



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:03 PM UTC

PDB ID : 5QTP / pdb_00005qtp
Title : PanDDA analysis group deposition – Crystal Structure of NUDT5 in complex with AE-0227
Authors : Dubianok, Y.; Krojer, T.; Kovacs, H.; Moriaud, F.; Wright, N.; Strain-Damerell, C.; Burgess-Brown, N.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; von Delft, F.
Deposited on : 2019-08-14
Resolution : 1.73 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

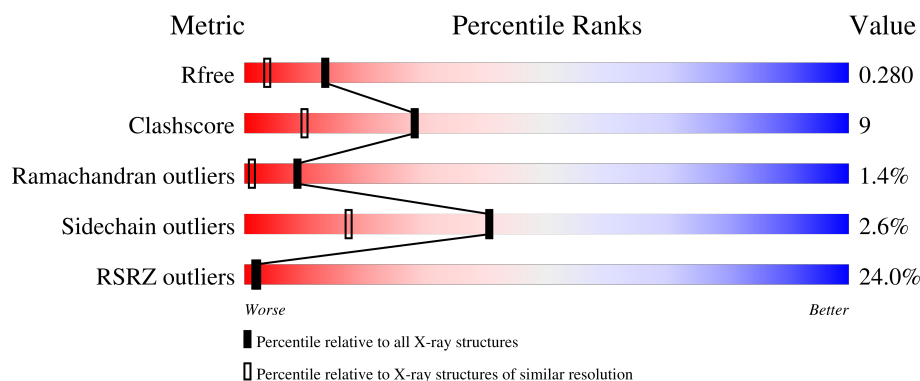
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	209	
1	B	209	
1	C	209	
1	D	209	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6177 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 ADP-sugar pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1466	927	245	286	8			
1	B	194	Total	C	N	O	S	0	0	0
			1468	926	245	289	8			
1	C	193	Total	C	N	O	S	0	0	0
			1430	901	239	282	8			
1	D	194	Total	C	N	O	S	0	0	0
			1450	915	242	285	8			

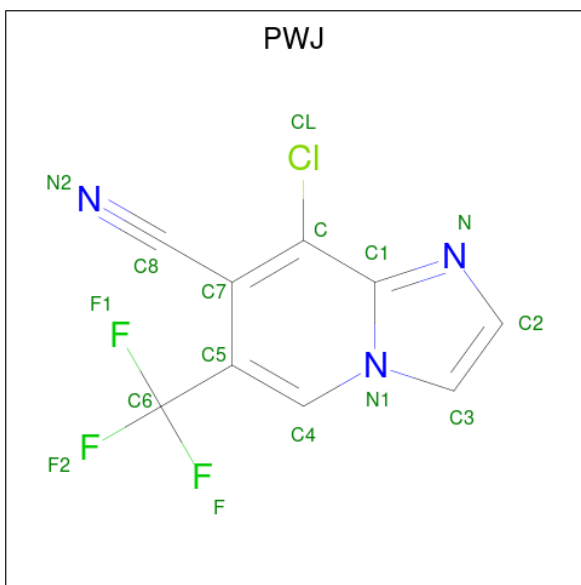
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9UUKK9
B	0	SER	-	expression tag	UNP Q9UUKK9
C	0	SER	-	expression tag	UNP Q9UUKK9
D	0	SER	-	expression tag	UNP Q9UUKK9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

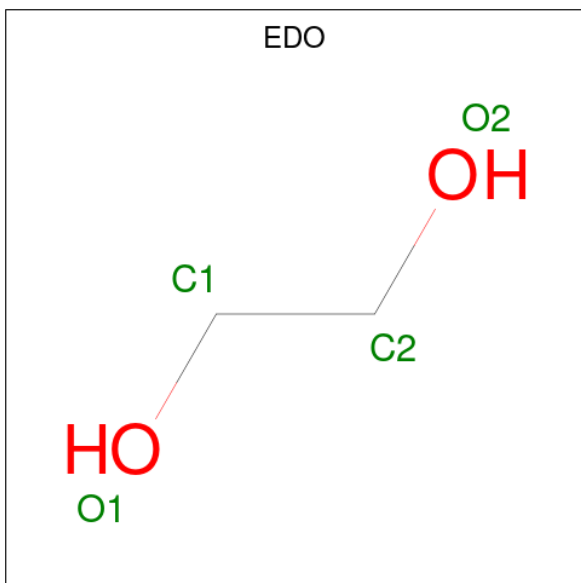
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 8-chloro-6-(trifluoromethyl)imidazo[1,2-a]pyridine-7-carbonitrile (CCD ID: PWJ) (formula: C₉H₃ClF₃N₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	0	0
			16	9	1	3	3		
3	B	1	Total	C	Cl	F	N	0	0
			16	9	1	3	3		
3	C	1	Total	C	Cl	F	N	0	0
			16	9	1	3	3		
3	D	1	Total	C	Cl	F	N	0	0
			16	9	1	3	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0

