



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:09 am GMT

PDB ID : 5FO8
Title : Crystal Structure of Human Complement C3b in Complex with MCP (CCP1-4)
Authors : Forneris, F.; Wu, J.; Xue, X.; Gros, P.
Deposited on : 2015-11-18
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

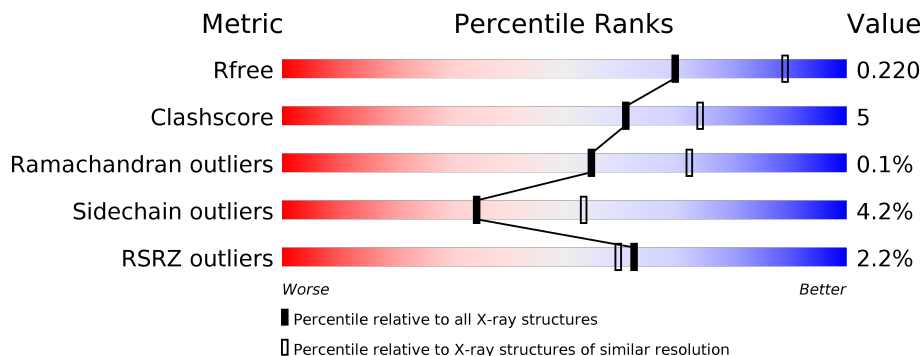
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	645	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 84%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 1% 84% 14% </div> </div>
2	B	915	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 14%, green 83%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 3% 83% 14% </div> </div>
3	C	252	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 46%, grey 49%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 2% 46% 49% </div> </div>

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
5	EDO	A	1668	-	-	-	X
5	EDO	B	2664	-	-	-	X
5	EDO	B	2667	-	-	-	X
5	EDO	B	2670	-	-	-	X
5	EDO	B	2674	-	-	-	X
5	EDO	B	2675	-	-	-	X
5	EDO	B	2676	-	-	-	X
5	EDO	B	2678	-	-	-	X
5	EDO	B	2680	-	-	-	X
5	EDO	B	2681	-	-	-	X
5	EDO	B	2682	-	-	-	X
5	EDO	B	2684	-	-	-	X
5	EDO	B	2686	-	-	-	X
5	EDO	B	2687	-	-	-	X
5	EDO	B	2688	-	-	-	X
5	EDO	B	2691	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13810 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 COMPLEMENT C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			4979	3169	844	951	15			

- Molecule 2 is a protein called COMPLEMENT C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	894	Total	C	N	O	S	0	1	0
			7145	4530	1201	1376	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called MEMBRANE COFACTOR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	0	0
			999	644	157	189	9			

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	N	O	0	0
			39	22	2	15		

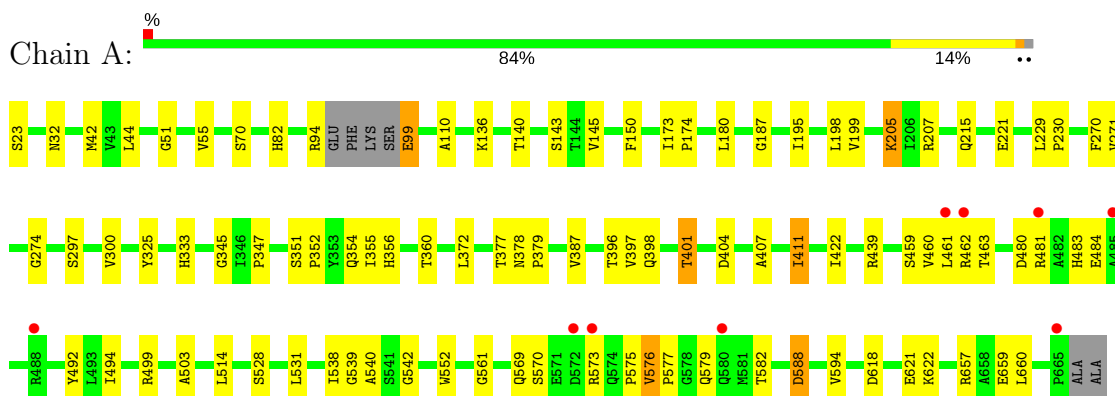
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	172	Total 172	O 172	0	0
7	B	293	Total 293	O 293	0	0
7	C	27	Total 27	O 27	0	0

