



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:10 PM UTC

PDB ID : 2A2O / pdb_00002a2o
Title : CRYSTAL STRUCTURE OF a putativeTenA family transcriptional regulator (BT_3146) FROM BACTEROIDES THETA IOTAOMICRON VPI-5482 AT 2.16 Å RESOLUTION
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-06-22
Resolution : 2.16 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

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

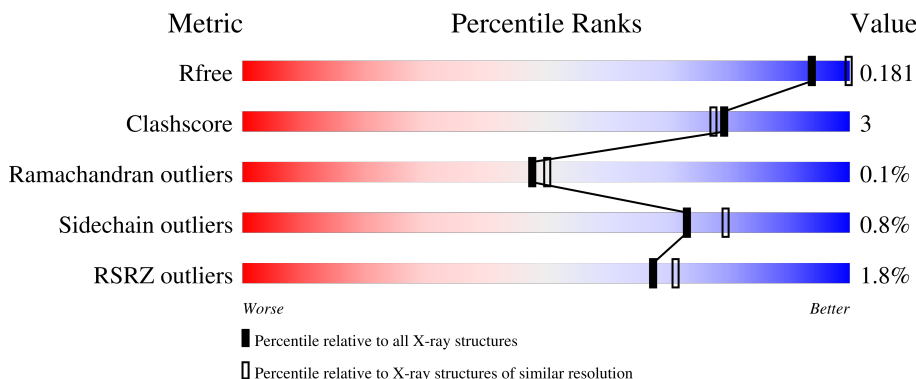
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

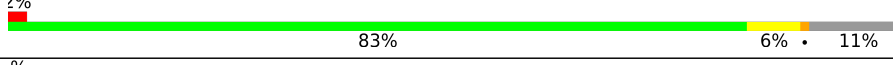
The reported resolution of this entry is 2.16 Å.

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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	258	
1	B	258	
1	C	258	
1	D	258	
1	E	258	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	258	2% 85% 11%
1	G	258	2% 84% 5% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14881 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 hypothetical protein BT3146.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	Se	0	4	0
			1863	1197	299	357	4	6			
1	B	230	Total	C	N	O	S	Se	0	5	0
			1861	1194	297	360	4	6			
1	C	230	Total	C	N	O	S	Se	0	7	0
			1864	1198	299	357	4	6			
1	D	229	Total	C	N	O	S	Se	0	3	0
			1847	1186	295	356	4	6			
1	E	230	Total	C	N	O	S	Se	0	10	0
			1889	1212	303	364	4	6			
1	F	229	Total	C	N	O	S	Se	0	4	0
			1850	1188	295	357	4	6			
1	G	230	Total	C	N	O	S	Se	0	6	0
			1872	1200	300	362	4	6			

There are 133 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP Q8A309
A	-10	GLY	-	expression tag	UNP Q8A309
A	-9	SER	-	expression tag	UNP Q8A309
A	-8	ASP	-	expression tag	UNP Q8A309
A	-7	LYS	-	expression tag	UNP Q8A309
A	-6	ILE	-	expression tag	UNP Q8A309
A	-5	HIS	-	expression tag	UNP Q8A309
A	-4	HIS	-	expression tag	UNP Q8A309
A	-3	HIS	-	expression tag	UNP Q8A309
A	-2	HIS	-	expression tag	UNP Q8A309
A	-1	HIS	-	expression tag	UNP Q8A309
A	0	HIS	-	expression tag	UNP Q8A309
A	1	MSE	MET	modified residue	UNP Q8A309
A	76	MSE	MET	modified residue	UNP Q8A309
A	157	MSE	MET	modified residue	UNP Q8A309

