



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2026 – 06:13 PM EDT

PDB ID : 9P3H / pdb_00009p3h
Title : Crystal Structure of Conserved Hypothetical Protein from *Stenotrophomonas maltophilia* (strain K279a)
Authors : Minasov, G.; Shuvalova, L.; Brunzelle, J.S.; Wawrzak, Z.; Kiryukhina, O.; Satchell, K.J.F.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on : 2025-06-13
Resolution : 1.85 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

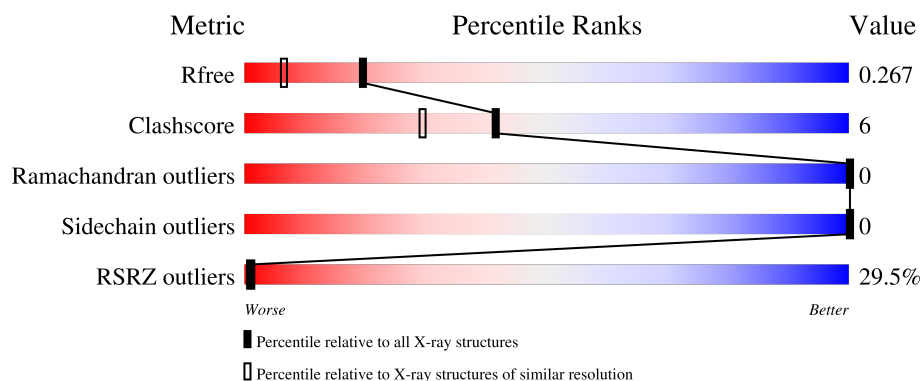
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


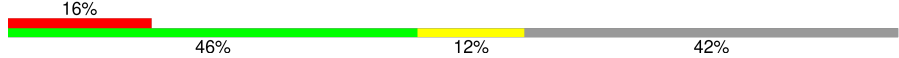


The reported resolution of this entry is 1.85 Å.

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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	444	
1	B	444	
1	C	444	
1	D	444	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9177 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 Conserved hyopthetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	Se	0	3	0
			2213	1379	402	428	1	3			
1	B	258	Total	C	N	O	S	Se	0	1	0
			2064	1283	375	403	1	2			
1	C	265	Total	C	N	O	S	Se	0	1	0
			2130	1329	383	415	1	2			
1	D	259	Total	C	N	O	S	Se	0	1	0
			2069	1285	375	406	1	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B2FKX1
A	-1	ASN	-	expression tag	UNP B2FKX1
A	0	ALA	-	expression tag	UNP B2FKX1
B	-2	SER	-	expression tag	UNP B2FKX1
B	-1	ASN	-	expression tag	UNP B2FKX1
B	0	ALA	-	expression tag	UNP B2FKX1
C	-2	SER	-	expression tag	UNP B2FKX1
C	-1	ASN	-	expression tag	UNP B2FKX1
C	0	ALA	-	expression tag	UNP B2FKX1
D	-2	SER	-	expression tag	UNP B2FKX1
D	-1	ASN	-	expression tag	UNP B2FKX1
D	0	ALA	-	expression tag	UNP B2FKX1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).