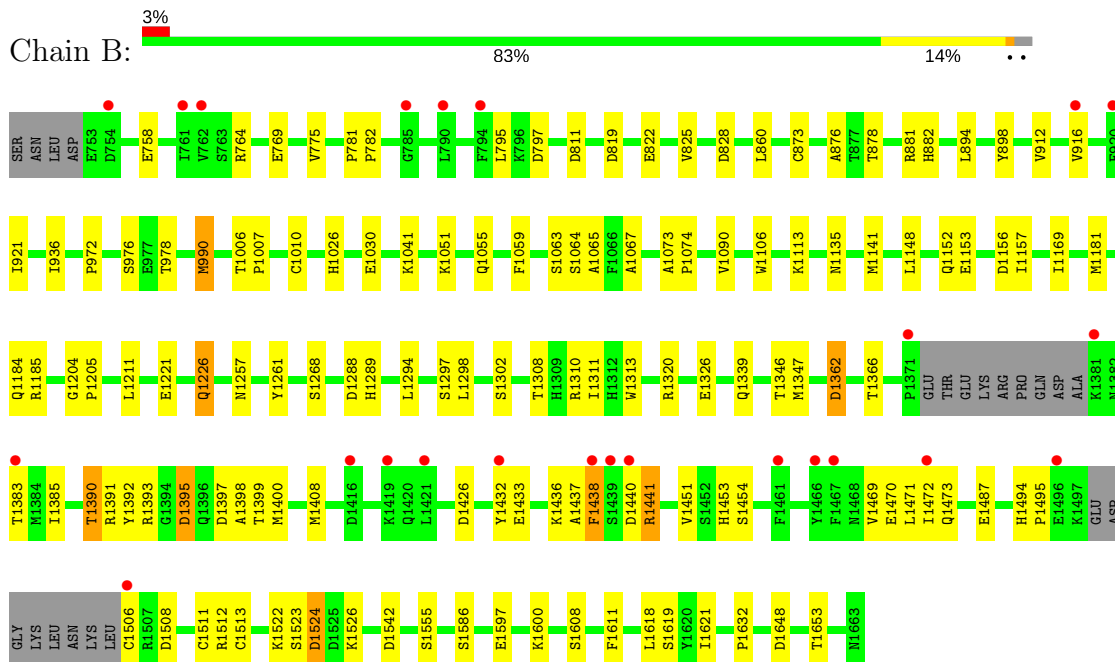
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: COMPLEMENT C3



• Molecule 2: COMPLEMENT C3



• Molecule 3: MEMBRANE COFACTOR PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	82.83Å 130.63Å 233.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.02 – 2.40 65.31 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (57.02-2.40) 95.2 (65.31-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.219 0.187 , 0.220	Depositor DCC
R_{free} test set	4928 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.5	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	0.94	EDS
Total number of atoms	13810	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: BMA, NAG, 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	0.27	0/5079	0.47	0/6902
2	B	0.29	1/7291 (0.0%)	0.46	1/9872 (0.0%)
3	C	0.25	0/1029	0.42	0/1399
All	All	0.28	1/13399 (0.0%)	0.46	1/18173 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1511	CYS	CB-SG	5.39	1.91	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1362	ASP	CB-CG-OD1	5.05	122.84	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	4979	0	5037	55	0
2	B	7145	0	7070	80	0
3	C	999	0	962	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	25	2	0
5	A	16	0	24	1	0
5	B	112	0	168	12	0
6	B	39	0	34	0	0
7	A	172	0	0	4	0
7	B	293	0	0	17	1
7	C	27	0	0	0	0
All	All	13810	0	13320	137	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 5.

