



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:28 AM UTC

PDB ID : 2Q4M / pdb_00002q4m
Title : Ensemble refinement of the crystal structure of protein from Arabidopsis thaliana At5g01750
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

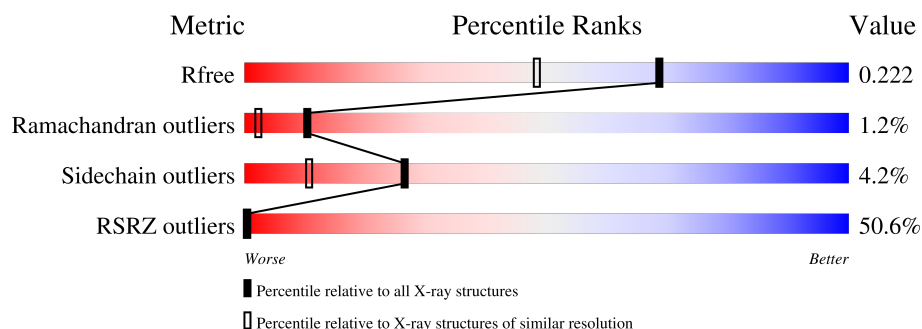
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	1-A	217	37% 71% 25%
1	10-A	217	71% 25%
1	11-A	217	71% 25%
1	12-A	217	72% 25%
1	13-A	217	71% 25%
1	14-A	217	72% 25%
1	15-A	217	70% 5% 25%

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Mol	Chain	Length	Quality of chain
1	16-A	217	 71% • 25%
1	2-A	217	 71% • 25%
1	3-A	217	 71% • 25%
1	4-A	217	 71% • 25%
1	5-A	217	 71% • 25%
1	6-A	217	 71% • 25%
1	7-A	217	 72% • 25%
1	8-A	217	 72% • 25%
1	9-A	217	 71% • 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22688 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.

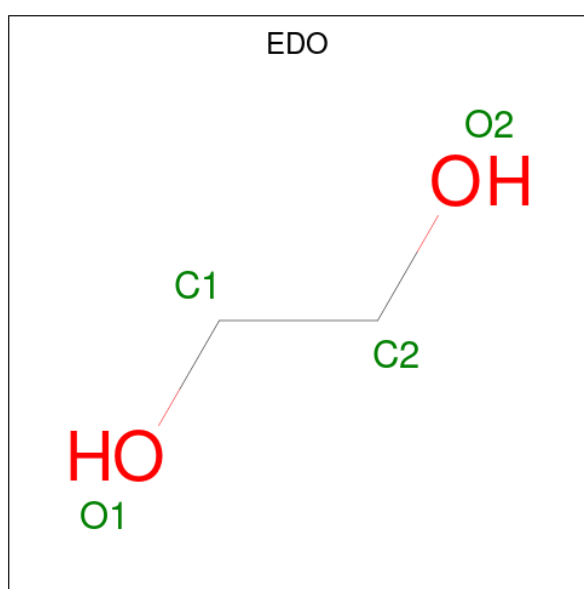
- Molecule 1 is a protein called Protein At5g01750.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	2-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	3-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	4-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	5-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	6-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	7-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	8-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	9-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	10-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	11-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	12-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	13-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	14-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	15-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			
1	16-A	162	Total	C	N	O	S	Se	0	0	0
			1287	820	228	234	3	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9LZX1
A	40	MSE	MET	modified residue	UNP Q9LZX1
A	46	MSE	MET	modified residue	UNP Q9LZX1
A	47	MSE	MET	modified residue	UNP Q9LZX1
A	95	MSE	MET	modified residue	UNP Q9LZX1
A	98	MSE	MET	modified residue	UNP Q9LZX1
A	124	MSE	MET	modified residue	UNP Q9LZX1
A	171	MSE	MET	modified residue	UNP Q9LZX1

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	1	Total C O 4 2 2	0	0
2	2-A	1	Total C O 4 2 2	0	0
2	3-A	1	Total C O 4 2 2	0	0
2	4-A	1	Total C O 4 2 2	0	0
2	5-A	1	Total C O 4 2 2	0	0
2	6-A	1	Total C O 4 2 2	0	0
2	7-A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	8-A	1	Total C O 4 2 2	0	0
2	9-A	1	Total C O 4 2 2	0	0
2	10-A	1	Total C O 4 2 2	0	0
2	11-A	1	Total C O 4 2 2	0	0
2	12-A	1	Total C O 4 2 2	0	0
2	13-A	1	Total C O 4 2 2	0	0
2	14-A	1	Total C O 4 2 2	0	0
2	15-A	1	Total C O 4 2 2	0	0
2	16-A	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	127	Total O 127 127	0	0
3	2-A	127	Total O 127 127	0	0
3	3-A	127	Total O 127 127	0	0
3	4-A	127	Total O 127 127	0	0
3	5-A	127	Total O 127 127	0	0
3	6-A	127	Total O 127 127	0	0
3	7-A	127	Total O 127 127	0	0
3	8-A	127	Total O 127 127	0	0
3	9-A	127	Total O 127 127	0	0
3	10-A	127	Total O 127 127	0	0