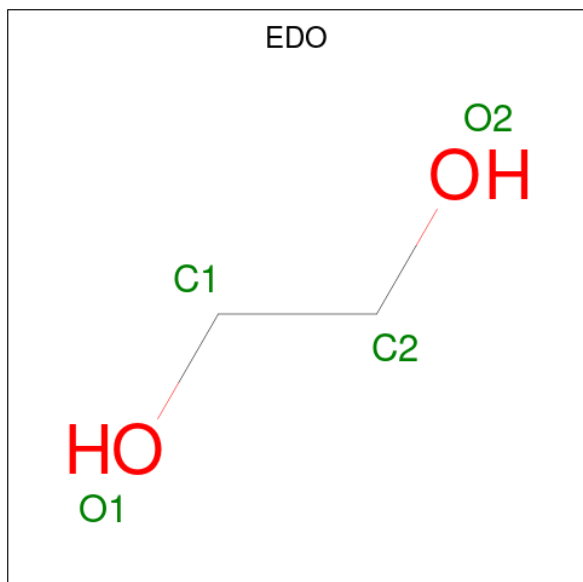


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

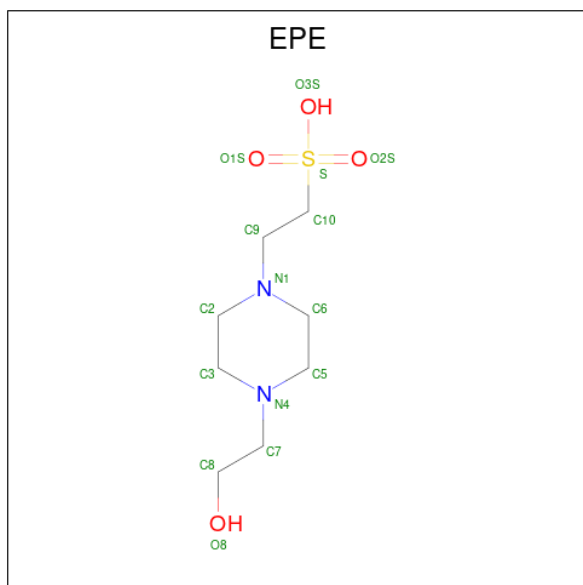
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	D	2	Total	Cl	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