All (137) 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)
2:B:1586:SER:OG	7:B:2246:HOH:O	1.83	0.91
2:B:873:CYS:HG	2:B:1513:CYS:HG	1.09	0.85
1:A:351:SER:O	7:A:2090:HOH:O	2.00	0.79
2:B:1010:CYS:SG	7:B:2078:HOH:O	2.42	0.77
2:B:819:ASP:O	7:B:2035:HOH:O	2.03	0.76
2:B:1297:SER:HG	2:B:1308:THR:HG1	1.31	0.73
2:B:1313:TRP:O	7:B:2231:HOH:O	2.07	0.71
1:A:503:ALA:H	4:A:1063:NAG:H81	1.55	0.70
2:B:822:GLU:OE1	7:B:2037:HOH:O	2.08	0.70
1:A:94:ARG:NH1	1:A:99:GLU:OE1	2.23	0.70
1:A:387:VAL:H	1:A:401:THR:HG22	1.56	0.70
1:A:576:VAL:HG12	1:A:579:GLN:HB2	1.74	0.69
1:A:462:ARG:NH2	1:A:552:TRP:O	2.27	0.68
2:B:1288:ASP:OD1	2:B:1289:HIS:ND1	2.29	0.67
2:B:1310:ARG:O	2:B:1320:ARG:NH2	2.29	0.66
2:B:1611:PHE:HD1	2:B:1618:LEU:HD21	1.59	0.65
1:A:569:GLN:HA	1:A:570:SER:HB3	1.77	0.65
2:B:1508:ASP:OD1	2:B:1512:ARG:NH2	2.29	0.65
2:B:1524:ASP:N	2:B:1524:ASP:OD1	2.26	0.64
1:A:32:ASN:OD1	7:A:2004:HOH:O	2.16	0.63
1:A:594:VAL:HG12	2:B:775:VAL:HG22	1.81	0.63
2:B:916:VAL:HG12	2:B:921:ILE:HB	1.82	0.62
1:A:136:LYS:NZ	2:B:769:GLU:OE1	2.33	0.61
2:B:1339:GLN:HG2	5:B:2682:EDO:H11	1.83	0.60
2:B:972:PRO:HB3	2:B:1621:ILE:HD12	1.83	0.60
1:A:481:ARG:HD3	1:A:484:GLU:HG2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ILE:HD13	1:A:531:LEU:HD23	1.84	0.59
1:A:480:ASP:OD1	1:A:483:HIS:ND1	2.34	0.58
2:B:758:GLU:OE1	2:B:881:ARG:NH2	2.36	0.58
1:A:51:GLY:O	1:A:82:HIS:HE1	1.86	0.57
1:A:588:ASP:OD1	1:A:588:ASP:N	2.33	0.56
1:A:576:VAL:HG22	1:A:577:PRO:HD2	1.87	0.56
1:A:205:LYS:HG3	1:A:221:GLU:HG2	1.88	0.56
1:A:198:LEU:HD13	2:B:1347:MET:HG3	1.87	0.55
3:C:213:ASN:HB2	3:C:215:VAL:HG22	1.87	0.55
1:A:140:THR:O	1:A:143:SER:OG	2.24	0.55
1:A:378:ASN:OD1	7:A:2091:HOH:O	2.18	0.55
1:A:360:THR:HG21	1:A:372:LEU:HD23	1.88	0.55
1:A:271:VAL:HG11	1:A:300:VAL:HG11	1.88	0.55
1:A:503:ALA:N	4:A:1063:NAG:H81	2.22	0.54
2:B:1141:MET:HG3	5:B:2678:EDO:H11	1.87	0.54
1:A:461:LEU:HD11	1:A:463:THR:HG23	1.88	0.54
2:B:1226:GLN:NE2	7:B:2200:HOH:O	2.40	0.53
1:A:99:GLU:OE1	1:A:99:GLU:HA	2.08	0.53
2:B:1261:TYR:OH	2:B:1268:SER:HB2	2.08	0.53
3:C:251:THR:HG22	3:C:269:VAL:HG22	1.90	0.53
2:B:1073:ALA:HA	5:B:2673:EDO:H22	1.90	0.53
2:B:1597:GLU:HB2	2:B:1600:LYS:HG3	1.91	0.52
2:B:1395:ASP:N	2:B:1395:ASP:OD1	2.42	0.52
