



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:06 AM UTC

PDB ID : 4XES / pdb\_00004xes  
Title : Structure of active-like neurotensin receptor  
Authors : Krumm, B.E.; White, J.F.; Shah, P.; Grisshammer, R.  
Deposited on : 2014-12-24  
Resolution : 2.60 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)

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<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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

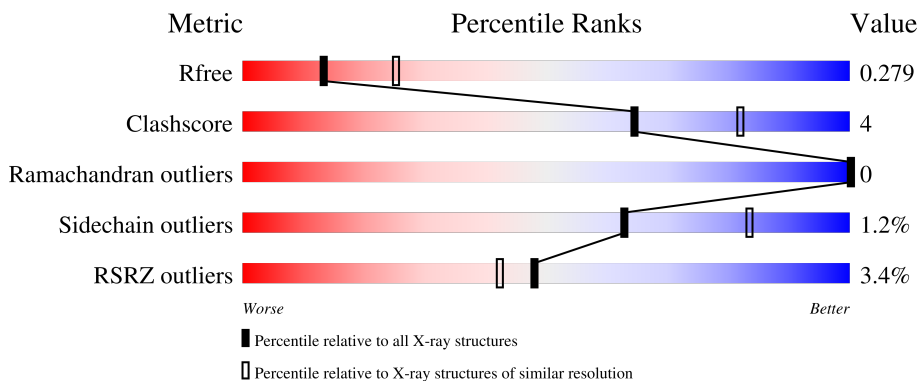
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	541	
2	B	6	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3923 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 Neurotensin receptor type 1, Endolysin chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	471	3714	2409	634	652	19	164	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ASP	-	expression tag	UNP P20789
A	34	TYR	-	expression tag	UNP P20789
A	35	LYS	-	expression tag	UNP P20789
A	36	ASP	-	expression tag	UNP P20789
A	37	ASP	-	expression tag	UNP P20789
A	38	ASP	-	expression tag	UNP P20789
A	39	ASP	-	expression tag	UNP P20789
A	40	ALA	-	expression tag	UNP P20789
A	41	THR	-	expression tag	UNP P20789
A	42	SER	-	expression tag	UNP P20789
A	86	LEU	ALA	engineered mutation	UNP P20789
A	166	ALA	GLU	engineered mutation	UNP P20789
A	215	ALA	GLY	engineered mutation	UNP P20789
A	360	ALA	VAL	engineered mutation	UNP P20789
A	989	ALA	-	linker	UNP P20789
A	990	HIS	-	linker	UNP P20789
A	991	HIS	-	linker	UNP P20789
A	992	HIS	-	linker	UNP P20789
A	993	HIS	-	linker	UNP P20789
A	994	HIS	-	linker	UNP P20789
A	995	HIS	-	linker	UNP P20789
A	996	HIS	-	linker	UNP P20789
A	997	HIS	-	linker	UNP P20789
A	998	HIS	-	linker	UNP P20789
A	999	HIS	-	linker	UNP P20789
A	1000	GLY	-	linker	UNP P20789
A	1001	GLY	-	linker	UNP P20789

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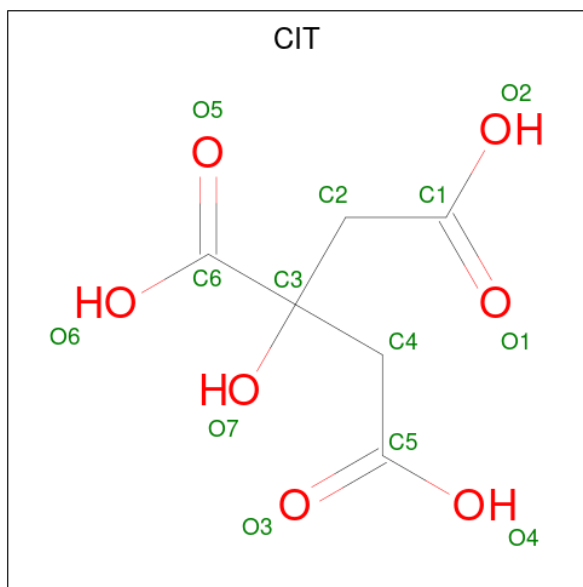
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1012	GLY	ARG	conflict	UNP P00720
A	1054	THR	CYS	conflict	UNP P00720
A	1097	ALA	CYS	conflict	UNP P00720
A	1122	ASN	GLN	conflict	UNP P00720
A	1123	ASN	GLN	conflict	UNP P00720
A	1137	ARG	ILE	conflict	UNP P00720
A	1162	GLY	-	expression tag	UNP P00720
A	1163	SER	-	expression tag	UNP P00720
A	1164	GLY	-	expression tag	UNP P00720
A	1165	SER	-	expression tag	UNP P00720

- Molecule 2 is a protein called Neurotensin/neuromedin N.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
2	B	6	58	38	12	8	0	0	0