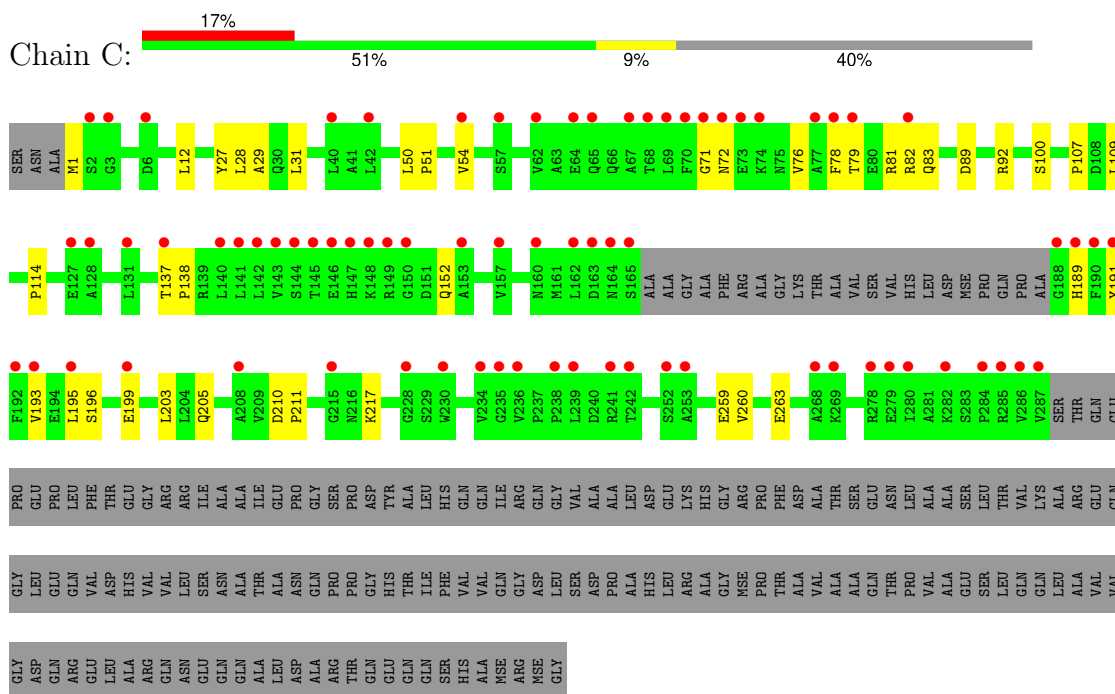


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C N O S 15 8 2 4 1	0	0

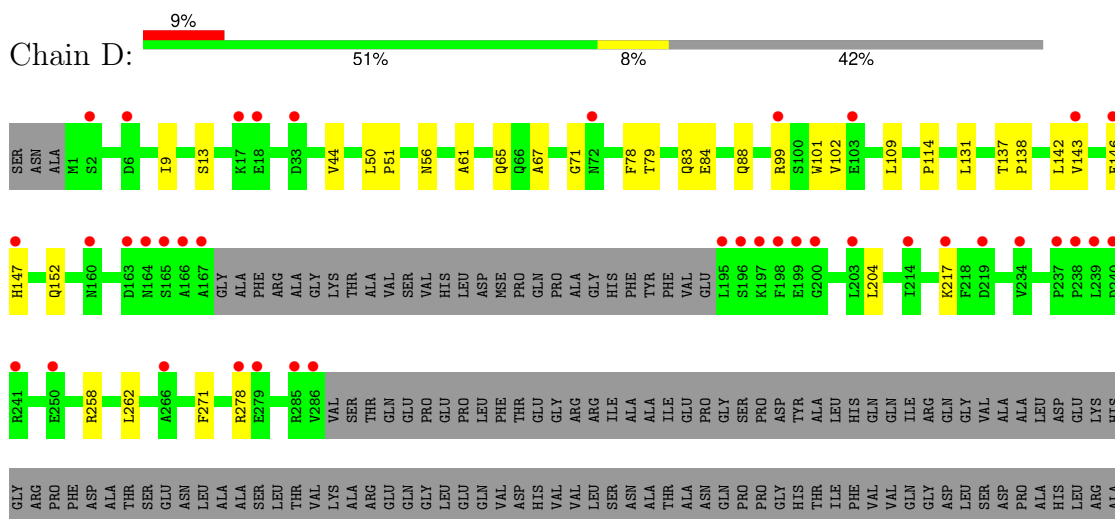
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	109	Total O 110 110	0	1
7	B	147	Total O 148 148	0	1
7	C	148	Total O 151 151	0	3
7	D	182	Total O 187 187	0	5

- Molecule 1: Conserved hypothetical protein



- Molecule 1: Conserved hypothetical protein



GLY MSE THR ALA VAL ALA ALA GLN THR PRO VAL ALA GLU SER LEU GLN LEU ALA VAL VAL GLY ASP GLN ARG GLO LEU ALA ARG GLN ASN GLO GLN GLN ALA LEU ASP ALA ARG THR GLN GLU GLN GLN SER HIS ALA MSE ARG MSE GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.40Å 144.74Å 79.04Å 90.00° 113.16° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	91.1 (30.00-1.85) 95.0 (30.00-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.192 , 0.215 0.244 , 0.267	Depositor DCC
R_{free} test set	5173 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9177	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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, PGE, EPE, EDO, SO4

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	0.44	0/2263	0.93	1/3068 (0.0%)
1	B	0.45	0/2105	0.95	1/2854 (0.0%)
1	C	0.45	0/2175	0.96	1/2950 (0.0%)
1	D	0.46	0/2110	1.00	1/2862 (0.0%)
All	All	0.45	0/8653	0.96	4/11734 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	PRO	N-CA-C	-5.41	103.29	111.41
1	D	114	PRO	N-CA-C	-5.17	103.70	111.57
1	A	114	PRO	N-CA-C	-5.08	103.84	111.57
1	C	114	PRO	N-CA-C	-5.04	103.86	111.41

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	2213	0	2133	38	0
1	B	2064	0	1999	33	0
1	C	2130	0	2048	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2069	0	1997	20	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	15	0	0	0	0
2	D	25	0	0	0	0
3	A	10	0	14	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
5	B	4	0	6	0	0
5	C	8	0	12	0	0
6	D	15	0	18	0	0
7	A	110	0	0	1	0
7	B	148	0	0	1	0
7	C	151	0	0	2	0
7	D	187	0	0	0	0
All	All	9177	0	8227	108	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 6.