1:A:539:GLY:HA2	1:A:540:ALA:HB3	1.91	0.52
3:C:166:PRO:HG2	3:C:220:ALA:HB2	1.92	0.52
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.92	0.51
2:B:1007:PRO:HG3	7:B:2095:HOH:O	2.09	0.51
2:B:1221:GLU:OE1	7:B:2194:HOH:O	2.20	0.51
2:B:882:HIS:NE2	2:B:898:TYR:HE1	2.10	0.50
2:B:1611:PHE:CD1	2:B:1618:LEU:HD21	2.44	0.50
5:B:2666:EDO:O2	7:B:2190:HOH:O	2.19	0.50
1:A:483:HIS:CE1	1:A:540:ALA:HB2	2.47	0.50
2:B:876:ALA:HB2	2:B:882:HIS:HB3	1.94	0.50
1:A:32:ASN:HD22	1:A:657:ARG:HH11	1.59	0.49
1:A:573:ARG:HG2	1:A:575:PRO:HD3	1.94	0.49
2:B:1041:LYS:O	5:B:2675:EDO:O2	2.30	0.49
2:B:1362:ASP:O	2:B:1390:THR:HA	2.12	0.49
1:A:401:THR:HA	1:A:407:ALA:HB2	1.94	0.49
1:A:657:ARG:NH2	7:A:2159:HOH:O	2.42	0.49
2:B:1156:ASP:OD2	3:C:245:LYS:NZ	2.39	0.49
2:B:873:CYS:HG	2:B:1513:CYS:CB	2.24	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1257:ASN:HB3	5:B:2691:EDO:H22	1.95	0.48
2:B:1051:LYS:HE3	2:B:1055:GLN:OE1	2.13	0.48
1:A:145:VAL:HG23	1:A:195:ILE:HD11	1.94	0.48
2:B:1398:ALA:HB3	2:B:1451:VAL:HB	1.95	0.48
2:B:1487:GLU:HG2	5:B:2671:EDO:H22	1.94	0.47
2:B:860:LEU:HD22	2:B:916:VAL:HG21	1.96	0.47
2:B:1454:SER:O	7:B:2241:HOH:O	2.20	0.47
1:A:44:LEU:HD13	1:A:55:VAL:HG11	1.96	0.47
1:A:539:GLY:HA3	1:A:542:GLY:N	2.29	0.47
1:A:274:GLY:HA3	1:A:325:TYR:CZ	2.49	0.47
1:A:561:GLY:HA3	1:A:588:ASP:OD2	2.14	0.47
1:A:492:TYR:HB2	1:A:531:LEU:HD21	1.97	0.47
2:B:1408:MET:SD	2:B:1495:PRO:HD3	2.55	0.46
2:B:1362:ASP:OD1	2:B:1393:ARG:NH2	2.48	0.46
2:B:1392:TYR:CG	2:B:1398:ALA:HB2	2.51	0.46
1:A:42:MET:HE1	1:A:110:ALA:HB2	1.98	0.45
2:B:1181:MET:HB3	5:B:2677:EDO:H21	1.98	0.45
2:B:1438:PHE:C	2:B:1440:ASP:H	2.20	0.45
2:B:978:THR:HG23	2:B:1346:THR:HG22	1.98	0.45
1:A:354:GLN:HG3	1:A:377:THR:OG1	2.17	0.45
2:B:1648:ASP:OD1	5:B:2687:EDO:O1	2.25	0.44
2:B:1437:ALA:HA	2:B:1441:ARG:NE	2.33	0.44
2:B:1135:ASN:O	7:B:2149:HOH:O	2.21	0.44
1:A:356:HIS:ND1	5:A:1666:EDO:H21	2.33	0.44
2:B:1113:LYS:HD3	2:B:1113:LYS:HA	1.83	0.44
2:B:1436:LYS:HA	2:B:1436:LYS:HD2	1.83	0.44
1:A:205:LYS:HD2	1:A:207:ARG:NH2	2.33	0.43
1:A:372:LEU:HD11	1:A:422:ILE:HG21	1.99	0.43
1:A:618:ASP:O	1:A:622:LYS:HG2	2.18	0.43
2:B:1397:ASP:OD1	2:B:1453:HIS:ND1	2.45	0.43
2:B:1026:HIS:ND1	7:B:2082:HOH:O	2.04	0.43