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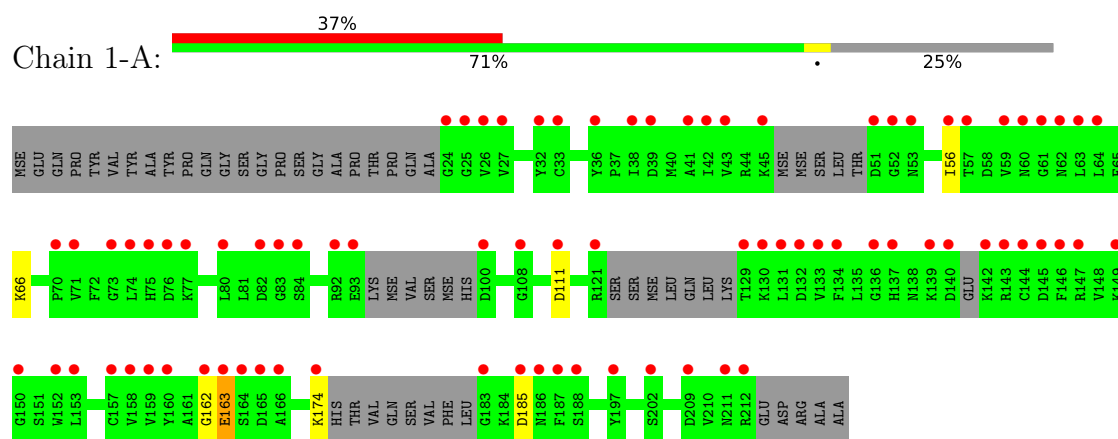
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	11-A	127	Total 127	O 127	0	0
3	12-A	127	Total 127	O 127	0	0
3	13-A	127	Total 127	O 127	0	0
3	14-A	127	Total 127	O 127	0	0
3	15-A	127	Total 127	O 127	0	0
3	16-A	127	Total 127	O 127	0	0

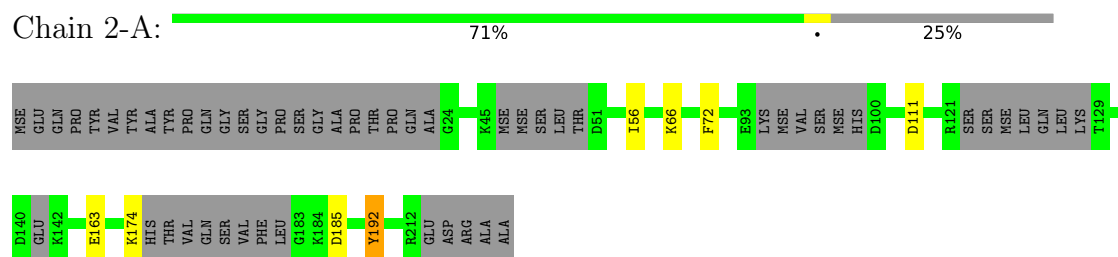
3 Residue-property plots [i](#)

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.