All (108) 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:D:13:SER:OG	1:D:99:ARG:NH2	2.21	0.74
1:C:89:ASP:OD1	1:C:92:ARG:NH2	2.27	0.68
1:A:137:THR:HB	1:A:138:PRO:HD3	1.79	0.65
1:B:204:LEU:HA	1:B:217:LYS:HE2	1.80	0.63
1:B:255:ASN:O	1:B:259:GLU:HG3	1.99	0.62
1:A:152:GLN:HG2	1:B:100:SER:CB	2.31	0.61
1:C:50:LEU:HB3	1:C:51:PRO:HD3	1.82	0.61
1:B:67:ALA:O	1:B:71:GLY:HA2	2.01	0.60
1:A:272:HIS:CG	1:A:273:PRO:HD2	2.37	0.60
1:B:146:GLU:OE1	1:B:146:GLU:C	2.46	0.59
1:B:78:PHE:CE2	1:B:83:GLN:HG2	2.37	0.59
1:C:12:LEU:HD11	1:C:28:LEU:HD21	1.85	0.58
1:C:76:VAL:HG13	1:C:82:ARG:NH2	2.18	0.58
1:A:255:ASN:O	1:A:259[A]:GLU:OE1	2.20	0.58
1:A:146:GLU:OE1	1:A:146:GLU:C	2.47	0.58
1:A:152:GLN:HG2	1:B:100:SER:HB3	1.84	0.58
1:D:204:LEU:HA	1:D:217:LYS:HE2	1.85	0.57
1:D:9:ILE:HD11	1:D:102:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLU:C	1:D:146:GLU:OE1	2.48	0.57
1:A:119:LEU:HD11	1:A:139:ARG:HG3	1.87	0.55
1:C:109:LEU:HD21	1:D:109:LEU:HD21	1.88	0.55
1:A:109:LEU:HD21	1:B:109:LEU:HD21	1.88	0.55
1:A:12:LEU:HD11	1:A:28:LEU:HD21	1.90	0.54
1:D:50:LEU:HB3	1:D:51:PRO:HD3	1.88	0.54
1:C:71:GLY:O	1:C:72:ASN:HB3	2.08	0.53
1:A:138:PRO:O	1:A:142:LEU:HG	2.08	0.53
1:D:137:THR:HB	1:D:138:PRO:HD3	1.90	0.53
1:B:137:THR:HB	1:B:138:PRO:HD3	1.90	0.52
1:A:140:LEU:HD12	1:A:141:LEU:N	2.24	0.52
1:C:137:THR:HB	1:C:138:PRO:HD3	1.92	0.52
1:A:205:GLN:O	1:A:217:LYS:HE3	2.10	0.52
1:A:183:MSE:HB3	1:A:188:GLY:HA3	1.91	0.51
1:B:50:LEU:HB3	1:B:51:PRO:HD3	1.92	0.51
1:A:183:MSE:HB3	1:A:188:GLY:CA	2.41	0.51
1:B:9:ILE:HD11	1:B:102:VAL:HG21	1.92	0.51
1:A:89:ASP:OD1	1:A:92:ARG:NH2	2.44	0.51
1:C:78:PHE:CE2	1:C:83:GLN:HG2	2.47	0.50
1:A:78:PHE:CE2	1:A:83:GLN:HG2	2.46	0.50
1:A:259[B]:GLU:OE1	1:A:259[B]:GLU:HA	2.13	0.48
1:A:181:LEU:H	1:A:181:LEU:HD12	1.79	0.47
1:A:185:GLN:HE21	1:A:185:GLN:HA	1.80	0.47
1:A:50:LEU:O	1:A:54:VAL:HG23	2.14	0.47
1:A:255:ASN:O	1:A:259[B]:GLU:HG2	2.14	0.47
1:B:216:ASN:OD1	1:B:219:ASP:N	2.49	0.46
1:B:250:GLU:O	1:B:254:LEU:HG	2.15	0.46
1:B:84:GLU:O	1:B:88:GLN:HG3	2.16	0.46
1:C:54:VAL:HG21	1:C:199:GLU:HG2	1.98	0.46
1:B:69:LEU:HD23	1:D:143:VAL:HG12	1.96	0.46
1:A:247:ASP:O	1:A:251:ILE:HG13	2.16	0.45
1:C:203:LEU:O	1:C:217:LYS:NZ	2.50	0.45
1:D:84:GLU:O	1:D:88:GLN:HG3	2.16	0.45
1:A:95:LEU:HD21	1:A:99[B]:ARG:HH11	1.82	0.45
1:A:181:LEU:HD12	1:A:181:LEU:N	2.32	0.44
1:C:189:HIS:O	1:C:193:VAL:HG23	2.18	0.44
1:B:78:PHE:CZ	1:B:83:GLN:HG2	2.52	0.44