2:B:1152:GLN:NE2	7:B:2157:HOH:O	2.40	0.43
1:A:352:PRO:O	1:A:379:PRO:HD3	2.18	0.43
2:B:1067:ALA:HB2	2:B:1074:PRO:HA	2.00	0.43
2:B:1090:VAL:HG21	2:B:1157:ILE:HD13	2.00	0.43
2:B:1632:PRO:O	5:B:2681:EDO:O1	2.28	0.43
3:C:263:ASP:HB2	3:C:284:LEU:HD22	2.01	0.43
1:A:173:ILE:HA	1:A:174:PRO:HD3	1.90	0.42
1:A:150:PHE:HA	1:A:187:GLY:O	2.19	0.42
2:B:1184:GLN:NE2	7:B:2173:HOH:O	2.50	0.42
2:B:1399:THR:OG1	2:B:1400:MET:N	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:VAL:HG11	1:A:411:ILE:HG22	2.01	0.42
1:A:528:SER:OG	1:A:621:GLU:OE2	2.28	0.42
2:B:873:CYS:SG	2:B:1513:CYS:C	2.98	0.42
2:B:1010:CYS:HA	2:B:1059:PHE:CZ	2.54	0.42
2:B:1362:ASP:OD2	2:B:1391:ARG:NH2	2.53	0.42
2:B:1608:SER:HA	2:B:1611:PHE:CE2	2.55	0.42
1:A:229:LEU:HA	1:A:230:PRO:HD3	1.91	0.42
1:A:404:ASP:N	1:A:404:ASP:OD1	2.53	0.42
2:B:1063:SER:O	2:B:1064:SER:HB2	2.20	0.42
1:A:355:ILE:O	1:A:439:ARG:NH1	2.52	0.42
2:B:1204:GLY:HA3	2:B:1205:PRO:HD3	1.91	0.41
2:B:1211:LEU:HB3	5:B:2666:EDO:H12	2.01	0.41
1:A:345:GLY:O	1:A:347:PRO:HD3	2.20	0.41
1:A:270:PHE:HD2	2:B:1400:MET:HE3	1.85	0.41
2:B:781:PRO:HA	2:B:782:PRO:HD3	1.82	0.41
2:B:976:SER:N	7:B:2056:HOH:O	2.13	0.41
2:B:1006:THR:HA	2:B:1007:PRO:HD3	1.86	0.41
2:B:1522:LYS:HA	2:B:1522:LYS:HD3	1.86	0.41
2:B:1185:ARG:NH1	7:B:2144:HOH:O	2.20	0.41
2:B:1065:ALA:HB2	2:B:1106:TRP:CD2	2.56	0.41
1:A:136:LYS:HB2	1:A:136:LYS:HE3	1.89	0.41
2:B:1294:LEU:HB2	2:B:1311:ILE:HB	2.01	0.41
2:B:795:LEU:HD13	2:B:825:VAL:HG22	2.03	0.41
2:B:1148:LEU:HD11	2:B:1169:ILE:HG23	2.02	0.41
2:B:1030:GLU:HG2	7:B:2081:HOH:O	2.20	0.40
3:C:194:ALA:HA	3:C:195:PRO:HD3	1.93	0.40
2:B:1653:THR:HG21	5:B:2680:EDO:H22	2.03	0.40
2:B:990:MET:HE2	2:B:990:MET:HB3	1.91	0.40
1:A:539:GLY:HA3	1:A:542:GLY:H	1.85	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)
7:B:2137:HOH:O	7:B:2291:HOH:O[1_545]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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	635/645 (98%)	617 (97%)	17 (3%)	1 (0%)	51	67
2	B	889/915 (97%)	860 (97%)	29 (3%)	0	100	100
3	C	127/252 (50%)	123 (97%)	4 (3%)	0	100	100
All	All	1651/1812 (91%)	1600 (97%)	50 (3%)	1 (0%)	55	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	659	GLU