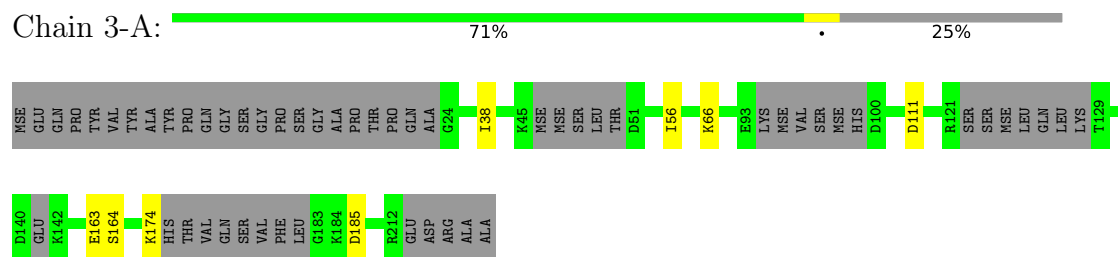
• Molecule 1: Protein At5g01750



• Molecule 1: Protein At5g01750

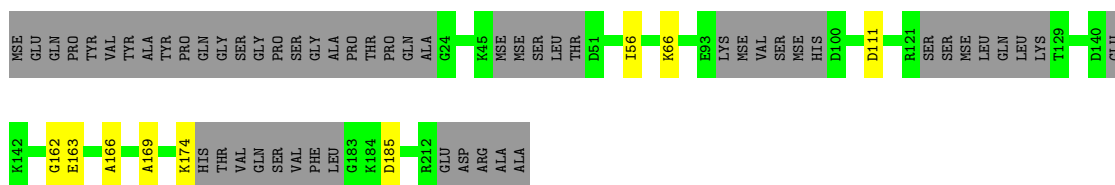


• Molecule 1: Protein At5g01750



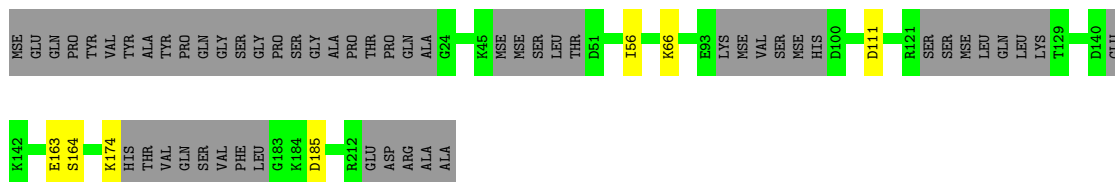
• Molecule 1: Protein At5g01750





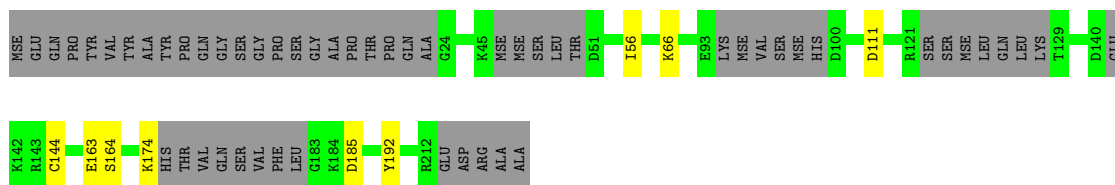
- Molecule 1: Protein At5g01750

Chain 5-A: 71% 25%



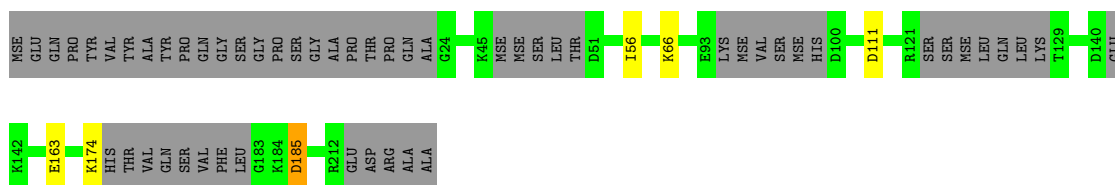
- Molecule 1: Protein At5g01750

Chain 6-A: 71% 25%



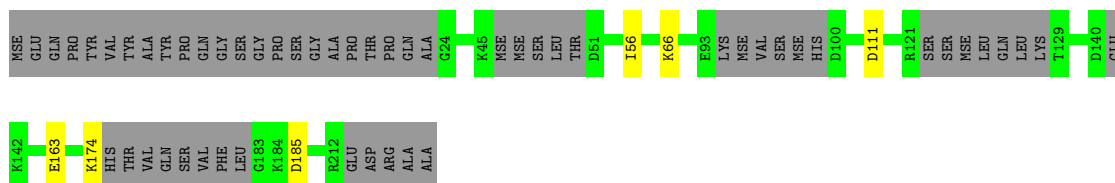
- Molecule 1: Protein At5g01750

Chain 7-A: 72% 25%



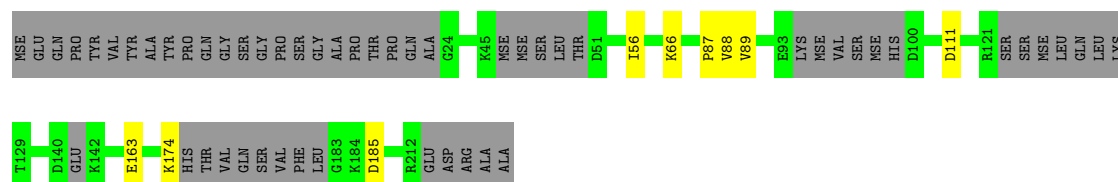
- Molecule 1: Protein At5g01750

Chain 8-A: 72% 25%

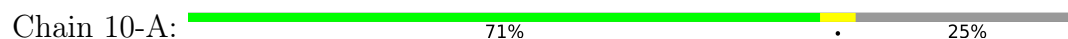


- Molecule 1: Protein At5g01750

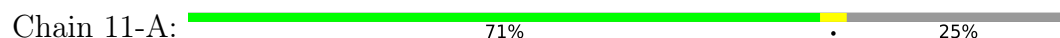
Chain 9-A: 71% 25%



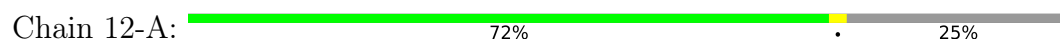
- Molecule 1: Protein At5g01750



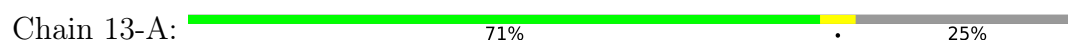
- Molecule 1: Protein At5g01750



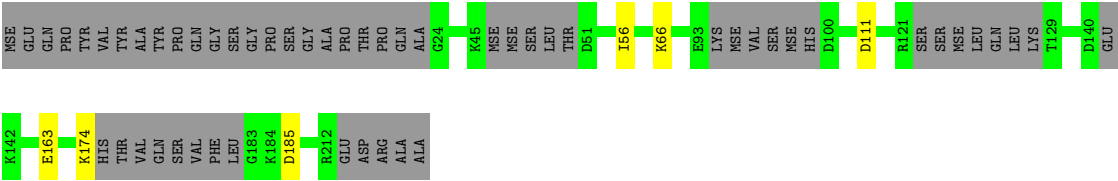
- Molecule 1: Protein At5g01750



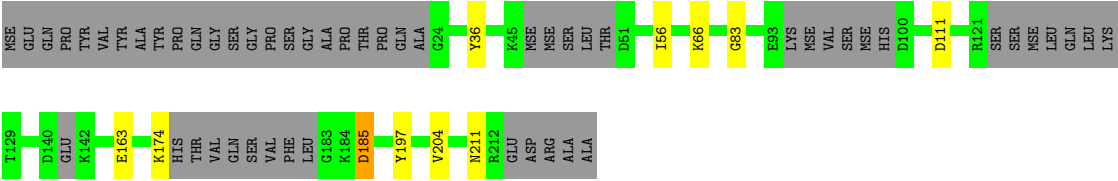
- Molecule 1: Protein At5g01750



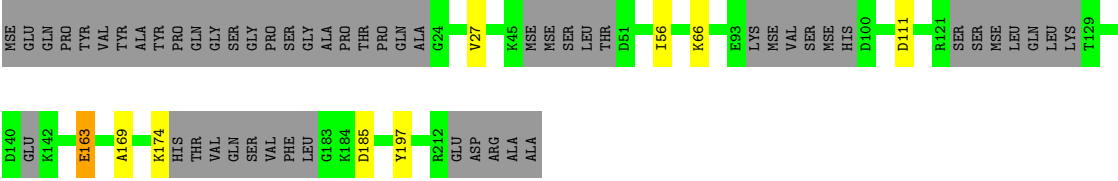
- Molecule 1: Protein At5g01750



