



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2022 – 01:23 pm BST

PDB ID : 7QRV
Title : Crystal structure of NHL domain of TRIM2 (full C-terminal)
Authors : Chaikuad, A.; Zhubi, R.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2022-01-12
Resolution : 1.45 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28

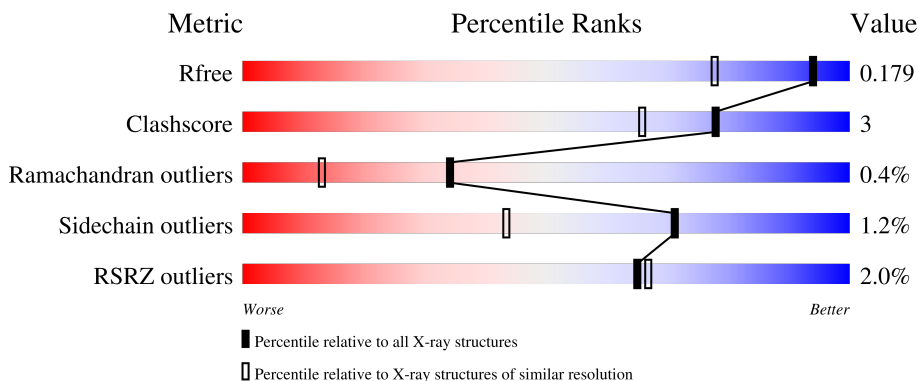
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	281	
1	B	281	
1	C	281	
1	D	281	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	D	801	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9997 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 Tripartite motif-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	278	Total 2155	C 1357	N 386	O 406	S 6	0	9	0
1	B	276	Total 2136	C 1345	N 382	O 403	S 6	0	8	0
1	C	278	Total 2161	C 1363	N 385	O 406	S 7	0	10	0
1	D	281	Total 2168	C 1362	N 387	O 412	S 7	0	8	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	464	SER	-	expression tag	UNP Q9C040
A	465	MET	-	expression tag	UNP Q9C040
B	464	SER	-	expression tag	UNP Q9C040
B	465	MET	-	expression tag	UNP Q9C040
C	464	SER	-	expression tag	UNP Q9C040
C	465	MET	-	expression tag	UNP Q9C040
D	464	SER	-	expression tag	UNP Q9C040
D	465	MET	-	expression tag	UNP Q9C040

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 8 4 4	0	1
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	348	Total O 348 348	0	0
3	B	271	Total O 271 271	0	0
3	C	313	Total O 313 313	0	0
3	D	337	Total O 337 337	0	0

3 Residue-property plots [i](#)

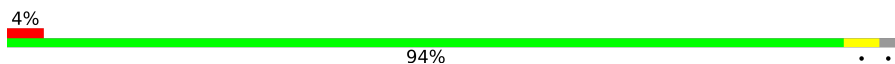
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tripartite motif-containing protein 2

Chain A: 



- Molecule 1: Tripartite motif-containing protein 2

Chain B: 



- Molecule 1: Tripartite motif-containing protein 2

Chain C: 



- Molecule 1: Tripartite motif-containing protein 2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.67Å 89.24Å 86.72Å 90.00° 106.99° 90.00°	Depositor
Resolution (Å)	45.47 – 1.45 45.43 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.47-1.45) 99.5 (45.43-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 1.45Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.152 , 0.178 0.153 , 0.179	Depositor DCC
R_{free} test set	8686 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9997	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.92 % 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 9.7472e-03. 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 [i](#)

5.1 Standard geometry [i](#)

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	0.84	0/2227	0.82	1/3004 (0.0%)
1	B	0.79	0/2204	0.79	1/2971 (0.0%)
1	C	0.83	0/2236	0.80	1/3014 (0.0%)
1	D	0.87	0/2237	0.88	3/3019 (0.1%)
All	All	0.83	0/8904	0.82	6/12008 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	615	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	C	615	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	475	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	B	615	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	D	619	ASP	CB-CG-OD2	-5.81	113.07	118.30

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	2155	0	2124	12	0
1	B	2136	0	2102	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2161	0	2136	14	0
1	D	2168	0	2123	12	0
2	A	36	0	54	4	0
2	B	16	0	24	1	0
2	C	28	0	39	5	0
2	D	28	0	40	6	0
3	A	348	0	0	4	0
3	B	271	0	0	3	0
3	C	313	0	0	8	0
3	D	337	0	0	7	0
All	All	9997	0	8642	50	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 3.