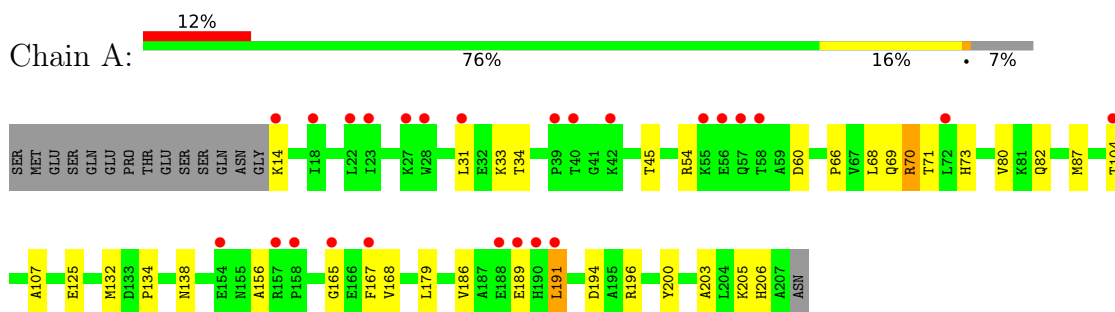
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	76	Total O 76 76	0	0
6	B	66	Total O 66 66	0	0
6	C	77	Total O 77 77	0	0
6	D	39	Total O 39 39	0	0

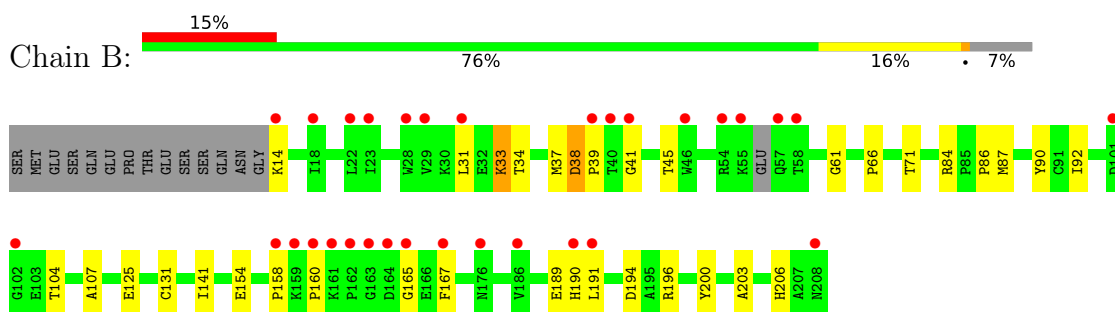
3 Residue-property plots [i](#)

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.