• Molecule 1: Protein At5g01750



• Molecule 1: Protein At5g01750



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.07Å 57.50Å 75.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.68 – 1.70 37.68 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.68-1.70) 99.9 (37.68-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.158 , 0.207 0.173 , 0.222	Depositor DCC
R_{free} test set	1037 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22688	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.64% 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: 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	1-A	0.43	0/1306	0.36	0/1756
1	2-A	0.43	0/1306	0.36	0/1756
1	3-A	0.43	0/1306	0.36	0/1756
1	4-A	0.43	0/1306	0.36	0/1756
1	5-A	0.43	0/1306	0.36	0/1756
1	6-A	0.43	0/1306	0.36	0/1756
1	7-A	0.43	0/1306	0.36	0/1756
1	8-A	0.43	0/1306	0.36	0/1756
1	9-A	0.43	0/1306	0.36	0/1756
1	10-A	0.43	0/1306	0.36	0/1756
1	11-A	0.43	0/1306	0.36	0/1756
1	12-A	0.43	0/1306	0.36	0/1756
1	13-A	0.43	0/1306	0.36	0/1756
1	14-A	0.43	0/1306	0.36	0/1756
1	15-A	0.43	0/1306	0.36	0/1756
1	16-A	0.43	0/1306	0.36	0/1756
All	All	0.43	0/20896	0.36	0/28096