The worst 5 of 50 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:468:ILE:HD13	1:C:611:ARG:HH21	1.52	0.74
1:A:514:SER:OG	1:A:516:ASP:OD1	2.05	0.73
1:B:514:SER:OG	1:B:516:ASP:OD1	2.07	0.72
1:C:514:SER:OG	1:C:516:ASP:OD1	2.09	0.69
1:C:467:PRO:HB2	3:C:1080:H0H:O	1.93	0.69

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	285/281 (101%)	274 (96%)	10 (4%)	1 (0%)	34 13
1	B	282/281 (100%)	269 (95%)	12 (4%)	1 (0%)	34 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	286/281 (102%)	272 (95%)	13 (4%)	1 (0%)	41	18
1	D	287/281 (102%)	275 (96%)	11 (4%)	1 (0%)	41	18
All	All	1140/1124 (101%)	1090 (96%)	46 (4%)	4 (0%)	34	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	577	GLY
1	A	577	GLY
1	B	577	GLY
1	D	577	GLY

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	236/230 (103%)	234 (99%)	2 (1%)	81	62
1	B	233/230 (101%)	230 (99%)	3 (1%)	69	40
1	C	237/230 (103%)	233 (98%)	4 (2%)	60	28
1	D	238/230 (104%)	235 (99%)	3 (1%)	69	40
All	All	944/920 (103%)	932 (99%)	12 (1%)	71	40

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

Mol	Chain	Res	Type
1	C	669	PHE
1	C	694	GLN
1	D	694	GLN
1	D	563	ASP
1	B	694	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	666	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](#)

27 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	EDO	D	806	-	3,3,3	0.52	0	2,2,2	0.60	0
2	EDO	C	805	-	3,3,3	0.42	0	2,2,2	0.18	0
2	EDO	D	807	-	3,3,3	1.14	0	2,2,2	0.25	0
2	EDO	A	801	-	3,3,3	0.31	0	2,2,2	0.09	0
2	EDO	A	804	-	3,3,3	0.11	0	2,2,2	0.20	0
2	EDO	A	809	-	3,3,3	0.36	0	2,2,2	0.31	0
2	EDO	B	801	-	3,3,3	0.19	0	2,2,2	0.15	0
2	EDO	D	801	-	3,3,3	0.78	0	2,2,2	0.14	0
2	EDO	A	803	-	3,3,3	0.27	0	2,2,2	0.18	0
2	EDO	C	801	-	3,3,3	0.19	0	2,2,2	0.47	0
2	EDO	C	802	-	3,3,3	0.08	0	2,2,2	0.06	0
2	EDO	C	806[B]	-	3,3,3	1.34	0	2,2,2	0.48	0
2	EDO	C	803	-	3,3,3	0.16	0	2,2,2	0.35	0
2	EDO	B	804	-	3,3,3	0.46	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	803	-	3,3,3	0.06	0	2,2,2	0.14	0
2	EDO	D	803	-	3,3,3	0.39	0	2,2,2	0.39	0
2	EDO	C	804	-	3,3,3	1.02	0	2,2,2	0.75	0
2	EDO	D	804	-	3,3,3	0.24	0	2,2,2	0.14	0
2	EDO	A	808	-	3,3,3	0.14	0	2,2,2	0.21	0
2	EDO	C	806[A]	-	3,3,3	1.27	0	2,2,2	0.43	0
2	EDO	A	805	-	3,3,3	0.14	0	2,2,2	0.43	0
2	EDO	D	802	-	3,3,3	0.22	0	2,2,2	0.47	0
2	EDO	A	802	-	3,3,3	0.05	0	2,2,2	0.11	0
2	EDO	D	805	-	3,3,3	0.19	0	2,2,2	0.20	0
2	EDO	A	807	-	3,3,3	0.21	0	2,2,2	0.24	0
2	EDO	B	802	-	3,3,3	0.15	0	2,2,2	0.19	0
2	EDO	A	806	-	3,3,3	0.13	0	2,2,2	0.16	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	EDO	D	806	-	-	1/1/1/1	-
2	EDO	C	805	-	-	0/1/1/1	-
2	EDO	D	807	-	-	0/1/1/1	-
2	EDO	A	801	-	-	0/1/1/1	-
2	EDO	A	804	-	-	1/1/1/1	-
2	EDO	A	809	-	-	0/1/1/1	-
2	EDO	B	801	-	-	1/1/1/1	-
2	EDO	D	801	-	-	1/1/1/1	-
2	EDO	A	803	-	-	1/1/1/1	-
2	EDO	C	801	-	-	1/1/1/1	-
2	EDO	C	802	-	-	0/1/1/1	-
2	EDO	C	806[B]	-	-	1/1/1/1	-
2	EDO	C	803	-	-	0/1/1/1	-
2	EDO	B	804	-	-	0/1/1/1	-
2	EDO	B	803	-	-	0/1/1/1	-
2	EDO	D	803	-	-	1/1/1/1	-
2	EDO	C	804	-	-	1/1/1/1	-
2	EDO	D	804	-	-	0/1/1/1	-
2	EDO	A	808	-	-	1/1/1/1	-
2	EDO	C	806[A]	-	-	0/1/1/1	-
2	EDO	A	805	-	-	0/1/1/1	-
2	EDO	D	802	-	-	0/1/1/1	-
2	EDO	A	802	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	805	-	-	0/1/1/1	-
2	EDO	A	807	-	-	0/1/1/1	-
2	EDO	B	802	-	-	1/1/1/1	-
2	EDO	A	806	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	EDO	O1-C1-C2-O2
2	B	802	EDO	O1-C1-C2-O2
2	C	806[B]	EDO	O1-C1-C2-O2
2	A	802	EDO	O1-C1-C2-O2
2	A	808	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	806	EDO	1	0
2	A	804	EDO	1	0
2	A	809	EDO	1	0
2	D	801	EDO	4	0
2	A	803	EDO	1	0
2	C	806[B]	EDO	3	0
2	C	803	EDO	2	0
2	D	803	EDO	1	0
2	A	802	EDO	1	0
2	A	807	EDO	1	0
2	B	802	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	278/281 (98%)	-0.41	4 (1%) 75 76	7, 12, 23, 53	0
1	B	276/281 (98%)	-0.06	10 (3%) 42 46	10, 18, 31, 56	0
1	C	278/281 (98%)	-0.26	6 (2%) 62 65	9, 15, 29, 67	0
1	D	281/281 (100%)	-0.33	2 (0%) 87 89	8, 12, 24, 45	0
All	All	1113/1124 (99%)	-0.27	22 (1%) 65 67	7, 14, 28, 67	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	744	GLN	6.3
1	A	744	GLN	5.9
1	B	744	GLN	5.1
1	C	743	LEU	4.9
1	A	468	ILE	4.6