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	MSE	MET	modified residue	UNP Q8A309
A	202	MSE	MET	modified residue	UNP Q8A309
A	205	MSE	MET	modified residue	UNP Q8A309
A	226	MSE	MET	modified residue	UNP Q8A309
B	-11	MSE	-	expression tag	UNP Q8A309
B	-10	GLY	-	expression tag	UNP Q8A309
B	-9	SER	-	expression tag	UNP Q8A309
B	-8	ASP	-	expression tag	UNP Q8A309
B	-7	LYS	-	expression tag	UNP Q8A309
B	-6	ILE	-	expression tag	UNP Q8A309
B	-5	HIS	-	expression tag	UNP Q8A309
B	-4	HIS	-	expression tag	UNP Q8A309
B	-3	HIS	-	expression tag	UNP Q8A309
B	-2	HIS	-	expression tag	UNP Q8A309
B	-1	HIS	-	expression tag	UNP Q8A309
B	0	HIS	-	expression tag	UNP Q8A309
B	1	MSE	MET	modified residue	UNP Q8A309
B	76	MSE	MET	modified residue	UNP Q8A309
B	157	MSE	MET	modified residue	UNP Q8A309
B	161	MSE	MET	modified residue	UNP Q8A309
B	202	MSE	MET	modified residue	UNP Q8A309
B	205	MSE	MET	modified residue	UNP Q8A309
B	226	MSE	MET	modified residue	UNP Q8A309
C	-11	MSE	-	expression tag	UNP Q8A309
C	-10	GLY	-	expression tag	UNP Q8A309
C	-9	SER	-	expression tag	UNP Q8A309
C	-8	ASP	-	expression tag	UNP Q8A309
C	-7	LYS	-	expression tag	UNP Q8A309
C	-6	ILE	-	expression tag	UNP Q8A309
C	-5	HIS	-	expression tag	UNP Q8A309
C	-4	HIS	-	expression tag	UNP Q8A309
C	-3	HIS	-	expression tag	UNP Q8A309
C	-2	HIS	-	expression tag	UNP Q8A309
C	-1	HIS	-	expression tag	UNP Q8A309
C	0	HIS	-	expression tag	UNP Q8A309
C	1	MSE	MET	modified residue	UNP Q8A309
C	76	MSE	MET	modified residue	UNP Q8A309
C	157	MSE	MET	modified residue	UNP Q8A309
C	161	MSE	MET	modified residue	UNP Q8A309
C	202	MSE	MET	modified residue	UNP Q8A309
C	205	MSE	MET	modified residue	UNP Q8A309
C	226	MSE	MET	modified residue	UNP Q8A309

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MSE	-	expression tag	UNP Q8A309
D	-10	GLY	-	expression tag	UNP Q8A309
D	-9	SER	-	expression tag	UNP Q8A309
D	-8	ASP	-	expression tag	UNP Q8A309
D	-7	LYS	-	expression tag	UNP Q8A309
D	-6	ILE	-	expression tag	UNP Q8A309
D	-5	HIS	-	expression tag	UNP Q8A309
D	-4	HIS	-	expression tag	UNP Q8A309
D	-3	HIS	-	expression tag	UNP Q8A309
D	-2	HIS	-	expression tag	UNP Q8A309
D	-1	HIS	-	expression tag	UNP Q8A309
D	0	HIS	-	expression tag	UNP Q8A309
D	1	MSE	MET	modified residue	UNP Q8A309
D	76	MSE	MET	modified residue	UNP Q8A309
D	157	MSE	MET	modified residue	UNP Q8A309
D	161	MSE	MET	modified residue	UNP Q8A309
D	202	MSE	MET	modified residue	UNP Q8A309
D	205	MSE	MET	modified residue	UNP Q8A309
D	226	MSE	MET	modified residue	UNP Q8A309
E	-11	MSE	-	expression tag	UNP Q8A309
E	-10	GLY	-	expression tag	UNP Q8A309
E	-9	SER	-	expression tag	UNP Q8A309
E	-8	ASP	-	expression tag	UNP Q8A309
E	-7	LYS	-	expression tag	UNP Q8A309
E	-6	ILE	-	expression tag	UNP Q8A309
E	-5	HIS	-	expression tag	UNP Q8A309
E	-4	HIS	-	expression tag	UNP Q8A309
E	-3	HIS	-	expression tag	UNP Q8A309
E	-2	HIS	-	expression tag	UNP Q8A309
E	-1	HIS	-	expression tag	UNP Q8A309
E	0	HIS	-	expression tag	UNP Q8A309
E	1	MSE	MET	modified residue	UNP Q8A309
E	76	MSE	MET	modified residue	UNP Q8A309
E	157	MSE	MET	modified residue	UNP Q8A309
E	161	MSE	MET	modified residue	UNP Q8A309
E	202	MSE	MET	modified residue	UNP Q8A309
E	205	MSE	MET	modified residue	UNP Q8A309
E	226	MSE	MET	modified residue	UNP Q8A309
F	-11	MSE	-	expression tag	UNP Q8A309
F	-10	GLY	-	expression tag	UNP Q8A309
F	-9	SER	-	expression tag	UNP Q8A309
F	-8	ASP	-	expression tag	UNP Q8A309