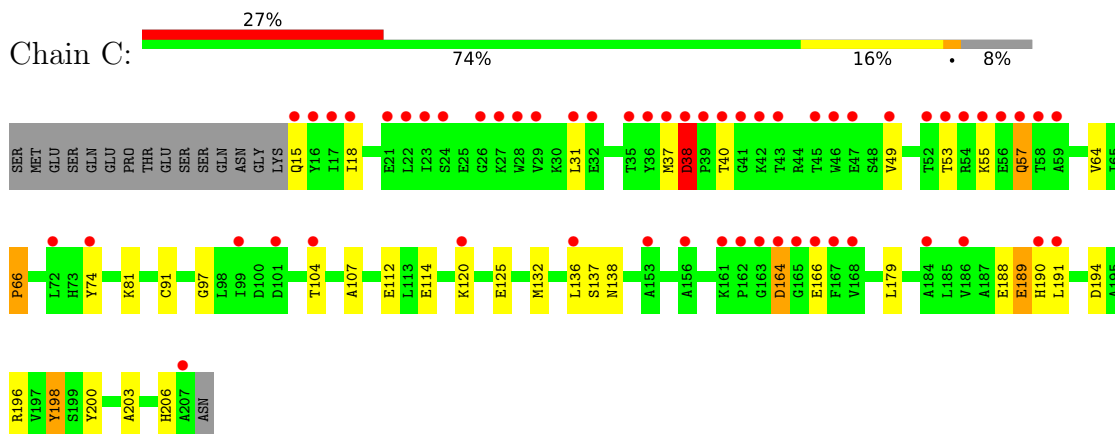
- Molecule 1: ADP-sugar pyrophosphatase



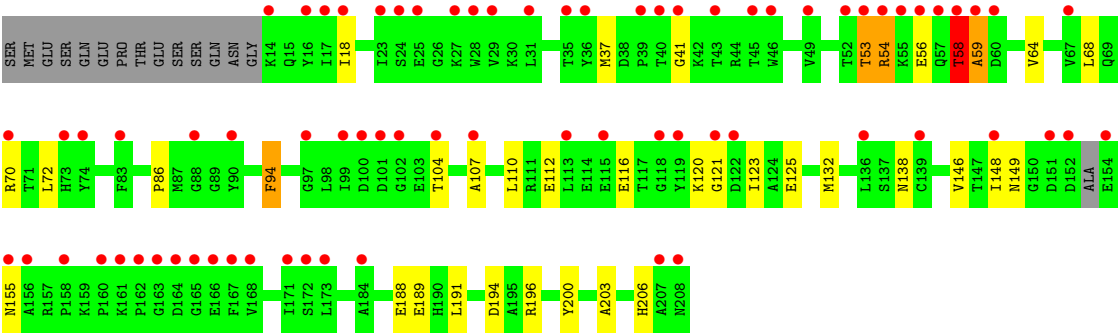
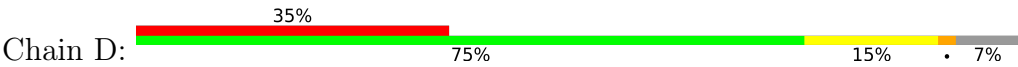
- Molecule 1: ADP-sugar pyrophosphatase



- Molecule 1: ADP-sugar pyrophosphatase



- Molecule 1: ADP-sugar pyrophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.25Å 59.83Å 80.05Å 79.42° 81.55° 75.70°	Depositor
Resolution (Å)	42.67 – 1.73 42.67 – 1.73	Depositor EDS
% Data completeness (in resolution range)	96.2 (42.67-1.73) 91.1 (42.67-1.73)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.229 , 0.261 (Not available) , 0.280	Depositor DCC
R_{free} test set	4561 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6177	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PWJ, EDO, MG

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	1.15	0/1494	1.30	0/2037
1	B	1.09	0/1496	1.35	3/2040 (0.1%)
1	C	1.11	0/1459	1.41	3/1998 (0.2%)
1	D	1.10	0/1478	1.42	4/2020 (0.2%)
All	All	1.11	0/5927	1.37	10/8095 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	THR	CA-C-N	7.43	135.73	121.54
1	D	58	THR	C-N-CA	7.43	135.73	121.54
1	B	38	ASP	CB-CA-C	6.66	121.50	109.45
1	B	71	THR	CA-CB-OG1	-6.43	99.96	109.60
1	C	38	ASP	CA-CB-CG	6.07	118.67	112.60
1	D	18	ILE	N-CA-C	-5.61	106.34	111.67
1	B	38	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	198	TYR	CA-C-N	5.18	127.18	120.44
1	C	198	TYR	C-N-CA	5.18	127.18	120.44
1	D	94	PHE	N-CA-C	-5.02	103.15	110.08

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	1466	0	1437	31	0
1	B	1468	0	1420	29	0
1	C	1430	0	1347	28	0
1	D	1450	0	1386	34	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
4	A	8	0	12	0	0
4	B	8	0	12	2	0
4	C	12	0	18	1	0
4	D	4	0	6	0	0
5	B	1	0	0	0	0
6	A	76	0	0	2	0
6	B	66	0	0	4	0
6	C	77	0	0	7	0
6	D	39	0	0	2	0
All	All	6177	0	5638	103	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 9.