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	2-A	0	2
1	6-A	0	1
1	11-A	0	1
1	15-A	0	2
1	16-A	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	11-A	192	TYR	Sidechain
1	15-A	197	TYR	Sidechain
1	15-A	36	TYR	Sidechain
1	16-A	197	TYR	Sidechain
1	2-A	192	TYR	Sidechain
1	2-A	72	PHE	Sidechain
1	6-A	192	TYR	Sidechain

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	1-A	1287	0	1289	0	0
1	2-A	1287	0	1289	0	0
1	3-A	1287	0	1289	0	0
1	4-A	1287	0	1289	0	0
1	5-A	1287	0	1289	0	0
1	6-A	1287	0	1289	0	0
1	7-A	1287	0	1289	0	0
1	8-A	1287	0	1289	0	0
1	9-A	1287	0	1289	0	0
1	10-A	1287	0	1289	0	0
1	11-A	1287	0	1289	0	0
1	12-A	1287	0	1289	0	0
1	13-A	1287	0	1289	0	0
1	14-A	1287	0	1289	0	0
1	15-A	1287	0	1289	0	0
1	16-A	1287	0	1289	0	0
2	1-A	4	0	6	0	0
2	2-A	4	0	6	0	0
2	3-A	4	0	6	0	0
2	4-A	4	0	6	0	0
2	5-A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-A	4	0	6	0	0
2	7-A	4	0	6	0	0
2	8-A	4	0	6	0	0
2	9-A	4	0	6	0	0
2	10-A	4	0	6	0	0
2	11-A	4	0	6	0	0
2	12-A	4	0	6	0	0
2	13-A	4	0	6	0	0
2	14-A	4	0	6	0	0
2	15-A	4	0	6	0	0
2	16-A	4	0	6	0	0
3	1-A	127	0	0	0	0
3	2-A	127	0	0	0	0
3	3-A	127	0	0	0	0
3	4-A	127	0	0	0	0
3	5-A	127	0	0	0	0
3	6-A	127	0	0	0	0
3	7-A	127	0	0	0	0
3	8-A	127	0	0	0	0
3	9-A	127	0	0	0	0
3	10-A	127	0	0	0	0
3	11-A	127	0	0	0	0
3	12-A	127	0	0	0	0
3	13-A	127	0	0	0	0
3	14-A	127	0	0	0	0
3	15-A	127	0	0	0	0
3	16-A	127	0	0	0	0
All	All	22688	0	20720	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	150/217 (69%)	139 (93%)	9 (6%)	2 (1%)	9	2
1	2-A	150/217 (69%)	140 (93%)	9 (6%)	1 (1%)	18	7
1	3-A	150/217 (69%)	136 (91%)	12 (8%)	2 (1%)	9	2
1	4-A	150/217 (69%)	132 (88%)	15 (10%)	3 (2%)	6	1
1	5-A	150/217 (69%)	139 (93%)	10 (7%)	1 (1%)	18	7
1	6-A	150/217 (69%)	142 (95%)	6 (4%)	2 (1%)	9	2
1	7-A	150/217 (69%)	140 (93%)	9 (6%)	1 (1%)	18	7
1	8-A	150/217 (69%)	141 (94%)	9 (6%)	0	100	100
1	9-A	150/217 (69%)	133 (89%)	14 (9%)	3 (2%)	6	1
1	10-A	150/217 (69%)	141 (94%)	7 (5%)	2 (1%)	9	2
1	11-A	150/217 (69%)	145 (97%)	5 (3%)	0	100	100
1	12-A	150/217 (69%)	137 (91%)	12 (8%)	1 (1%)	18	7
1	13-A	150/217 (69%)	137 (91%)	9 (6%)	4 (3%)	4	0
1	14-A	150/217 (69%)	139 (93%)	11 (7%)	0	100	100
1	15-A	150/217 (69%)	135 (90%)	11 (7%)	4 (3%)	4	0
1	16-A	150/217 (69%)	136 (91%)	11 (7%)	3 (2%)	6	1
All	All	2400/3472 (69%)	2212 (92%)	159 (7%)	29 (1%)	10	2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	163	GLU
1	4-A	169	ALA
1	13-A	163	GLU
1	1-A	162	GLY
1	4-A	162	GLY
1	6-A	164	SER
1	7-A	185	ASP
1	10-A	109	SER
1	12-A	163	GLU
1	13-A	162	GLY
1	13-A	164	SER
1	15-A	185	ASP
1	15-A	211	ASN
1	16-A	163	GLU