1:C:71:GLY:O	1:C:72:ASN:CB	2.66	0.44
1:D:78:PHE:CE1	1:D:131:LEU:HD11	2.53	0.44
1:C:205:GLN:O	7:C:601:HOH:O	2.21	0.44
1:A:44:VAL:HG13	1:A:56:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ALA:O	1:B:264:ARG:NH2	2.49	0.43
1:B:245:GLU:O	1:B:251:ILE:HD11	2.18	0.43
1:A:64:GLU:O	1:A:65:GLN:HB2	2.19	0.43
1:A:221:HIS:CG	1:A:254:LEU:HD11	2.52	0.43
1:A:132:ASN:O	1:A:135:CYS:SG	2.73	0.43
1:A:64:GLU:C	1:A:66:GLN:H	2.26	0.43
1:B:99:ARG:O	1:B:103:GLU:HG3	2.18	0.43
1:C:193:VAL:O	1:C:196:SER:OG	2.29	0.43
1:A:100:SER:CB	1:B:152:GLN:HG2	2.49	0.43
1:C:29:ALA:HA	7:C:697:HOH:O	2.19	0.43
1:D:67:ALA:O	1:D:71:GLY:HA2	2.19	0.42
1:D:138:PRO:O	1:D:142:LEU:HG	2.19	0.42
1:D:61:ALA:O	1:D:65:GLN:HG2	2.19	0.42
1:B:164:ASN:O	1:B:165:SER:C	2.62	0.42
1:C:1:MSE:SE	1:C:107:PRO:HD2	2.70	0.42
1:B:221:HIS:CE1	1:B:232:HIS:CD2	3.08	0.42
1:C:152:GLN:HE21	1:D:101:TRP:NE1	2.16	0.42
1:C:259:GLU:O	1:C:263:GLU:HG3	2.19	0.42
1:B:196:SER:N	7:B:612:HOH:O	2.52	0.42
1:B:221:HIS:HA	1:B:231:ASN:O	2.20	0.42
1:B:77:ALA:O	1:B:82:ARG:HD2	2.19	0.42
1:B:216:ASN:ND2	1:B:218:PHE:CE1	2.88	0.41
1:A:30:GLN:OE1	1:A:277:TYR:HB3	2.19	0.41
1:B:146:GLU:OE1	1:B:147:HIS:N	2.53	0.41
1:C:27:TYR:CE2	1:C:31:LEU:HD21	2.55	0.41
1:D:146:GLU:OE1	1:D:147:HIS:N	2.53	0.41
1:A:274:GLU:O	1:A:276:PRO:HD3	2.21	0.41
1:B:89:ASP:OD1	1:B:92:ARG:NH2	2.53	0.41
1:C:79:THR:O	1:C:83:GLN:HG3	2.20	0.41
1:D:258:ARG:O	1:D:262:LEU:HG	2.21	0.41
1:A:50:LEU:N	1:A:51:PRO:CD	2.83	0.41
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.86	0.41
1:A:258:ARG:NH1	1:A:262:LEU:HD11	2.36	0.41
1:B:74[B]:LYS:HD2	1:B:74[B]:LYS:O	2.21	0.41
1:B:258:ARG:O	1:B:262:LEU:HG	2.21	0.41
1:D:44:VAL:HG13	1:D:56:ASN:OD1	2.21	0.41
1:D:271:PHE:HB2	1:D:278:ARG:NH1	2.36	0.41
1:A:138:PRO:HA	7:A:625:HOH:O	2.20	0.41
1:C:81:ARG:CZ	1:C:260:VAL:HG22	2.51	0.41
1:B:237:PRO:HA	1:B:238:PRO:HA	1.81	0.40
1:C:210:ASP:HA	1:C:211:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:THR:O	1:D:83:GLN:HG3	2.21	0.40
1:A:12:LEU:HD21	1:A:27:TYR:HD2	1.86	0.40
1:B:7:ARG:NH1	1:B:27:TYR:OH	2.54	0.40
1:C:27:TYR:O	1:C:31:LEU:HG	2.22	0.40
1:C:100:SER:CB	1:D:152:GLN:HG2	2.51	0.40
1:A:185:GLN:HA	1:A:185:GLN:NE2	2.35	0.40
1:C:191:TYR:O	1:C:195:LEU:HG	2.22	0.40
1:B:220:TYR:CD1	1:B:220:TYR:N	2.89	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	275/444 (62%)	264 (96%)	11 (4%)	0	100	100
1	B	255/444 (57%)	247 (97%)	8 (3%)	0	100	100