All (103) 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:104:THR:HG23	1:A:107:ALA:H	1.32	0.92
1:D:120:LYS:H	1:D:155:ASN:HD21	1.19	0.91
1:A:186:VAL:HA	1:A:191:LEU:HD21	1.56	0.88
1:B:92:ILE:HD11	1:B:191:LEU:HD13	1.59	0.83
1:A:31:LEU:HB2	1:B:31:LEU:HD11	1.64	0.78
1:C:206:HIS:HD2	1:D:200:TYR:OH	1.67	0.78
6:C:427:HOH:O	1:D:196:ARG:HD2	1.85	0.77
1:D:58:THR:HG23	1:D:59:ALA:H	1.48	0.77
1:A:203:ALA:HB3	1:B:203:ALA:HB3	1.66	0.76
1:C:104:THR:HG23	1:C:107:ALA:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:302:EDO:C2	6:B:403:HOH:O	2.35	0.74
1:D:53:THR:HG23	6:D:638:HOH:O	1.88	0.73
1:D:191:LEU:C	1:D:191:LEU:HD12	2.16	0.70
1:D:58:THR:HG23	1:D:59:ALA:N	2.04	0.69
1:D:194:ASP:OD1	1:D:196:ARG:HD3	1.91	0.69
1:D:64:VAL:O	1:D:94:PHE:HB3	1.93	0.68
1:C:125:GLU:OE1	6:C:402:HOH:O	2.13	0.67
1:B:154:GLU:OE1	6:B:401:HOH:O	2.12	0.66
1:D:132:MET:HE1	1:D:196:ARG:CZ	2.26	0.66
1:C:166:GLU:OE2	6:C:401:HOH:O	2.13	0.65
4:B:302:EDO:H22	6:B:403:HOH:O	1.96	0.64
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.79	0.64
1:D:104:THR:HG23	1:D:107:ALA:H	1.64	0.63
6:C:427:HOH:O	1:D:196:ARG:CD	2.45	0.62
1:A:179:LEU:HD23	1:A:205:LYS:HD2	1.81	0.62
1:D:191:LEU:HD12	1:D:191:LEU:O	1.99	0.61
1:C:200:TYR:CD1	1:D:203:ALA:HB2	2.36	0.60
6:C:402:HOH:O	1:D:206:HIS:HE1	1.85	0.57
1:C:74:TYR:HB3	6:C:416:HOH:O	2.03	0.57
1:A:68:LEU:HG	1:A:70:ARG:HD2	1.89	0.56
1:C:194:ASP:OD2	1:C:196:ARG:NH2	2.39	0.55
1:D:37:MET:SD	1:D:41:GLY:O	2.64	0.55
1:A:31:LEU:HB2	1:B:31:LEU:CD1	2.34	0.55
1:C:132:MET:HE1	1:C:196:ARG:CZ	2.37	0.55
1:C:206:HIS:CD2	1:D:200:TYR:OH	2.55	0.54
1:C:203:ALA:HB2	1:D:200:TYR:CD1	2.42	0.54
1:B:158:PRO:O	1:B:160:PRO:HD3	2.08	0.53
1:A:54:ARG:HD3	1:A:60:ASP:OD1	2.09	0.53
1:A:14:LYS:N	1:B:90:TYR:HH	2.07	0.53
1:C:18:ILE:HD11	1:C:37:MET:HE2	1.91	0.53
1:A:206:HIS:HE1	1:B:125:GLU:OE1	1.94	0.51
1:D:120:LYS:H	1:D:155:ASN:ND2	1.99	0.51
1:A:132:MET:HE1	1:A:196:ARG:CZ	2.41	0.50
1:C:179:LEU:HD11	1:C:198:TYR:CZ	2.46	0.50
1:D:58:THR:CG2	1:D:59:ALA:N	2.73	0.50
1:C:191:LEU:HD12	1:C:191:LEU:C	2.36	0.49
1:B:190:HIS:O	1:B:190:HIS:CG	2.65	0.49
1:C:188:GLU:C	1:C:189:GLU:HG3	2.37	0.49
1:D:110:LEU:HG	1:D:123:ILE:HD11	1.93	0.49
1:A:165:GLY:HA2	1:A:167:PHE:CE1	2.47	0.49
1:C:138:ASN:HB3	1:D:86:PRO:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ASN:C	1:D:149:ASN:HD22	2.20	0.48
1:A:104:THR:HG22	1:A:107:ALA:CB	2.43	0.48
1:C:200:TYR:OH	1:D:206:HIS:HD2	1.95	0.48
1:B:37:MET:SD	1:B:41:GLY:HA2	2.55	0.47
1:D:191:LEU:C	1:D:191:LEU:CD1	2.87	0.47
1:A:125:GLU:OE1	1:B:206:HIS:HE1	1.97	0.47
1:D:70:ARG:HD3	6:D:609:HOH:O	2.14	0.47
1:A:69:GLN:C	1:A:70:ARG:HG3	2.40	0.47
1:D:188:GLU:HG3	1:D:189:GLU:HG3	1.97	0.46
1:C:136:LEU:C	1:C:136:LEU:HD13	2.41	0.46
1:A:167:PHE:CG	1:B:39:PRO:HG3	2.51	0.46
1:A:206:HIS:HD2	1:B:200:TYR:OH	1.99	0.46
1:B:61:GLY:O	1:B:141:ILE:HA	2.16	0.46
1:B:189:GLU:HB3	1:B:191:LEU:HD12	1.98	0.46
1:C:49:VAL:O	1:C:137:SER:HA	2.16	0.45
1:D:121:GLY:HA3	1:D:146:VAL:CG1	2.45	0.45
1:A:80:VAL:HB	1:A:168:VAL:CG1	2.47	0.45
1:A:70:ARG:HD3	6:A:412:HOH:O	2.16	0.45
1:A:71:THR:O	1:A:73:HIS:HD2	2.00	0.45
1:C:81:LYS:HA	1:C:91:CYS:O	2.17	0.45
1:A:70:ARG:CD	6:A:412:HOH:O	2.65	0.44
1:B:34:THR:O	1:B:45:THR:HA	2.16	0.44
1:B:87:MET:HE3	1:B:87:MET:HB3	1.89	0.44
1:C:132:MET:HE2	4:C:305:EDO:O1	2.18	0.44
1:A:82:GLN:HG2	1:A:168:VAL:HG22	2.00	0.44
1:B:190:HIS:O	1:B:190:HIS:CD2	2.71	0.44
1:A:104:THR:CG2	1:A:107:ALA:H	2.17	0.43
1:D:112:GLU:O	1:D:116:GLU:HG3	2.18	0.43
1:B:165:GLY:HA2	1:B:167:PHE:CZ	2.54	0.43
1:A:194:ASP:HA	1:B:131:CYS:SG	2.59	0.43
1:A:200:TYR:OH	1:B:206:HIS:HD2	2.01	0.43
1:B:37:MET:SD	1:B:41:GLY:C	3.02	0.43
1:B:104:THR:HG23	1:B:107:ALA:H	1.83	0.43
1:A:134:PRO:HB2	1:B:84:ARG:HG3	2.01	0.43
1:C:114:GLU:OE2	1:C:120:LYS:HE3	2.19	0.43
1:C:206:HIS:HE1	1:D:125:GLU:OE1	2.02	0.42
1:B:33:LYS:HD2	6:B:464:HOH:O	2.18	0.42
1:A:138:ASN:HB3	1:B:86:PRO:O	2.20	0.42
1:A:34:THR:O	1:A:45:THR:HA	2.19	0.42
1:C:97:GLY:HA3	1:C:112:GLU:CD	2.45	0.42
1:A:87:MET:HE3	1:A:87:MET:HB3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:VAL:O	1:C:66:PRO:HD3	2.20	0.41
1:D:37:MET:SD	1:D:41:GLY:C	3.03	0.41
1:B:14:LYS:HE3	1:B:39:PRO:HB2	2.02	0.41
1:A:203:ALA:HB3	1:B:203:ALA:CB	2.45	0.41
1:C:15:GLN:N	6:C:410:HOH:O	2.54	0.41
1:C:38:ASP:OD1	1:C:38:ASP:C	2.63	0.41
1:C:38:ASP:OD1	1:C:40:THR:N	2.51	0.41
1:D:68:LEU:HA	1:D:148:ILE:HB	2.02	0.41
1:A:104:THR:HG22	1:A:107:ALA:HB2	2.03	0.41
1:B:194:ASP:OD2	1:B:196:ARG:NH2	2.42	0.40
1:D:54:ARG:NH1	1:D:138:ASN:O	2.50	0.40