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Mol	Chain	Res	Type
1	3-A	164	SER
1	4-A	166	ALA
1	9-A	87	PRO
1	10-A	83	GLY
1	15-A	83	GLY
1	15-A	204	VAL
1	16-A	169	ALA
1	5-A	164	SER
1	6-A	144	CYS
1	9-A	88	VAL
1	2-A	192	TYR
1	3-A	38	ILE
1	9-A	89	VAL
1	16-A	27	VAL
1	13-A	79	VAL

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	1-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	2-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	3-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	4-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	5-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	6-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	7-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	8-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	9-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	10-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	11-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	12-A	142/181 (78%)	136 (96%)	6 (4%)	26	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	13-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	14-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	15-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
1	16-A	142/181 (78%)	136 (96%)	6 (4%)	26	11
All	All	2272/2896 (78%)	2176 (96%)	96 (4%)	26	11

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	56	ILE
1	1-A	66	LYS
1	1-A	111	ASP
1	1-A	163	GLU
1	1-A	174	LYS
1	1-A	185	ASP
1	2-A	56	ILE
1	2-A	66	LYS
1	2-A	111	ASP
1	2-A	163	GLU
1	2-A	174	LYS
1	2-A	185	ASP
1	3-A	56	ILE
1	3-A	66	LYS
1	3-A	111	ASP
1	3-A	163	GLU
1	3-A	174	LYS
1	3-A	185	ASP
1	4-A	56	ILE
1	4-A	66	LYS
1	4-A	111	ASP
1	4-A	163	GLU
1	4-A	174	LYS
1	4-A	185	ASP
1	5-A	56	ILE
1	5-A	66	LYS
1	5-A	111	ASP
1	5-A	163	GLU
1	5-A	174	LYS
1	5-A	185	ASP
1	6-A	56	ILE
1	6-A	66	LYS

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Mol	Chain	Res	Type
1	6-A	111	ASP
1	6-A	163	GLU
1	6-A	174	LYS
1	6-A	185	ASP
1	7-A	56	ILE
1	7-A	66	LYS
1	7-A	111	ASP
1	7-A	163	GLU
1	7-A	174	LYS
1	7-A	185	ASP
1	8-A	56	ILE
1	8-A	66	LYS
1	8-A	111	ASP
1	8-A	163	GLU
1	8-A	174	LYS
1	8-A	185	ASP
1	9-A	56	ILE
1	9-A	66	LYS
1	9-A	111	ASP
1	9-A	163	GLU
1	9-A	174	LYS
1	9-A	185	ASP
1	10-A	56	ILE
1	10-A	66	LYS
1	10-A	111	ASP
1	10-A	163	GLU
1	10-A	174	LYS
1	10-A	185	ASP
1	11-A	56	ILE
1	11-A	66	LYS
1	11-A	111	ASP
1	11-A	163	GLU
1	11-A	174	LYS
1	11-A	185	ASP
1	12-A	56	ILE
1	12-A	66	LYS
1	12-A	111	ASP
1	12-A	163	GLU
1	12-A	174	LYS
1	12-A	185	ASP
1	13-A	56	ILE
1	13-A	66	LYS

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Mol	Chain	Res	Type
1	13-A	111	ASP
1	13-A	163	GLU
1	13-A	174	LYS
1	13-A	185	ASP
1	14-A	56	ILE
1	14-A	66	LYS
1	14-A	111	ASP
1	14-A	163	GLU
1	14-A	174	LYS
1	14-A	185	ASP
1	15-A	56	ILE
1	15-A	66	LYS
1	15-A	111	ASP
1	15-A	163	GLU
1	15-A	174	LYS
1	15-A	185	ASP
1	16-A	56	ILE
1	16-A	66	LYS
1	16-A	111	ASP
1	16-A	163	GLU
1	16-A	174	LYS
1	16-A	185	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	60	ASN
1	1-A	112	GLN
1	1-A	172	HIS
1	2-A	60	ASN
1	2-A	75	HIS
1	2-A	103	GLN
1	2-A	112	GLN
1	2-A	211	ASN
1	3-A	60	ASN
1	3-A	103	GLN
1	3-A	112	GLN
1	3-A	172	HIS
1	3-A	211	ASN
1	4-A	60	ASN
1	4-A	103	GLN
1	4-A	170	GLN