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	LYS	-	expression tag	UNP Q8A309
F	-6	ILE	-	expression tag	UNP Q8A309
F	-5	HIS	-	expression tag	UNP Q8A309
F	-4	HIS	-	expression tag	UNP Q8A309
F	-3	HIS	-	expression tag	UNP Q8A309
F	-2	HIS	-	expression tag	UNP Q8A309
F	-1	HIS	-	expression tag	UNP Q8A309
F	0	HIS	-	expression tag	UNP Q8A309
F	1	MSE	MET	modified residue	UNP Q8A309
F	76	MSE	MET	modified residue	UNP Q8A309
F	157	MSE	MET	modified residue	UNP Q8A309
F	161	MSE	MET	modified residue	UNP Q8A309
F	202	MSE	MET	modified residue	UNP Q8A309
F	205	MSE	MET	modified residue	UNP Q8A309
F	226	MSE	MET	modified residue	UNP Q8A309
G	-11	MSE	-	expression tag	UNP Q8A309
G	-10	GLY	-	expression tag	UNP Q8A309
G	-9	SER	-	expression tag	UNP Q8A309
G	-8	ASP	-	expression tag	UNP Q8A309
G	-7	LYS	-	expression tag	UNP Q8A309
G	-6	ILE	-	expression tag	UNP Q8A309
G	-5	HIS	-	expression tag	UNP Q8A309
G	-4	HIS	-	expression tag	UNP Q8A309
G	-3	HIS	-	expression tag	UNP Q8A309
G	-2	HIS	-	expression tag	UNP Q8A309
G	-1	HIS	-	expression tag	UNP Q8A309
G	0	HIS	-	expression tag	UNP Q8A309
G	1	MSE	MET	modified residue	UNP Q8A309
G	76	MSE	MET	modified residue	UNP Q8A309
G	157	MSE	MET	modified residue	UNP Q8A309
G	161	MSE	MET	modified residue	UNP Q8A309
G	202	MSE	MET	modified residue	UNP Q8A309
G	205	MSE	MET	modified residue	UNP Q8A309
G	226	MSE	MET	modified residue	UNP Q8A309

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	C	1	Total K 1 1	0	0
3	D	2	Total K 2 2	0	0
3	E	1	Total K 1 1	0	0
3	F	1	Total K 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total K 1 1	0	0

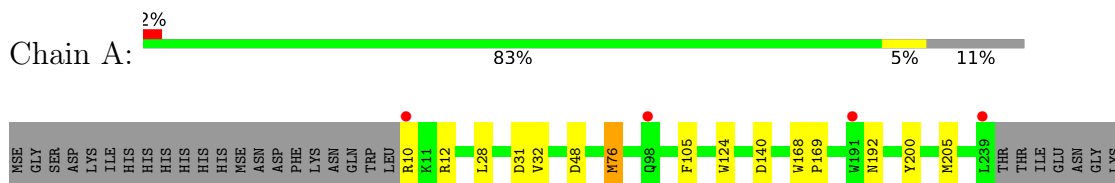
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	243	Total O 243 243	0	0
4	B	232	Total O 232 232	0	0
4	C	266	Total O 266 266	0	0
4	D	234	Total O 234 234	0	0
4	E	251	Total O 251 251	0	0
4	F	248	Total O 248 248	0	0
4	G	241	Total O 241 241	0	0

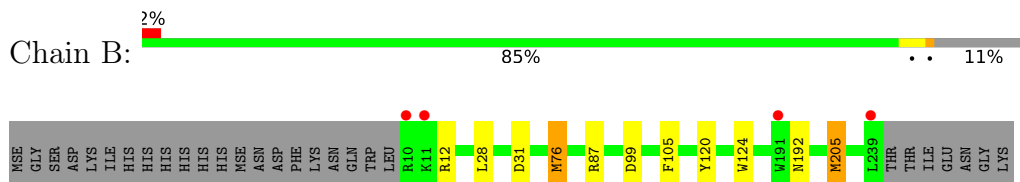
3 Residue-property plots [i](#)

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.

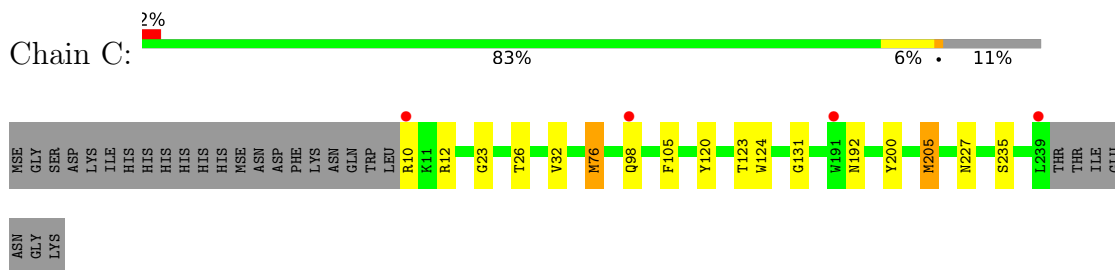
- Molecule 1: hypothetical protein BT3146