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	563/567 (99%)	541 (96%)	22 (4%)	37	56
2	B	792/810 (98%)	757 (96%)	35 (4%)	33	51
3	C	114/222 (51%)	110 (96%)	4 (4%)	41	61
All	All	1469/1599 (92%)	1408 (96%)	61 (4%)	34	53

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	70	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	99	GLU
1	A	180	LEU
1	A	199	VAL
1	A	205	LYS
1	A	215	GLN
1	A	297	SER
1	A	333	HIS
1	A	396	THR
1	A	398	GLN
1	A	401	THR
1	A	411	ILE
1	A	459	SER
1	A	460	VAL
1	A	499	ARG
1	A	514	LEU
1	A	538	ILE
1	A	576	VAL
1	A	582	THR
1	A	588	ASP
1	A	660	LEU
2	B	811	ASP
2	B	828	ASP
2	B	878	THR
2	B	894	LEU
2	B	912	VAL
2	B	936	ILE
2	B	990	MET
2	B	1153	GLU
2	B	1226	GLN
2	B	1298	LEU
2	B	1302	SER
2	B	1326	GLU
2	B	1366	THR
2	B	1383	THR
2	B	1385	ILE
2	B	1390	THR
2	B	1395	ASP
2	B	1426	ASP
2	B	1432	TYR
2	B	1433	GLU
2	B	1438	PHE
2	B	1441	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1469	VAL
2	B	1470	GLU
2	B	1471	LEU
2	B	1472	ILE
2	B	1473	GLN
2	B	1494	HIS
2	B	1506	CYS
2	B	1523	SER
2	B	1524	ASP
2	B	1526	LYS
2	B	1542	ASP
2	B	1555	SER
2	B	1619	SER
3	C	179	GLU
3	C	215	VAL
3	C	284	LEU
3	C	286	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	82	HIS
2	B	919	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](#)