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Mol	Chain	Res	Type
1	4-A	172	HIS
1	5-A	60	ASN
1	5-A	170	GLN
1	5-A	172	HIS
1	6-A	60	ASN
1	6-A	103	GLN
1	6-A	112	GLN
1	6-A	172	HIS
1	7-A	60	ASN
1	7-A	137	HIS
1	7-A	172	HIS
1	7-A	194	ASN
1	8-A	103	GLN
1	8-A	172	HIS
1	9-A	103	GLN
1	9-A	112	GLN
1	9-A	172	HIS
1	9-A	194	ASN
1	10-A	53	ASN
1	10-A	170	GLN
1	10-A	172	HIS
1	10-A	194	ASN
1	11-A	60	ASN
1	11-A	112	GLN
1	11-A	137	HIS
1	11-A	172	HIS
1	11-A	194	ASN
1	12-A	60	ASN
1	12-A	103	GLN
1	12-A	112	GLN
1	12-A	172	HIS
1	12-A	194	ASN
1	12-A	211	ASN
1	13-A	60	ASN
1	13-A	172	HIS
1	14-A	103	GLN
1	14-A	112	GLN
1	14-A	172	HIS
1	15-A	60	ASN
1	15-A	170	GLN
1	15-A	172	HIS

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](#)

16 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	15-A	700	-	3,3,3	0.57	0	2,2,2	0.26	0
2	EDO	13-A	700	-	3,3,3	0.52	0	2,2,2	0.27	0
2	EDO	8-A	700	-	3,3,3	0.53	0	2,2,2	0.28	0
2	EDO	14-A	700	-	3,3,3	0.56	0	2,2,2	0.27	0
2	EDO	7-A	700	-	3,3,3	0.55	0	2,2,2	0.25	0
2	EDO	10-A	700	-	3,3,3	0.48	0	2,2,2	0.29	0
2	EDO	1-A	700	-	3,3,3	0.50	0	2,2,2	0.30	0
2	EDO	6-A	700	-	3,3,3	0.54	0	2,2,2	0.28	0
2	EDO	5-A	700	-	3,3,3	0.53	0	2,2,2	0.28	0
2	EDO	9-A	700	-	3,3,3	0.54	0	2,2,2	0.26	0
2	EDO	4-A	700	-	3,3,3	0.52	0	2,2,2	0.28	0
2	EDO	11-A	700	-	3,3,3	0.51	0	2,2,2	0.29	0
2	EDO	16-A	700	-	3,3,3	0.59	0	2,2,2	0.26	0
2	EDO	2-A	700	-	3,3,3	0.49	0	2,2,2	0.29	0
2	EDO	12-A	700	-	3,3,3	0.49	0	2,2,2	0.28	0
2	EDO	3-A	700	-	3,3,3	0.52	0	2,2,2	0.27	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	15-A	700	-	-	1/1/1/1	-
2	EDO	13-A	700	-	-	0/1/1/1	-
2	EDO	8-A	700	-	-	0/1/1/1	-
2	EDO	14-A	700	-	-	0/1/1/1	-
2	EDO	7-A	700	-	-	0/1/1/1	-
2	EDO	10-A	700	-	-	0/1/1/1	-
2	EDO	1-A	700	-	-	0/1/1/1	-
2	EDO	6-A	700	-	-	0/1/1/1	-
2	EDO	5-A	700	-	-	0/1/1/1	-
2	EDO	9-A	700	-	-	0/1/1/1	-
2	EDO	4-A	700	-	-	0/1/1/1	-
2	EDO	11-A	700	-	-	0/1/1/1	-
2	EDO	16-A	700	-	-	0/1/1/1	-
2	EDO	2-A	700	-	-	0/1/1/1	-
2	EDO	12-A	700	-	-	0/1/1/1	-
2	EDO	3-A	700	-	-	0/1/1/1	-