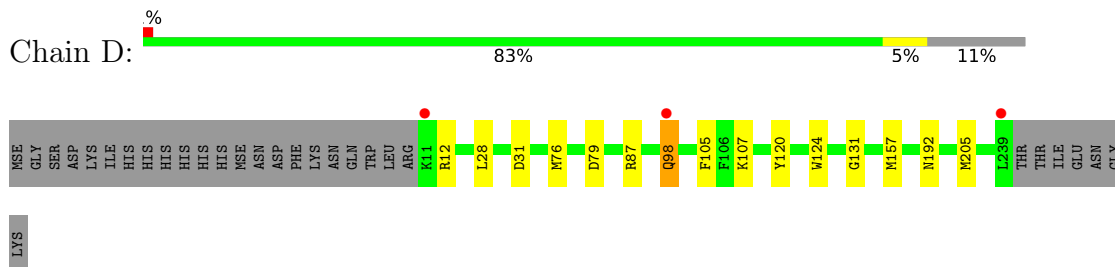
- Molecule 1: hypothetical protein BT3146



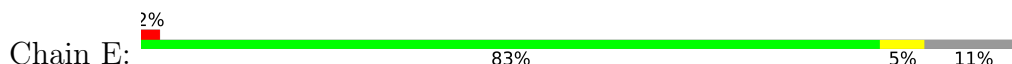
- Molecule 1: hypothetical protein BT3146

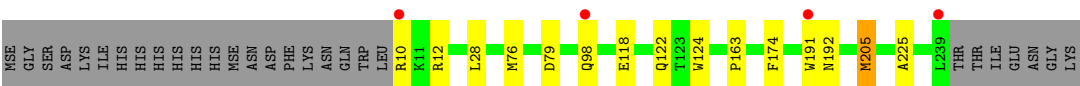


- Molecule 1: hypothetical protein BT3146

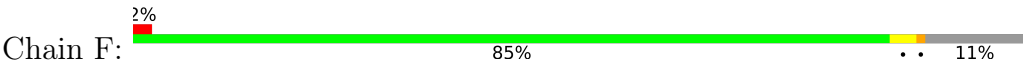


- Molecule 1: hypothetical protein BT3146

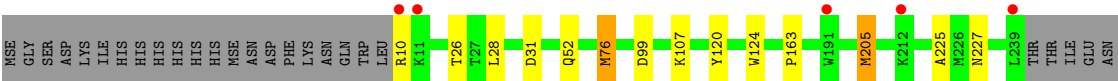
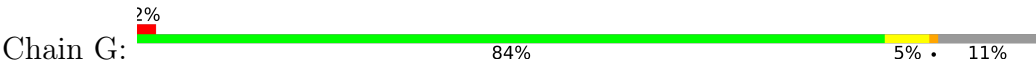




• Molecule 1: hypothetical protein BT3146



• Molecule 1: hypothetical protein BT3146



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	201.24Å 201.24Å 291.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 2.16 48.85 – 2.16	Depositor EDS
% Data completeness (in resolution range)	95.3 (48.85-2.16) 95.3 (48.85-2.16)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.145 , 0.173 0.155 , 0.181	Depositor DCC
R_{free} test set	8818 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	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	0.97	EDS
Total number of atoms	14881	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, K

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	0.87	0/1925	0.83	0/2612
1	B	0.86	1/1927 (0.1%)	0.84	1/2615 (0.0%)
1	C	0.94	1/1938 (0.1%)	0.89	1/2631 (0.0%)
1	D	0.91	0/1905	0.86	1/2586 (0.0%)
1	E	0.90	1/1975 (0.1%)	0.85	0/2681
1	F	0.93	2/1912 (0.1%)	0.86	0/2596
1	G	0.91	1/1942 (0.1%)	0.85	1/2635 (0.0%)
All	All	0.90	6/13524 (0.0%)	0.85	4/18356 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	205	MSE	SE-CE	-9.88	1.65	1.95
1	F	76	MSE	SE-CE	-8.23	1.70	1.95
1	B	205	MSE	SE-CE	-6.32	1.76	1.95
1	G	205	MSE	SE-CE	-5.91	1.77	1.95
1	F	205	MSE	SE-CE	-5.87	1.77	1.95
1	E	205	MSE	SE-CE	-5.82	1.77	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	MSE	CG-SE-CE	5.51	111.05	98.92
1	G	76	MSE	CG-SE-CE	5.47	110.95	98.92
1	D	157	MSE	CG-SE-CE	-5.41	87.03	98.92
1	B	76	MSE	CG-SE-CE	5.30	110.58	98.92

There are no chirality outliers.