1	C	262/444 (59%)	255 (97%)	7 (3%)	0	100	100
1	D	256/444 (58%)	254 (99%)	2 (1%)	0	100	100
All	All	1048/1776 (59%)	1020 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/359 (65%)	234 (100%)	0	100	100
1	B	221/359 (62%)	221 (100%)	0	100	100
1	C	228/359 (64%)	228 (100%)	0	100	100
1	D	221/359 (62%)	221 (100%)	0	100	100
All	All	904/1436 (63%)	904 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	GLN
1	B	72	ASN
1	C	129	ASN
1	C	134	ASN
1	C	212	ASN
1	D	30	GLN
1	D	160	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, 3 are monoatomic - leaving 18 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	SO4	D	504	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	B	502	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	C	501	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	D	505	-	4,4,4	0.32	0	6,6,6	0.06	0
5	EDO	C	504	-	3,3,3	0.08	0	2,2,2	0.10	0
5	EDO	B	504	-	3,3,3	0.07	0	2,2,2	0.16	0
5	EDO	C	505	-	3,3,3	0.07	0	2,2,2	0.16	0
2	SO4	C	503	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	A	502	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	D	506	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	C	502	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	501	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	D	503	-	4,4,4	0.33	0	6,6,6	0.08	0
3	PGE	A	504	-	9,9,9	0.17	0	8,8,8	0.09	0
2	SO4	D	507	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	A	503	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	503	-	4,4,4	0.34	0	6,6,6	0.07	0
6	EPE	D	508	-	15,15,15	0.59	1 (6%)	19,20,20	0.59	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	C	504	-	-	1/1/1/1	-
5	EDO	B	504	-	-	0/1/1/1	-
5	EDO	C	505	-	-	1/1/1/1	-
3	PGE	A	504	-	-	4/7/7/7	-
6	EPE	D	508	-	-	1/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	508	EPE	O3S-S	2.15	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	PGE	O1-C1-C2-O2
3	A	504	PGE	O3-C5-C6-O4
3	A	504	PGE	O2-C3-C4-O3
5	C	505	EDO	O1-C1-C2-O2
3	A	504	PGE	C6-C5-O3-C4
6	D	508	EPE	N4-C7-C8-O8
5	C	504	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	A	273/444 (61%)	2.19	122 (44%) 0 0	11, 27, 70, 104	3 (1%)
1	B	256/444 (57%)	1.44	73 (28%) 1 1	11, 21, 43, 53	1 (0%)
1	C	263/444 (59%)	1.54	75 (28%) 1 1	7, 21, 52, 73	1 (0%)
1	D	257/444 (57%)	0.97	39 (15%) 5 5	8, 19, 38, 63	1 (0%)
All	All	1049/1776 (59%)	1.54	309 (29%) 1 1	7, 22, 53, 104	6 (0%)