5 carbohydrates 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	$\# Z > 2$
4	NAG	A	1063	1,4	14,14,15	0.53	0	15,19,21	1.13	1 (6%)
4	NAG	A	1064	4	14,14,15	0.52	0	15,19,21	0.78	0
6	NAG	B	1939	2,6	14,14,15	0.51	0	15,19,21	1.05	1 (6%)
6	NAG	B	1940	6	14,14,15	0.57	0	15,19,21	1.22	2 (13%)
6	BMA	B	1941	6	11,11,12	0.82	0	13,15,17	0.75	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	NAG	A	1063	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1064	4	-	0/6/23/26	0/1/1/1
6	NAG	B	1939	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1940	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1941	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1063	NAG	O5-C1-C2	-2.60	107.86	111.47
6	B	1940	NAG	C4-C3-C2	2.49	114.67	111.02
6	B	1939	NAG	C1-O5-C5	2.71	115.91	112.17
6	B	1940	NAG	C3-C4-C5	2.73	115.03	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1063	NAG	2	0

5.6 Ligand geometry

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	1666	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	A	1667	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	A	1668	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	A	1669	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	B	2664	-	3,3,3	0.44	0	2,2,2	0.44	0
5	EDO	B	2665	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	B	2666	-	3,3,3	0.45	0	2,2,2	0.33	0
5	EDO	B	2667	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	B	2668	-	3,3,3	0.47	0	2,2,2	0.25	0
5	EDO	B	2669	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	B	2670	-	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	B	2671	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	B	2672	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	B	2673	-	3,3,3	0.46	0	2,2,2	0.42	0
5	EDO	B	2674	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	B	2675	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	B	2676	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	B	2677	-	3,3,3	0.47	0	2,2,2	0.35	0
5	EDO	B	2678	-	3,3,3	0.44	0	2,2,2	0.40	0
5	EDO	B	2679	-	3,3,3	0.45	0	2,2,2	0.39	0
5	EDO	B	2680	-	3,3,3	0.42	0	2,2,2	0.39	0
5	EDO	B	2681	-	3,3,3	0.45	0	2,2,2	0.33	0
5	EDO	B	2682	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	B	2683	-	3,3,3	0.47	0	2,2,2	0.35	0
5	EDO	B	2684	-	3,3,3	0.46	0	2,2,2	0.15	0
5	EDO	B	2685	-	3,3,3	0.43	0	2,2,2	0.43	0
5	EDO	B	2686	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	B	2687	-	3,3,3	0.45	0	2,2,2	0.39	0
5	EDO	B	2688	-	3,3,3	0.48	0	2,2,2	0.33	0
5	EDO	B	2689	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	B	2690	-	3,3,3	0.47	0	2,2,2	0.43	0
5	EDO	B	2691	-	3,3,3	0.42	0	2,2,2	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1666	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1667	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1668	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1669	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2664	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2665	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2666	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2667	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2668	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2669	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2670	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2671	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2672	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2673	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2674	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2675	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2676	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2677	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2678	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2679	