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	192/209 (92%)	184 (96%)	6 (3%)	2 (1%)	12	2
1	B	190/209 (91%)	182 (96%)	7 (4%)	1 (0%)	24	12
1	C	191/209 (91%)	184 (96%)	3 (2%)	4 (2%)	5	0
1	D	190/209 (91%)	177 (93%)	9 (5%)	4 (2%)	5	0
All	All	763/836 (91%)	727 (95%)	25 (3%)	11 (1%)	9	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	57	GLN
1	D	54	ARG
1	C	55	LYS
1	D	59	ALA

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Mol	Chain	Res	Type
1	D	56	GLU
1	A	156	ALA
1	C	164	ASP
1	D	58	THR
1	A	66	PRO
1	B	66	PRO
1	C	66	PRO

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	155/179 (87%)	151 (97%)	4 (3%)	40	17
1	B	155/179 (87%)	153 (99%)	2 (1%)	61	43
1	C	146/179 (82%)	139 (95%)	7 (5%)	23	5
1	D	151/179 (84%)	148 (98%)	3 (2%)	48	26
All	All	607/716 (85%)	591 (97%)	16 (3%)	40	17

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	70	ARG
1	A	189	GLU
1	A	191	LEU
1	B	33	LYS
1	B	38	ASP
1	C	31	LEU
1	C	38	ASP
1	C	53	THR
1	C	57	GLN
1	C	164	ASP
1	C	189	GLU
1	C	190	HIS
1	D	53	THR