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
2	15-A	700	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1-A	160/217 (73%)	2.34	81 (50%) 0 0	0, 1, 2, 3	160 (100%)
1	2-A	0/217	-	-	-	-
1	3-A	0/217	-	-	-	-
1	4-A	0/217	-	-	-	-
1	5-A	0/217	-	-	-	-
1	6-A	0/217	-	-	-	-
1	7-A	0/217	-	-	-	-
1	8-A	0/217	-	-	-	-
1	9-A	0/217	-	-	-	-
1	10-A	0/217	-	-	-	-
1	11-A	0/217	-	-	-	-
1	12-A	0/217	-	-	-	-
1	13-A	0/217	-	-	-	-
1	14-A	0/217	-	-	-	-
1	15-A	0/217	-	-	-	-
1	16-A	0/217	-	-	-	-
All	All	160/3472 (4%)	2.34	81 (50%) 0 0	0, 1, 2, 3	160 (100%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	144	CYS	11.7
1	1-A	59	VAL	7.9
1	1-A	129	THR	5.6
1	1-A	130	LYS	5.5
1	1-A	162	GLY	5.3
1	1-A	143	ARG	5.2
1	1-A	57	THR	5.0
1	1-A	145	ASP	4.9
1	1-A	70	PRO	4.8
1	1-A	142	LYS	4.8
1	1-A	75	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
1	1-A	38	ILE	4.8
1	1-A	39	ASP	4.7
1	1-A	140	ASP	4.6
1	1-A	51	ASP	4.5
1	1-A	212	ARG	4.5
1	1-A	53	ASN	4.4
1	1-A	186	ASN	4.4
1	1-A	73	GLY	4.3
1	1-A	74	LEU	4.1
1	1-A	134	PHE	4.1
1	1-A	56	ILE	4.1
1	1-A	139	LYS	4.0
1	1-A	45	LYS	4.0
1	1-A	52	GLY	3.8
1	1-A	131	LEU	3.8
1	1-A	163	GLU	3.8
1	1-A	36	TYR	3.7
1	1-A	26	VAL	3.6
1	1-A	84	SER	3.5
1	1-A	185	ASP	3.5
1	1-A	60	ASN	3.5
1	1-A	100	ASP	3.4
1	1-A	41	ALA	3.3
1	1-A	24	GLY	3.3
1	1-A	76	ASP	3.2
1	1-A	153	LEU	3.2
1	1-A	165	ASP	3.2
1	1-A	71	VAL	3.2
1	1-A	188	SER	3.1
1	1-A	83	GLY	3.1
1	1-A	133	VAL	3.1
1	1-A	80	LEU	3.1
1	1-A	132	ASP	3.1
1	1-A	183	GLY	3.1
1	1-A	32	TYR	3.0
1	1-A	202	SER	3.0
1	1-A	146	PHE	3.0
1	1-A	160	TYR	2.9
1	1-A	197	TYR	2.9
1	1-A	211	ASN	2.9
1	1-A	164	SER	2.9
1	1-A	157	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	1-A	25	GLY	2.8
1	1-A	137	HIS	2.8
1	1-A	152	TRP	2.7
1	1-A	42	ILE	2.7
1	1-A	77	LYS	2.6
1	1-A	61	GLY	2.5
1	1-A	149	LYS	2.5
1	1-A	147	ARG	2.5
1	1-A	43	VAL	2.5
1	1-A	121	ARG	2.5
1	1-A	33	CYS	2.5
1	1-A	111	ASP	2.4
1	1-A	93	GLU	2.4
1	1-A	187	PHE	2.4
1	1-A	209	ASP	2.4
1	1-A	108	GLY	2.4
1	1-A	62	ASN	2.4
1	1-A	63	LEU	2.4
1	1-A	136	GLY	2.3
1	1-A	82	ASP	2.2
1	1-A	150	GLY	2.2
1	1-A	64	LEU	2.1
1	1-A	166	ALA	2.1
1	1-A	158	VAL	2.1
1	1-A	92	ARG	2.0
1	1-A	27	VAL	2.0
1	1-A	159	VAL	2.0
1	1-A	174	LYS	2.0

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	EDO	1-A	700	4/4	0.63	0.26	47,48,49,51	4
2	EDO	2-A	700	4/4	-	-	47,48,49,51	4
2	EDO	3-A	700	4/4	-	-	48,48,49,50	4
2	EDO	4-A	700	4/4	-	-	48,48,49,50	4
2	EDO	5-A	700	4/4	-	-	48,48,49,50	4
2	EDO	6-A	700	4/4	-	-	48,48,49,50	4
2	EDO	7-A	700	4/4	-	-	48,49,49,50	4
2	EDO	8-A	700	4/4	-	-	48,48,49,50	4
2	EDO	9-A	700	4/4	-	-	48,49,49,50	4
2	EDO	10-A	700	4/4	-	-	46,48,48,50	4
2	EDO	11-A	700	4/4	-	-	48,48,49,50	4
2	EDO	12-A	700	4/4	-	-	47,48,49,51	4
2	EDO	13-A	700	4/4	-	-	46,48,49,51	4
2	EDO	14-A	700	4/4	-	-	47,49,49,50	4
2	EDO	15-A	700	4/4	-	-	47,49,49,50	4
2	EDO	16-A	700	4/4	-	-	48,49,49,50	4

6.5 Other polymers [i](#)

There are no such residues in this entry.