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2680	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2681	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2682	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2683	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2684	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2685	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2686	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2687	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2688	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2689	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2690	-	-	0/1/1/1	0/0/0/0
5	EDO	B	2691	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1666	EDO	1	0
5	B	2666	EDO	2	0
5	B	2671	EDO	1	0
5	B	2673	EDO	1	0
5	B	2675	EDO	1	0
5	B	2677	EDO	1	0
5	B	2678	EDO	1	0
5	B	2680	EDO	1	0
5	B	2681	EDO	1	0
5	B	2682	EDO	1	0
5	B	2687	EDO	1	0
5	B	2691	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	639/645 (99%)	-0.13	9 (1%) 75 74	38, 64, 99, 164	0
2	B	894/915 (97%)	-0.04	24 (2%) 55 52	26, 64, 118, 157	0
3	C	129/252 (51%)	-0.04	4 (3%) 49 47	43, 71, 101, 122	0
All	All	1662/1812 (91%)	-0.07	37 (2%) 62 59	26, 65, 110, 164	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	PRO	6.7
2	B	1466	TYR	5.9
2	B	1438	PHE	4.4
2	B	790	LEU	4.2
1	A	481	ARG	3.8
3	C	160	VAL	3.8
1	A	461	LEU	3.5
3	C	213	ASN	3.4
2	B	916	VAL	3.3
2	B	1432	TYR	3.2
3	C	177	GLU	3.2
2	B	762	VAL	3.1
1	A	572	ASP	3.1
2	B	1416	ASP	3.1
2	B	785	GLY	2.8
2	B	1381	LYS	2.8
2	B	761	ILE	2.7
1	A	573	ARG	2.6
2	B	1467	PHE	2.6
3	C	159	LYS	2.6
2	B	1419	LYS	2.5
2	B	1383	THR	2.4
2	B	1439	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	485	ALA	2.4
2	B	754	ASP	2.3
1	A	580	GLN	2.3
2	B	1421	LEU	2.3
2	B	1472	ILE	2.3
2	B	1496	GLU	2.2
2	B	920	PHE	2.2
1	A	462	ARG	2.2
1	A	488	ARG	2.2
2	B	1461	PHE	2.1
2	B	1440	ASP	2.1
2	B	1506	CYS	2.1
2	B	794	PHE	2.1
2	B	1371	PRO	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	A	1063	14/15	0.93	0.14	-0.87	67,79,90,101	0
6	BMA	B	1941	11/12	0.74	0.26	-	122,143,153,153	0
6	NAG	B	1940	14/15	0.76	0.23	-	102,132,138,142	0
4	NAG	A	1064	14/15	0.82	0.17	-	94,112,117,117	0
6	NAG	B	1939	14/15	0.89	0.16	-	94,100,108,121	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	B	2678	4/4	0.92	0.33	16.21	62,63,64,65	0
5	EDO	B	2674	4/4	0.68	0.34	13.43	82,87,93,96	0
5	EDO	B	2682	4/4	0.85	0.48	13.29	77,81,86,91	0
5	EDO	B	2681	4/4	0.89	0.21	7.76	91,92,92,98	0
5	EDO	B	2670	4/4	0.97	0.27	7.47	45,47,48,49	3
5	EDO	B	2680	4/4	0.90	0.23	6.77	78,86,89,91	0
5	EDO	B	2675	4/4	0.90	0.22	6.58	48,50,51,55	3
5	EDO	B	2691	4/4	0.94	0.26	5.15	47,54,66,77	0
5	EDO	B	2667	4/4	0.95	0.20	4.95	64,65,68,76	1
5	EDO	B	2686	4/4	0.83	0.23	4.75	70,75,86,92	0
5	EDO	B	2684	4/4	0.92	0.19	4.72	36,43,55,66	0
5	EDO	B	2676	4/4	0.86	0.24	4.50	65,66,77,82	0
5	EDO	B	2687	4/4	0.94	0.21	3.58	51,53,55,59	0
5	EDO	B	2664	4/4	0.95	0.18	3.25	42,56,63,72	0
5	EDO	A	1668	4/4	0.79	0.18	2.98	92,92,95,96	0
5	EDO	B	2688	4/4	0.82	0.20	2.79	76,78,82,85	0
5	EDO	B	2673	4/4	0.83	0.19	1.33	70,70,75,77	1
5	EDO	B	2683	4/4	0.96	0.17	0.98	55,56,56,57	0
5	EDO	B	2685	4/4	0.93	0.18	0.98	48,58,61,64	0
5	EDO	B	2690	4/4	0.97	0.17	0.94	33,38,48,54	0
5	EDO	B	2671	4/4	0.84	0.17	0.61	76,76,76,85	1
5	EDO	B	2665	4/4	0.77	0.15	0.51	88,90,92,93	0
5	EDO	B	2666	4/4	0.87	0.23	-	59,60,62,63	2
5	EDO	B	2677	4/4	0.84	0.21	-	85,87,88,88	0
5	EDO	B	2668	4/4	0.75	0.27	-	82,82,84,84	0
5	EDO	A	1667	4/4	0.89	0.19	-	90,90,92,93	0
5	EDO	A	1666	4/4	0.92	0.19	-	79,82,83,85	0
5	EDO	B	2669	4/4	0.93	0.14	-	87,87,88,88	0
5	EDO	A	1669	4/4	0.63	0.27	-	99,99,100,101	0
5	EDO	B	2679	4/4	0.86	0.21	-	68,73,77,82	0
5	EDO	B	2672	4/4	0.85	0.17	-	74,74,76,78	0
5	EDO	B	2689	4/4	0.92	0.21	-	62,65,71,73	0

6.5 Other polymers

There are no such residues in this entry.