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	VAL	9.8
1	A	67	ALA	8.8
1	A	136	TRP	8.0
1	B	286	VAL	7.5
1	A	135	CYS	7.4
1	D	195	LEU	7.3
1	A	61	ALA	7.0
1	A	63	ALA	7.0
1	A	192	PHE	6.9
1	A	195	LEU	6.9
1	A	187	ALA	6.8
1	C	286	VAL	6.7
1	A	58	PHE	6.4
1	C	189	HIS	6.3
1	A	190	PHE	6.1
1	C	190	PHE	6.0
1	A	131	LEU	5.9
1	C	287	VAL	5.7
1	B	166	ALA	5.6
1	A	181	LEU	5.6
1	A	184	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	77	ALA	5.5
1	A	57	SER	5.4
1	A	140	LEU	5.4
1	A	193	VAL	5.4
1	A	133	VAL	5.2
1	A	186	PRO	5.1
1	D	238	PRO	4.9
1	A	137	THR	4.9
1	B	246	THR	4.9
1	C	72	ASN	4.8
1	A	64	GLU	4.7
1	A	65	GLN	4.7
1	C	160	ASN	4.7
1	C	71	GLY	4.7
1	A	66	GLN	4.6
1	B	71	GLY	4.6
1	C	147	HIS	4.5
1	A	60	THR	4.5
1	A	189	HIS	4.5
1	C	140	LEU	4.5
1	C	285	ARG	4.4
1	A	78	PHE	4.4
1	B	253	ALA	4.4
1	C	191	TYR	4.4
1	D	237	PRO	4.4
1	B	72	ASN	4.4
1	A	59	ALA	4.4
1	C	188	GLY	4.3
1	C	192	PHE	4.3
1	C	195	LEU	4.2
1	A	180	HIS	4.2
1	C	3	GLY	4.2
1	C	252	SER	4.2
1	A	132	ASN	4.2
1	B	73	GLU	4.1
1	B	251	ILE	4.1
1	C	238	PRO	4.1
1	D	240	ASP	4.1
1	D	165	SER	4.1
1	A	119	LEU	4.1
1	B	67	ALA	4.0
1	A	191	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	227	ASP	4.0
1	D	163	ASP	4.0
1	A	237	PRO	4.0
1	D	234	VAL	4.0
1	C	127	GLU	3.9
1	B	195	LEU	3.9
1	A	2	SER	3.9
1	A	170	PHE	3.9
1	B	74[A]	LYS	3.9
1	B	249	ALA	3.9
1	D	239	LEU	3.9
1	B	201	ALA	3.8
1	A	196	SER	3.8
1	C	69	LEU	3.8
1	C	144	SER	3.8
1	A	199	GLU	3.8
1	C	143	VAL	3.7
1	C	235	GLY	3.7
1	C	142	LEU	3.7
1	A	285	ARG	3.7
1	C	162	LEU	3.7
1	A	182	ASP	3.7
1	D	199	GLU	3.7
1	A	126	PHE	3.7
1	C	70	PHE	3.7
1	D	197	LYS	3.7
1	A	238	PRO	3.7
1	B	217	LYS	3.6
1	B	236	VAL	3.6
1	A	55	ALA	3.6
1	D	241	ARG	3.6
1	A	198	PHE	3.6
1	D	286	VAL	3.5
1	C	164	ASN	3.5
1	A	188	GLY	3.5
1	C	68	THR	3.4
1	A	185	GLN	3.4
1	B	226	LYS	3.4
1	A	173	GLY	3.4
1	B	239	LEU	3.4
1	C	141	LEU	3.4
1	C	73	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	237	PRO	3.4
1	A	197	LYS	3.3