There are no planarity outliers.

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	1863	0	1758	8	0
1	B	1861	0	1742	8	0
1	C	1864	0	1754	14	0
1	D	1847	0	1736	11	0
1	E	1889	0	1778	11	0
1	F	1850	0	1739	9	0
1	G	1872	0	1761	9	0
2	A	20	0	30	0	0
2	B	8	0	12	0	0
2	C	12	0	18	0	0
2	D	16	0	24	0	0
2	E	20	0	30	0	0
2	F	20	0	30	3	0
2	G	16	0	24	1	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	243	0	0	0	0
4	B	232	0	0	0	0
4	C	266	0	0	5	0
4	D	234	0	0	2	0
4	E	251	0	0	1	0
4	F	248	0	0	4	0
4	G	241	0	0	1	1
All	All	14881	0	12436	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 3.

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:C:23:GLY:O	1:C:26:THR:HG23	1.75	0.86
1:D:28:LEU:HD22	1:D:205:MSE:HE2	1.76	0.67
1:C:227[B]:ASN:CG	4:C:382:HOH:O	2.39	0.64
1:E:76:MSE:HA	1:E:76:MSE:HE3	1.80	0.62
1:B:76:MSE:HG2	1:B:124:TRP:CE2	2.39	0.58
1:E:76:MSE:HG2	1:E:124:TRP:CE2	2.40	0.56
1:F:98:GLN:NE2	4:F:379:HOH:O	2.11	0.56
1:B:87:ARG:HD3	1:B:87:ARG:C	2.32	0.55
1:G:52:GLN:HG2	4:G:473:HOH:O	2.07	0.54
1:A:32[B]:VAL:HG22	1:A:200:TYR:CE2	2.43	0.54
1:A:105:PHE:CD1	1:A:205:MSE:HE3	2.43	0.54
1:D:105:PHE:CD1	1:D:205:MSE:HE3	2.43	0.54
1:C:227[B]:ASN:ND2	4:C:382:HOH:O	2.40	0.53
1:C:105:PHE:CD1	1:C:205:MSE:HE3	2.44	0.53
1:C:32[B]:VAL:HG22	1:C:200:TYR:CE2	2.44	0.52
1:D:76:MSE:HG2	1:D:124:TRP:CE2	2.44	0.52
1:A:28:LEU:HD22	1:A:205:MSE:HE2	1.91	0.52
1:F:76:MSE:HG2	1:F:124:TRP:CE2	2.45	0.52
1:B:28:LEU:HD22	1:B:205:MSE:HE2	1.92	0.51
1:A:12:ARG:HD3	1:A:192:ASN:OD1	2.11	0.50
1:B:12:ARG:HD3	1:B:192:ASN:OD1	2.10	0.50
1:D:76:MSE:HE3	1:D:76:MSE:HA	1.93	0.50
1:F:235:SER:HB3	2:F:252:EDO:H21	1.94	0.50
1:A:76:MSE:HE3	1:A:76:MSE:HA	1.95	0.49
1:D:98:GLN:HG3	4:D:350:HOH:O	2.12	0.49
1:B:76:MSE:HE3	1:B:76:MSE:HA	1.95	0.48
1:D:87:ARG:NH1	4:D:357:HOH:O	2.39	0.48
1:G:76:MSE:HG2	1:G:124:TRP:CE2	2.48	0.48
1:F:28:LEU:HD22	1:F:205:MSE:HE2	1.95	0.48
1:F:60:LYS:NZ	4:F:376:HOH:O	2.47	0.48
1:F:76:MSE:HE1	2:F:251:EDO:H22	1.96	0.47
1:F:76:MSE:CE	2:F:251:EDO:H22	2.44	0.47
1:A:76:MSE:HG2	1:A:124:TRP:CE2	2.50	0.47
1:C:10:ARG:HH12	1:C:123:THR:HG21	1.80	0.47
1:G:76:MSE:HE2	1:G:120:TYR:OH	2.16	0.46
1:C:76:MSE:HE2	1:C:120:TYR:OH	2.16	0.46
1:G:76:MSE:HE2	1:G:120:TYR:CE1	2.51	0.46
1:C:76:MSE:HG2	1:C:124:TRP:CE2	2.50	0.45
1:G:163:PRO:HG2	1:G:225:ALA:HB3	1.98	0.45
1:E:10:ARG:HD2	1:E:191:TRP:CH2	2.52	0.44
1:D:76:MSE:HE2	1:D:120:TYR:CE1	2.53	0.44
1:D:12:ARG:HD3	1:D:192:ASN:OD1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:PRO:HG2	1:E:225:ALA:HB3	2.00	0.44
1:F:26[A]:THR:CG2	4:F:472:HOH:O	2.66	0.44
1:A:168:TRP:HB2	1:A:169:PRO:HD3	2.00	0.43
1:E:76:MSE:CE	1:E:79:ASP:HB2	2.48	0.43
1:G:227[B]:ASN:HD22	2:G:251:EDO:H22	1.82	0.43
1:E:10:ARG:HD2	1:E:191:TRP:CZ2	2.54	0.43
1:C:12:ARG:HD3	1:C:192:ASN:OD1	2.19	0.43
1:E:118[B]:GLU:OE1	1:E:122:GLN:NE2	2.43	0.43
1:E:28:LEU:HD22	1:E:205:MSE:HE2	2.02	0.42
1:G:99:ASP:OD1	1:G:99:ASP:C	2.61	0.42
1:E:12:ARG:HD3	1:E:192:ASN:OD1	2.19	0.42
1:C:235:SER:OG	4:C:315:HOH:O	2.22	0.42
1:D:76:MSE:HE3	1:D:79:ASP:HB2	2.01	0.42
1:C:32[B]:VAL:HG23	4:C:427:HOH:O	2.21	0.41
1:C:98:GLN:N	4:C:345:HOH:O	2.44	0.41
1:B:76:MSE:HE2	1:B:120:TYR:OH	2.20	0.41
1:D:76:MSE:HE2	1:D:120:TYR:OH	2.19	0.41
1:E:174:PHE:CD1	1:E:174:PHE:C	2.99	0.41
1:C:76:MSE:HE2	1:C:120:TYR:CE1	2.55	0.41
1:C:131:GLY:HA3	1:D:131:GLY:HA3	2.03	0.41
1:B:105:PHE:CD1	1:B:205:MSE:HE3	2.56	0.41
1:E:76:MSE:HE1	4:E:433:HOH:O	2.20	0.40
1:A:140:ASP:OD2	1:G:107:LYS:NZ	2.52	0.40
1:B:99:ASP:OD1	1:B:99:ASP:C	2.65	0.40
1:F:165:GLU:OE2	4:F:275:HOH:O	2.22	0.40
1:G:28:LEU:HD13	1:G:205:MSE:HE2	2.02	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)
4:G:437:HOH:O	4:G:466:HOH:O[10_775]	2.13	0.07