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Mol	Chain	Res	Type
1	D	58	THR
1	D	72	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	73	HIS
1	A	82	GLN
1	A	180	GLN
1	A	206	HIS
1	B	82	GLN
1	B	190	HIS
1	B	206	HIS
1	B	208	ASN
1	C	206	HIS
1	D	149	ASN
1	D	155	ASN
1	D	190	HIS
1	D	206	HIS
1	D	208	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 [i](#)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	$\# Z > 2$
4	EDO	B	302	-	3,3,3	0.31	0	2,2,2	0.26	0
3	PWJ	A	303	-	16,17,17	1.68	2 (12%)	19,26,26	1.91	4 (21%)
3	PWJ	D	501	-	16,17,17	1.96	6 (37%)	19,26,26	1.52	3 (15%)
4	EDO	D	504	-	3,3,3	0.17	0	2,2,2	0.63	0
3	PWJ	C	306	-	16,17,17	1.63	2 (12%)	19,26,26	1.66	3 (15%)
3	PWJ	B	305	-	16,17,17	1.40	2 (12%)	19,26,26	2.19	7 (36%)
4	EDO	B	306	-	3,3,3	0.20	0	2,2,2	0.03	0
4	EDO	A	304	-	3,3,3	0.29	0	2,2,2	0.29	0
4	EDO	C	305	-	3,3,3	0.15	0	2,2,2	0.18	0
4	EDO	C	301	-	3,3,3	0.21	0	2,2,2	0.41	0
4	EDO	A	305	-	3,3,3	0.27	0	2,2,2	0.30	0
4	EDO	C	304	-	3,3,3	0.14	0	2,2,2	0.41	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
4	EDO	B	302	-	-	1/1/1/1	-
3	PWJ	A	303	-	-	3/6/8/8	0/2/2/2
3	PWJ	D	501	-	-	0/6/8/8	0/2/2/2
4	EDO	D	504	-	-	0/1/1/1	-
3	PWJ	C	306	-	-	6/6/8/8	0/2/2/2
3	PWJ	B	305	-	-	1/6/8/8	0/2/2/2
4	EDO	B	306	-	-	0/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
4	EDO	C	305	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-
4	EDO	A	305	-	-	1/1/1/1	-
4	EDO	C	304	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	PWJ	C6-C5	5.27	1.59	1.49
3	C	306	PWJ	C6-C5	4.66	1.57	1.49
3	D	501	PWJ	C1-N1	3.48	1.45	1.38
3	B	305	PWJ	C6-C5	3.36	1.55	1.49
3	D	501	PWJ	C6-C5	3.24	1.55	1.49
3	B	305	PWJ	C1-N1	3.17	1.45	1.38
3	D	501	PWJ	C3-C2	2.94	1.42	1.35
3	D	501	PWJ	C1-N	2.66	1.38	1.33
3	D	501	PWJ	C-CL	-2.60	1.66	1.72
3	C	306	PWJ	C1-N1	2.32	1.43	1.38
3	D	501	PWJ	C2-N	2.25	1.42	1.38
3	A	303	PWJ	C-CL	-2.06	1.67	1.72

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	305	PWJ	C5-C4-N1	-5.57	116.45	123.20
3	A	303	PWJ	C8-C7-C5	5.53	123.89	118.25
3	C	306	PWJ	C8-C7-C5	4.92	123.27	118.25
3	B	305	PWJ	C8-C7-C5	4.73	123.08	118.25
3	A	303	PWJ	C5-C4-N1	-3.96	118.41	123.20
3	D	501	PWJ	C5-C4-N1	-3.90	118.47	123.20
3	D	501	PWJ	C6-C5-C7	-3.41	118.45	123.06
3	D	501	PWJ	C8-C7-C5	3.26	121.57	118.25
3	C	306	PWJ	C5-C4-N1	-3.13	119.41	123.20
3	B	305	PWJ	F1-C6-C5	2.92	118.32	112.68
3	A	303	PWJ	F1-C6-C5	2.74	117.96	112.68
3	A	303	PWJ	C6-C5-C4	-2.69	117.27	120.12
3	B	305	PWJ	C2-N-C1	-2.61	102.50	105.08
3	C	306	PWJ	F-C6-C5	2.50	117.50	112.68
3	B	305	PWJ	C3-C2-N	2.28	113.72	110.74
3	B	305	PWJ	C6-C5-C7	-2.13	120.18	123.06
3	B	305	PWJ	C3-N1-C1	-2.08	105.40	106.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	306	PWJ	C4-C5-C6-F
3	C	306	PWJ	C4-C5-C6-F1
3	C	306	PWJ	C4-C5-C6-F2
3	C	306	PWJ	C7-C5-C6-F