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 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, 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(\AA^2)	Q<0.9
2	EDO	B	802	4/4	0.70	0.19	46,47,47,49	0
2	EDO	C	804	4/4	0.76	0.17	21,25,25,26	0
2	EDO	A	803	4/4	0.80	0.21	39,39,42,45	0
2	EDO	B	801	4/4	0.83	0.16	31,34,36,42	0
2	EDO	A	802	4/4	0.83	0.16	38,41,41,42	0
2	EDO	A	809	4/4	0.83	0.19	29,29,30,33	0
2	EDO	B	803	4/4	0.84	0.13	38,40,40,42	0
2	EDO	A	806	4/4	0.84	0.18	19,23,31,32	0
2	EDO	D	804	4/4	0.84	0.18	30,34,37,40	0
2	EDO	C	805	4/4	0.85	0.13	32,33,34,46	0
2	EDO	D	803	4/4	0.88	0.14	25,27,27,31	0
2	EDO	D	805	4/4	0.88	0.11	20,24,30,30	0
2	EDO	D	806	4/4	0.88	0.13	23,25,26,29	0
2	EDO	B	804	4/4	0.89	0.18	18,23,25,32	0
2	EDO	C	802	4/4	0.89	0.08	32,33,34,40	0
2	EDO	C	806[A]	4/4	0.89	0.21	13,16,19,19	4
2	EDO	C	806[B]	4/4	0.89	0.21	10,15,17,18	4
2	EDO	C	803	4/4	0.90	0.20	14,22,25,31	0
2	EDO	D	801	4/4	0.90	0.20	19,21,25,36	0
2	EDO	C	801	4/4	0.90	0.13	28,31,32,34	0
2	EDO	D	807	4/4	0.90	0.18	20,23,26,33	0
2	EDO	A	804	4/4	0.91	0.10	34,35,38,44	0
2	EDO	A	808	4/4	0.92	0.09	35,35,36,38	0
2	EDO	A	801	4/4	0.93	0.10	22,22,22,26	0
2	EDO	D	802	4/4	0.94	0.13	12,19,21,27	0
2	EDO	A	805	4/4	0.94	0.10	12,18,20,24	0
2	EDO	A	807	4/4	0.94	0.14	22,31,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.