01	0.43
1:A:396:HIS:CE1	1:B:415:GLY:HA3	2.53	0.43
1:C:359:MET:HE3	1:C:416:LYS:HB3	2.01	0.43
1:A:441:GLU:HG3	3:A:597:HOH:O	2.18	0.43
1:C:370:LYS:NZ	3:C:563:HOH:O	2.52	0.43
1:A:406:GLN:OE1	3:A:612:HOH:O	2.21	0.42
1:C:348:ALA:O	1:C:351:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:HIS:HB2	3:E:530:HOH:O	2.19	0.42
1:E:421:LEU:N	1:E:422:PRO:CD	2.82	0.42
1:D:235:ASN:HB3	1:D:238:VAL:HB	2.01	0.42
2:E:505:TXF:C24	2:E:505:TXF:H132	2.49	0.42
1:E:276:LEU:O	1:E:280:ILE:HD12	2.20	0.41
1:C:421:LEU:N	1:C:422:PRO:CD	2.84	0.41
1:E:410:ASP:O	1:E:413:ARG:HB2	2.19	0.41
1:D:310:ILE:HG21	1:D:427:THR:HG21	2.02	0.41
1:D:242:LEU:HD11	1:D:364:GLU:HG3	2.03	0.41
1:E:349:ILE:CG1	1:E:427:THR:HG21	2.51	0.41
1:B:305:TRP:HZ3	2:B:502:TXF:H10	1.86	0.41
1:D:432:VAL:O	1:D:435:PHE:HB3	2.21	0.40
1:E:280:ILE:CD1	1:E:453:MET:SD	3.10	0.40
1:E:451:LEU:O	1:E:455:GLU:HG2	2.21	0.40
1:E:433:GLN:NE2	1:E:437:ASN:HD21	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:GLU:OE2	3:D:548:HOH:O[1_545]	2.17	0.03

## 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	230/226 (102%)	226 (98%)	4 (2%)	0	100	100
1	B	232/226 (103%)	227 (98%)	4 (2%)	1 (0%)	38	47
1	C	225/226 (100%)	218 (97%)	7 (3%)	0	100	100
1	D	225/226 (100%)	222 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	212/226 (94%)	205 (97%)	5 (2%)	2 (1%)	20	23
All	All	1124/1130 (100%)	1098 (98%)	23 (2%)	3 (0%)	44	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	ASN
1	E	287	PRO
1	E	413	ARG

### 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	205/200 (102%)	203 (99%)	2 (1%)	80	90
1	B	207/200 (104%)	201 (97%)	6 (3%)	48	64
1	C	200/200 (100%)	198 (99%)	2 (1%)	80	90
1	D	202/200 (101%)	195 (96%)	7 (4%)	41	56
1	E	185/200 (92%)	182 (98%)	3 (2%)	68	82
All	All	999/1000 (100%)	979 (98%)	20 (2%)	60	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	LYS
1	A	302	GLN
1	B	236	LYS
1	B	243	VAL
1	B	338	LYS
1	B	354	LYS
1	B	443	LYS
1	B	444	VAL
1	C	345	LEU

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Mol	Chain	Res	Type
1	C	455	GLU
1	D	236[A]	LYS
1	D	236[B]	LYS
1	D	259	ASP
1	D	261	ASP
1	D	270	ASP
1	D	338	LYS
1	D	352	LEU
1	E	293	SER
1	E	413	ARG
1	E	416	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	ASN
1	A	396	HIS
1	A	437	ASN
1	B	285	HIS
1	B	336	GLN
1	B	346	ASN
1	B	396	HIS
1	B	426	GLN
1	C	285	HIS
1	C	336	GLN
1	C	400	GLN
1	C	433	GLN
1	C	437	ASN
1	D	336	GLN
1	D	396	HIS
1	D	400	GLN
1	D	433	GLN
1	D	437	ASN
1	E	336	GLN
1	E	433	GLN
1	E	437	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	TXF	A	501	-	33,33,33	0.59	0	42,43,43	1.03	2 (4%)
2	TXF	B	502	-	33,33,33	0.54	0	42,43,43	1.21	5 (11%)
2	TXF	C	503	-	33,33,33	0.69	0	42,43,43	0.95	2 (4%)
2	TXF	D	504	-	33,33,33	0.65	0	42,43,43	1.08	3 (7%)
2	TXF	E	505	-	33,33,33	0.57	0	42,43,43	0.81	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
2	TXF	A	501	-	-	0/26/26/26	0/3/3/3
2	TXF	B	502	-	-	0/26/26/26	0/3/3/3
2	TXF	C	503	-	-	0/26/26/26	0/3/3/3
2	TXF	D	504	-	-	0/26/26/26	0/3/3/3
2	TXF	E	505	-	-	0/26/26/26	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	502	TXF	C9-C8-C11	-3.01	116.53	120.91
2	B	502	TXF	C18-C17-C12	-2.83	117.12	121.01
2	B	502	TXF	C8-C11-C23	-2.63	110.46	115.59
2	D	504	TXF	C8-C11-C23	-2.48	110.74	115.59
2	C	503	TXF	C18-C17-C12	-2.22	117.95	121.01
2	B	502	TXF	C14-C13-C12	-2.19	109.62	113.31
2	B	502	TXF	C23-C11-C12	2.15	125.64	122.88
2	C	503	TXF	C3-O4-C5	2.28	123.94	117.90
2	A	501	TXF	C23-C11-C12	2.46	126.03	122.88
2	D	504	TXF	C23-C11-C12	2.93	126.64	122.88
2	A	501	TXF	C3-O4-C5	3.33	126.72	117.90
2	D	504	TXF	C3-O4-C5	3.42	126.97	117.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	TXF	1	0
2	B	502	TXF	1	0
2	E	505	TXF	2	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.