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Mol	Chain	Res	Type	Atoms
3	C	306	PWJ	C7-C5-C6-F2
4	A	305	EDO	O1-C1-C2-O2
4	B	302	EDO	O1-C1-C2-O2
3	C	306	PWJ	C7-C5-C6-F1
3	A	303	PWJ	C4-C5-C6-F2
4	C	304	EDO	O1-C1-C2-O2
3	A	303	PWJ	C4-C5-C6-F
3	A	303	PWJ	C4-C5-C6-F1
3	B	305	PWJ	C4-C5-C6-F

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	EDO	2	0
4	C	305	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	194/209 (92%)	0.95	25 (12%) 7 10	15, 28, 50, 65	13 (6%)
1	B	194/209 (92%)	1.03	31 (15%) 5 6	17, 32, 60, 78	6 (3%)
1	C	193/209 (92%)	1.62	57 (29%) 1 1	14, 32, 55, 67	25 (12%)
1	D	194/209 (92%)	2.01	73 (37%) 1 1	15, 36, 59, 81	29 (14%)
All	All	775/836 (92%)	1.40	186 (24%) 2 2	14, 32, 57, 81	73 (9%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	GLY	12.4
1	A	191	LEU	10.9
1	A	14	LYS	10.1
1	C	163	GLY	10.0
1	C	162	PRO	9.6
1	D	152	ASP	9.1
1	D	208	ASN	8.9
1	B	54	ARG	8.4
1	C	161	LYS	8.1
1	B	55	LYS	7.8
1	D	58	THR	7.2
1	C	120	LYS	7.0
1	A	188	GLU	6.9
1	C	190	HIS	6.9
1	C	23	ILE	6.8
1	D	57	GLN	6.7
1	C	166	GLU	6.6
1	D	151	ASP	6.3
1	B	57	GLN	6.2
1	D	167	PHE	6.2
1	B	31	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	74	TYR	6.0
1	C	31	LEU	6.0
1	D	154	GLU	6.0
1	D	73	HIS	5.7
1	D	29	VAL	5.7
1	A	189	GLU	5.5
1	A	190	HIS	5.4
1	C	18	ILE	5.4
1	D	53	THR	5.2
1	C	40	THR	5.2
1	D	162	PRO	5.0
1	D	55	LYS	4.9
1	D	40	THR	4.9
1	D	163	GLY	4.7
1	A	28	TRP	4.7
1	C	16	TYR	4.6
1	D	31	LEU	4.6
1	D	56	GLU	4.6
1	A	55	LYS	4.5
1	C	164	ASP	4.5
1	C	37	MET	4.5
1	D	122	ASP	4.5
1	A	157	ARG	4.4
1	D	168	VAL	4.4
1	C	17	ILE	4.3
1	D	59	ALA	4.2
1	A	167	PHE	4.2
1	A	158	PRO	4.2
1	C	136	LEU	4.1
1	C	28	TRP	4.1
1	C	39	PRO	4.1
1	D	45	THR	4.1
1	B	46	TRP	4.0
1	B	167	PHE	3.9
1	B	163	GLY	3.8
1	A	56	GLU	3.8
1	D	113	LEU	3.8
1	C	54	ARG	3.7
1	D	54	ARG	3.7
1	D	158	PRO	3.7
1	C	74	TYR	3.7
1	D	23	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	160	PRO	3.6
1	D	16	TYR	3.6
1	C	191	LEU	3.6
1	D	90	TYR	3.5
1	C	21	GLU	3.5
1	D	156	ALA	3.5
1	D	100	ASP	3.5
1	C	43	THR	3.5
1	D	28	TRP	3.4
1	D	155	ASN	3.4
1	A	72	LEU	3.4
1	B	22	LEU	3.4
1	C	22	LEU	3.4
1	B	14	LYS	3.4
1	D	102	GLY	3.4
1	B	58	THR	3.3
1	A	42	LYS	3.3
1	B	39	PRO	3.2
1	D	14	LYS	3.2
1	B	28	TRP	3.2
1	B	191	LEU	3.2
1	C	46	TRP	3.2
1	C	41	GLY	3.2
1	C	167	PHE	3.2
1	C	104	THR	3.2
1	B	102	GLY	3.1
1	D	148	ILE	3.1
1	D	52	THR	3.0
1	C	168	VAL	3.0
1	C	36	TYR	3.0
1	D	119	TYR	3.0
1	B	160	PRO	3.0
1	D	49	VAL	2.9
1	C	56	GLU	2.9
1	C	52	THR	2.9
1	B	165	GLY	2.9