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



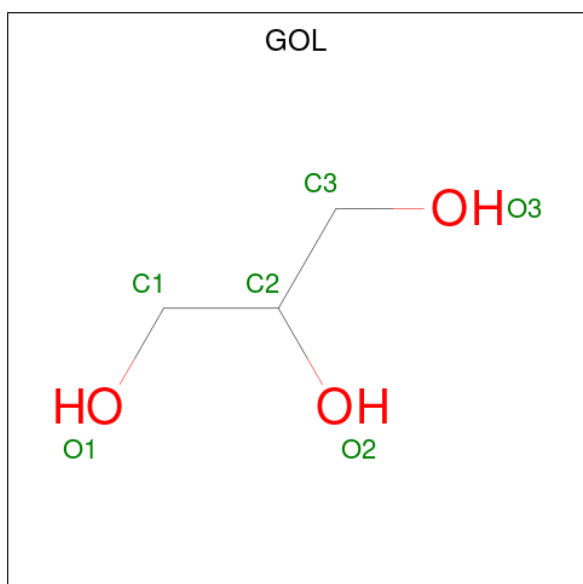
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	13	6	7	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



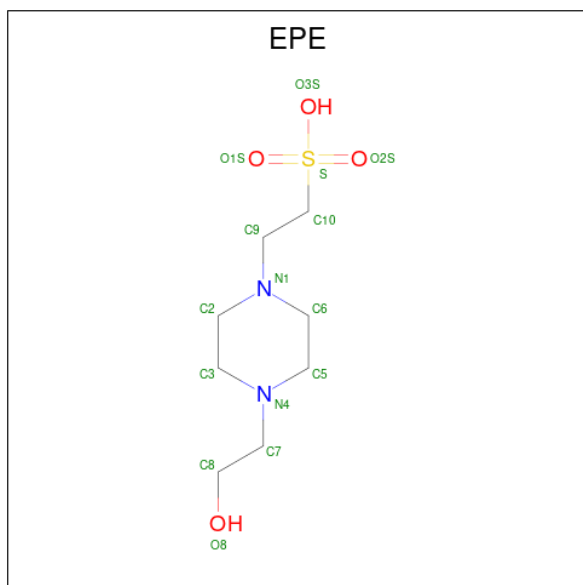
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

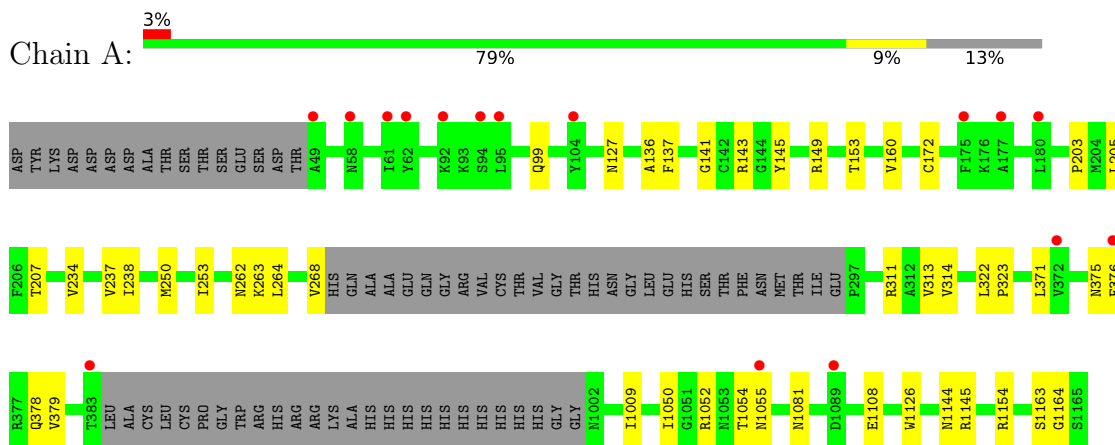
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	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: Neurotensin receptor type 1, Endolysin chimera



- Molecule 2: Neurotensin/neuromedin N



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.84Å 88.44Å 161.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.00 – 2.60 34.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.00-2.60) 99.4 (34.00-2.60)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.230 , 0.280 0.235 , 0.279	Depositor DCC
$R_{free}$ test set	1209 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.3	Xtrriage
Anisotropy	0.551	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.68	0/3797	0.86	1/5159 (0.0%)
2	B	0.62	0/59	0.87	0/77
All	All	0.68	0/3856	0.86	1/5236 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	VAL	CB-CA-C	-5.09	105.18	111.70

There are no chirality outliers.

There are no planarity outliers.

### 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	3714	0	3787	29	0
2	B	58	0	63	0	0
3	A	13	0	5	0	0
4	A	35	0	50	1	0
5	A	18	0	24	2	0
6	A	30	0	36	0	0
7	A	53	0	0	1	0
7	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3923	0	3965	29	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 4.