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	232/258 (90%)	231 (100%)	1 (0%)	0	100	100
1	B	233/258 (90%)	233 (100%)	0	0	100	100
1	C	235/258 (91%)	235 (100%)	0	0	100	100
1	D	230/258 (89%)	229 (100%)	0	1 (0%)	30	26
1	E	238/258 (92%)	236 (99%)	2 (1%)	0	100	100
1	F	231/258 (90%)	231 (100%)	0	0	100	100
1	G	234/258 (91%)	233 (100%)	1 (0%)	0	100	100
All	All	1633/1806 (90%)	1628 (100%)	4 (0%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	98	GLN

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	194/210 (92%)	190 (98%)	4 (2%)	47	52
1	B	194/210 (92%)	193 (100%)	1 (0%)	81	87
1	C	195/210 (93%)	195 (100%)	0	100	100
1	D	192/210 (91%)	190 (99%)	2 (1%)	68	75
1	E	201/210 (96%)	199 (99%)	2 (1%)	68	75
1	F	193/210 (92%)	193 (100%)	0	100	100
1	G	197/210 (94%)	193 (98%)	4 (2%)	48	54
All	All	1366/1470 (93%)	1353 (99%)	13 (1%)	73	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	31	ASP
1	A	48	ASP
1	A	76	MSE
1	B	31	ASP
1	D	31	ASP
1	D	107	LYS
1	E	98[A]	GLN
1	E	98[B]	GLN
1	G	10	ARG
1	G	26[A]	THR
1	G	26[B]	THR
1	G	31	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	D	98	GLN
1	D	204	ASN
1	G	52	GLN

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](#)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 for Mogul analysis.