1	D	97	GLY	2.9
1	B	164	ASP	2.9
1	C	55	LYS	2.9
1	C	35	THR	2.8
1	D	115	GLU	2.8
1	B	159	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	88	GLY	2.8
1	A	23	ILE	2.8
1	D	104	THR	2.8
1	C	26	GLY	2.8
1	D	39	PRO	2.8
1	D	18	ILE	2.8
1	C	58	THR	2.8
1	D	164	ASP	2.7
1	B	208	ASN	2.7
1	B	190	HIS	2.7
1	A	57	GLN	2.7
1	D	101	ASP	2.7
1	B	162	PRO	2.7
1	D	161	LYS	2.6
1	C	53	THR	2.6
1	A	27	LYS	2.6
1	B	176	ASN	2.6
1	C	32	GLU	2.6
1	D	36	TYR	2.6
1	D	67	VAL	2.6
1	D	99	ILE	2.6
1	D	46	TRP	2.6
1	C	29	VAL	2.5
1	C	99	ILE	2.5
1	D	60	ASP	2.5
1	C	38	ASP	2.5
1	C	101	ASP	2.5
1	D	118	GLY	2.5
1	B	40	THR	2.5
1	A	31	LEU	2.4
1	D	121	GLY	2.4
1	D	165	GLY	2.4
1	C	49	VAL	2.4
1	D	24	SER	2.4
1	B	23	ILE	2.4
1	D	70	ARG	2.4
1	D	41	GLY	2.4
1	A	58	THR	2.4
1	A	40	THR	2.3
1	D	136	LEU	2.3
1	B	161	LYS	2.3
1	B	101	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	27	LYS	2.3
1	D	107	ALA	2.3
1	D	173	LEU	2.3
1	B	18	ILE	2.3
1	D	25	GLU	2.3
1	D	43	THR	2.3
1	C	207	ALA	2.3
1	C	47	GLU	2.3
1	B	186	VAL	2.3
1	C	57	GLN	2.2
1	C	184	ALA	2.2
1	C	24	SER	2.2
1	C	15	GLN	2.2
1	A	154	GLU	2.2
1	A	104	THR	2.2
1	D	172	SER	2.2
1	D	184	ALA	2.2
1	D	207	ALA	2.2
1	C	42	LYS	2.2
1	A	39	PRO	2.2
1	D	35	THR	2.2
1	C	186	VAL	2.1
1	D	166	GLU	2.1
1	D	139	CYS	2.1
1	B	41	GLY	2.1
1	A	22	LEU	2.1
1	D	27	LYS	2.1
1	B	158	PRO	2.1
1	C	45	THR	2.1
1	D	171	ILE	2.1
1	C	156	ALA	2.1
1	C	72	LEU	2.1
1	A	18	ILE	2.1
1	D	17	ILE	2.1
1	A	165	GLY	2.1
1	C	59	ALA	2.1
1	D	83	PHE	2.1
1	C	153	ALA	2.0
1	B	29	VAL	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($\text{\AA}^2$)	Q<0.9
4	EDO	B	302	4/4	0.75	0.20	37,37,38,38	0
3	PWJ	D	501	16/16	0.79	0.14	37,46,58,68	16
5	CL	B	301	1/1	0.81	0.23	69,69,69,69	0
4	EDO	C	301	4/4	0.82	0.17	32,42,43,47	0
4	EDO	C	305	4/4	0.83	0.16	30,31,33,36	4
3	PWJ	A	303	16/16	0.84	0.14	33,41,45,47	16
4	EDO	A	305	4/4	0.84	0.18	46,47,47,52	0
3	PWJ	B	305	16/16	0.85	0.17	30,35,45,47	16
3	PWJ	C	306	16/16	0.86	0.15	43,48,56,58	16
4	EDO	C	304	4/4	0.87	0.14	34,35,35,39	4
2	MG	B	304	1/1	0.89	0.09	59,59,59,59	0
4	EDO	D	504	4/4	0.90	0.17	36,36,40,40	4
2	MG	A	302	1/1	0.90	0.10	65,65,65,65	0
4	EDO	A	304	4/4	0.92	0.09	25,28,28,30	0
4	EDO	B	306	4/4	0.93	0.10	28,29,30,30	4
2	MG	C	302	1/1	0.94	0.18	55,55,55,55	0
2	MG	C	303	1/1	0.96	0.05	31,31,31,31	0
2	MG	D	503	1/1	0.96	0.12	36,36,36,36	0
2	MG	B	303	1/1	0.96	0.04	31,31,31,31	0
2	MG	A	301	1/1	0.98	0.06	29,29,29,29	0
2	MG	D	502	1/1	0.98	0.05	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.