The worst 5 of 29 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:234:VAL:O	1:A:238:ILE:HG13	1.83	0.78
1:A:1052:ARG:HG2	1:A:1052:ARG:HH11	1.56	0.68
1:A:371:LEU:HA	7:A:1335:HOH:O	1.94	0.66
1:A:1009:ILE:HD11	1:A:1164:GLY:HA2	1.77	0.66
1:A:1052:ARG:HG2	1:A:1052:ARG:NH1	2.08	0.64

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	465/541 (86%)	443 (95%)	22 (5%)	0	100	100
2	B	4/6 (67%)	4 (100%)	0	0	100	100
All	All	469/547 (86%)	447 (95%)	22 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	400/459 (87%)	395 (99%)	5 (1%)	61	82
2	B	6/6 (100%)	6 (100%)	0	100	100
All	All	406/465 (87%)	401 (99%)	5 (1%)	63	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	153	THR
1	A	313	VAL
1	A	376	PHE
1	A	1163	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1068	ASN
1	A	1141	GLN
1	A	1144	ASN
1	A	127	ASN
1	A	82	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

11 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
5	GOL	A	1207	-	5,5,5	0.37	0	5,5,5	0.35	0
5	GOL	A	1208	-	5,5,5	0.38	0	5,5,5	0.20	0
3	CIT	A	1201	-	12,12,12	1.13	0	17,17,17	1.42	2 (11%)
4	PEG	A	1203	-	6,6,6	0.69	0	5,5,5	0.54	0
4	PEG	A	1202	-	6,6,6	0.58	0	5,5,5	0.17	0
6	EPE	A	1211	-	15,15,15	1.94	1 (6%)	19,20,20	1.09	2 (10%)
4	PEG	A	1204	-	6,6,6	0.30	0	5,5,5	0.35	0
5	GOL	A	1209	-	5,5,5	0.17	0	5,5,5	0.66	0
6	EPE	A	1210	-	15,15,15	2.14	1 (6%)	19,20,20	1.14	2 (10%)
4	PEG	A	1205	-	6,6,6	0.55	0	5,5,5	0.11	0
4	PEG	A	1206	-	6,6,6	0.66	0	5,5,5	0.56	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
5	GOL	A	1207	-	-	2/4/4/4	-
5	GOL	A	1208	-	-	3/4/4/4	-
3	CIT	A	1201	-	-	8/16/16/16	-
4	PEG	A	1203	-	-	1/4/4/4	-
4	PEG	A	1202	-	-	2/4/4/4	-
6	EPE	A	1211	-	-	5/9/19/19	0/1/1/1
4	PEG	A	1204	-	-	3/4/4/4	-
5	GOL	A	1209	-	-	1/4/4/4	-
6	EPE	A	1210	-	-	6/9/19/19	0/1/1/1
4	PEG	A	1205	-	-	2/4/4/4	-
4	PEG	A	1206	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1210	EPE	C10-S	-7.81	1.66	1.77
6	A	1211	EPE	C10-S	-7.06	1.67	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1201	CIT	O6-C6-C3	3.57	119.99	113.14
6	A	1211	EPE	O1S-S-C10	3.00	111.26	106.73
6	A	1210	EPE	O2S-S-C10	2.81	110.98	106.73
6	A	1211	EPE	O3S-S-C10	2.47	110.83	106.00
3	A	1201	CIT	O5-C6-C3	-2.24	117.76	122.09

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1207	GOL	C1-C2-C3-O3
5	A	1208	GOL	C1-C2-C3-O3
6	A	1210	EPE	C10-C9-N1-C6
6	A	1211	EPE	S-C10-C9-N1
3	A	1201	CIT	C1-C2-C3-O7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1203	PEG	1	0
5	A	1209	GOL	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 [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	471/541 (87%)	0.39	16 (3%) 48 42	29, 60, 80, 108	53 (11%)
2	B	6/6 (100%)	0.59	0 100 100	49, 52, 61, 69	0
All	All	477/547 (87%)	0.39	16 (3%) 48 42	29, 60, 80, 108	53 (11%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	PHE	3.2
1	A	104	TYR	2.9
1	A	61	ILE	2.8
1	A	95	LEU	2.8
1	A	94	SER	2.6

### 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, 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
6	EPE	A	1211	15/15	0.74	0.19	82,92,113,121	0
4	PEG	A	1206	7/7	0.82	0.22	63,64,72,74	0
5	GOL	A	1208	6/6	0.86	0.14	64,70,73,74	0
5	GOL	A	1209	6/6	0.87	0.14	56,57,64,68	0
4	PEG	A	1205	7/7	0.88	0.17	73,76,78,78	0
5	GOL	A	1207	6/6	0.89	0.12	69,73,74,77	0
4	PEG	A	1204	7/7	0.90	0.17	86,88,94,95	0
4	PEG	A	1202	7/7	0.91	0.10	58,60,62,63	0
4	PEG	A	1203	7/7	0.92	0.12	48,56,60,64	0
3	CIT	A	1201	13/13	0.92	0.08	51,56,62,62	0
6	EPE	A	1210	15/15	0.95	0.10	47,49,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.