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	G	250	-	3,3,3	0.38	0	2,2,2	0.20	0
2	EDO	A	250	-	3,3,3	0.53	0	2,2,2	0.64	0
2	EDO	B	249	-	3,3,3	0.70	0	2,2,2	0.10	0
2	EDO	B	250	-	3,3,3	0.74	0	2,2,2	0.60	0
2	EDO	A	248	-	3,3,3	0.64	0	2,2,2	0.25	0
2	EDO	E	251	-	3,3,3	0.23	0	2,2,2	0.95	0
2	EDO	D	249	-	3,3,3	0.59	0	2,2,2	0.37	0
2	EDO	G	249	-	3,3,3	0.81	0	2,2,2	0.80	0
2	EDO	G	251	-	3,3,3	0.58	0	2,2,2	0.51	0
2	EDO	G	248	-	3,3,3	0.63	0	2,2,2	0.24	0
2	EDO	E	249	-	3,3,3	0.73	0	2,2,2	0.54	0
2	EDO	F	251	-	3,3,3	0.41	0	2,2,2	0.16	0
2	EDO	E	250	-	3,3,3	0.83	0	2,2,2	0.43	0
2	EDO	E	252	-	3,3,3	0.72	0	2,2,2	0.22	0
2	EDO	A	249	-	3,3,3	0.89	0	2,2,2	0.65	0
2	EDO	C	250	-	3,3,3	0.36	0	2,2,2	0.46	0
2	EDO	C	249	-	3,3,3	0.80	0	2,2,2	0.66	0
2	EDO	F	249	-	3,3,3	0.83	0	2,2,2	0.50	0
2	EDO	D	250	-	3,3,3	0.91	0	2,2,2	0.81	0
2	EDO	E	248	-	3,3,3	0.61	0	2,2,2	0.35	0
2	EDO	C	248	-	3,3,3	0.63	0	2,2,2	0.21	0
2	EDO	F	250	-	3,3,3	0.46	0	2,2,2	0.43	0
2	EDO	D	251	-	3,3,3	0.62	0	2,2,2	0.31	0
2	EDO	A	247	-	3,3,3	0.62	0	2,2,2	0.35	0
2	EDO	F	252	-	3,3,3	0.71	0	2,2,2	0.42	0
2	EDO	F	248	-	3,3,3	0.69	0	2,2,2	0.42	0
2	EDO	A	251	-	3,3,3	0.56	0	2,2,2	0.19	0
2	EDO	D	252	-	3,3,3	0.33	0	2,2,2	0.13	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	G	250	-	-	1/1/1/1	-
2	EDO	A	250	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	249	-	-	1/1/1/1	-
2	EDO	B	250	-	-	1/1/1/1	-
2	EDO	A	248	-	-	0/1/1/1	-
2	EDO	E	251	-	-	0/1/1/1	-
2	EDO	D	249	-	-	0/1/1/1	-
2	EDO	G	249	-	-	1/1/1/1	-
2	EDO	G	251	-	-	1/1/1/1	-
2	EDO	G	248	-	-	0/1/1/1	-
2	EDO	E	249	-	-	1/1/1/1	-
2	EDO	F	251	-	-	0/1/1/1	-
2	EDO	E	250	-	-	1/1/1/1	-
2	EDO	E	252	-	-	1/1/1/1	-
2	EDO	A	249	-	-	0/1/1/1	-
2	EDO	C	250	-	-	1/1/1/1	-
2	EDO	C	249	-	-	0/1/1/1	-
2	EDO	F	249	-	-	0/1/1/1	-
2	EDO	D	250	-	-	1/1/1/1	-
2	EDO	E	248	-	-	1/1/1/1	-
2	EDO	C	248	-	-	0/1/1/1	-
2	EDO	F	250	-	-	0/1/1/1	-
2	EDO	D	251	-	-	0/1/1/1	-
2	EDO	A	247	-	-	1/1/1/1	-
2	EDO	F	252	-	-	1/1/1/1	-
2	EDO	F	248	-	-	0/1/1/1	-
2	EDO	A	251	-	-	0/1/1/1	-
2	EDO	D	252	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	247	EDO	O1-C1-C2-O2
2	B	250	EDO	O1-C1-C2-O2
2	E	250	EDO	O1-C1-C2-O2
2	E	252	EDO	O1-C1-C2-O2
2	G	249	EDO	O1-C1-C2-O2
2	G	251	EDO	O1-C1-C2-O2
2	D	250	EDO	O1-C1-C2-O2
2	F	252	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	249	EDO	O1-C1-C2-O2
2	B	249	EDO	O1-C1-C2-O2
2	C	250	EDO	O1-C1-C2-O2
2	E	248	EDO	O1-C1-C2-O2
2	G	250	EDO	O1-C1-C2-O2
2	A	250	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	251	EDO	1	0
2	F	251	EDO	2	0
2	F	252	EDO	1	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

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	224/258 (86%)	-0.08	4 (1%) 67 71	24, 36, 50, 76	4 (1%)
1	B	224/258 (86%)	-0.23	4 (1%) 67 71	24, 36, 50, 82	5 (2%)
1	C	224/258 (86%)	-0.29	4 (1%) 67 71	24, 36, 51, 77	7 (3%)
1	D	223/258 (86%)	-0.27	3 (1%) 75 78	26, 36, 50, 65	3 (1%)
1	E	224/258 (86%)	-0.25	4 (1%) 67 71	22, 36, 50, 85	10 (4%)
1	F	223/258 (86%)	-0.24	4 (1%) 67 71	24, 36, 50, 66	4 (1%)
1	G	224/258 (86%)	-0.21	5 (2%) 62 66	23, 36, 50, 80	6 (2%)
All	All	1566/1806 (86%)	-0.22	28 (1%) 67 71	22, 36, 50, 85	39 (2%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	LEU	8.6
1	F	239	LEU	6.3
1	A	239	LEU	6.2
1	G	239	LEU	5.8
1	D	239	LEU	5.6
1	E	191	TRP	5.1
1	F	191	TRP	5.0
1	B	10	ARG	5.0
1	E	239	LEU	4.7
1	E	10	ARG	4.6
1	G	10	ARG	4.5
1	C	239	LEU	4.5
1	A	191	TRP	4.5
1	A	10	ARG	4.4
1	C	10	ARG	3.6
1	A	98	GLN	3.6
1	G	191	TRP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	11	LYS	3.5
1	E	98[A]	GLN	3.5
1	F	238	ILE	3.1
1	B	191	TRP	2.9
1	C	98	GLN	2.9
1	C	191	TRP	2.8
1	D	11	LYS	2.5
1	B	11	LYS	2.2
1	G	212	LYS	2.1
1	G	11	LYS	2.1
1	D	98	GLN	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
3	K	C	247	1/1	0.87	0.23	93,93,93,93	0
3	K	D	248	1/1	0.87	0.21	96,96,96,96	0
3	K	F	247	1/1	0.87	0.21	92,92,92,92	0
2	EDO	A	251	4/4	0.88	0.15	72,75,75,78	0
2	EDO	E	250	4/4	0.88	0.21	60,67,67,74	0
2	EDO	G	251	4/4	0.88	0.21	60,63,65,67	0
2	EDO	A	247	4/4	0.89	0.20	66,72,74,77	0
2	EDO	E	249	4/4	0.90	0.20	45,50,50,58	0
2	EDO	C	249	4/4	0.90	0.17	41,48,49,56	0
2	EDO	F	252	4/4	0.91	0.23	58,60,63,68	0
2	EDO	F	249	4/4	0.91	0.16	53,57,59,64	0
3	K	B	247	1/1	0.91	0.14	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	F	248	4/4	0.92	0.16	43,52,56,62	0
2	EDO	B	250	4/4	0.92	0.17	46,48,51,63	0
3	K	B	248	1/1	0.93	0.13	82,82,82,82	0
2	EDO	A	249	4/4	0.93	0.16	43,50,55,64	0
2	EDO	E	252	4/4	0.93	0.18	45,51,58,62	0
2	EDO	F	251	4/4	0.93	0.20	36,60,61,62	0
2	EDO	C	250	4/4	0.94	0.11	48,48,52,55	0
2	EDO	D	252	4/4	0.94	0.11	50,54,56,61	0
2	EDO	A	248	4/4	0.94	0.17	35,45,48,51	0
2	EDO	G	248	4/4	0.94	0.16	35,43,52,55	0
2	EDO	G	249	4/4	0.94	0.14	44,48,53,57	0
2	EDO	G	250	4/4	0.94	0.11	56,59,63,64	0
3	K	G	247	1/1	0.94	0.15	78,78,78,78	1
3	K	E	247	1/1	0.95	0.11	82,82,82,82	0
2	EDO	A	250	4/4	0.95	0.13	48,52,53,54	0
2	EDO	C	248	4/4	0.95	0.16	34,48,50,54	0
3	K	D	247	1/1	0.96	0.10	85,85,85,85	0
2	EDO	E	248	4/4	0.96	0.19	37,51,51,55	0
2	EDO	D	251	4/4	0.96	0.10	43,52,53,61	0
2	EDO	D	249	4/4	0.96	0.17	30,45,52,55	0
2	EDO	E	251	4/4	0.96	0.10	50,50,51,58	0
2	EDO	F	250	4/4	0.97	0.09	48,53,54,55	0
2	EDO	D	250	4/4	0.97	0.11	39,40,46,50	0
2	EDO	B	249	4/4	0.97	0.18	32,49,50,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.