1	A	164	ASN	3.3
1	A	128	ALA	3.3
1	B	198	PHE	3.3
1	A	178	SER	3.3
1	B	202	ALA	3.3
1	B	242	THR	3.3
1	A	147	HIS	3.2
1	A	54	VAL	3.2
1	D	285	ARG	3.2
1	B	250	GLU	3.2
1	D	217	LYS	3.2
1	D	6	ASP	3.2
1	A	271	PHE	3.2
1	B	241	ARG	3.2
1	C	228	GLY	3.2
1	A	31	LEU	3.1
1	D	196	SER	3.1
1	B	284	PRO	3.1
1	C	165	SER	3.1
1	C	239	LEU	3.1
1	B	256	GLU	3.1
1	A	177	VAL	3.1
1	A	222	SER	3.1
1	C	150	GLY	3.1
1	C	268	ALA	3.1
1	A	148	LYS	3.0
1	A	124	VAL	3.0
1	D	198	PHE	3.0
1	A	281	ALA	3.0
1	C	149	ARG	3.0
1	A	209	VAL	3.0
1	B	234	VAL	3.0
1	B	269	LYS	3.0
1	C	131	LEU	2.9
1	B	231	ASN	2.9
1	B	162	LEU	2.9
1	D	160	ASN	2.9
1	B	229	SER	2.9
1	C	2	SER	2.9
1	A	129	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	2	SER	2.9
1	B	265	GLU	2.9
1	A	130	ASN	2.8
1	A	89	ASP	2.8
1	A	123	ASP	2.8
1	A	194	GLU	2.8
1	B	203	LEU	2.8
1	C	54	VAL	2.8
1	D	17	LYS	2.8
1	B	266	ALA	2.8
1	C	215	GLY	2.8
1	C	57	SER	2.8
1	D	164	ASN	2.8
1	A	280	ILE	2.8
1	A	143	VAL	2.8
1	A	268	ALA	2.7
1	D	200	GLY	2.7
1	A	246[A]	THR	2.7
1	A	134	ASN	2.7
1	A	226	LYS	2.7
1	C	67	ALA	2.7
1	B	240	ASP	2.7
1	B	254	LEU	2.7
1	B	146	GLU	2.7
1	C	234	VAL	2.7
1	B	218	PHE	2.7
1	C	78	PHE	2.7
1	C	163	ASP	2.7
1	C	145	THR	2.7
1	B	2	SER	2.7
1	B	165	SER	2.7
1	B	213	VAL	2.7
1	A	202	ALA	2.6
1	C	208	ALA	2.6
1	B	220	TYR	2.6
1	C	74	LYS	2.6
1	C	236	VAL	2.6
1	C	65	GLN	2.6
1	C	64	GLU	2.6
1	B	230	TRP	2.6
1	C	284	PRO	2.6
1	B	278	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	146	GLU	2.6
1	D	250	GLU	2.6
1	B	252	SER	2.6
1	C	230	TRP	2.6
1	C	148	LYS	2.6
1	C	157	VAL	2.6
1	A	149	ARG	2.5
1	B	259	GLU	2.5
1	C	279	GLU	2.5
1	C	40	LEU	2.5
1	D	147	HIS	2.5
1	A	241	ARG	2.5
1	A	6	ASP	2.5
1	A	151	ASP	2.5
1	A	269	LYS	2.5
1	C	282	LYS	2.5
1	D	72	ASN	2.5
1	C	153	ALA	2.5
1	A	79	THR	2.5
1	A	277	TYR	2.5
1	B	223	TYR	2.5
1	C	278	ARG	2.5
1	A	250	GLU	2.5
1	D	103	GLU	2.5
1	A	217	LYS	2.5
1	B	219	ASP	2.5
1	B	238	PRO	2.5
1	A	265	GLU	2.4
1	C	280	ILE	2.4
1	C	253	ALA	2.4
1	A	138	PRO	2.4
1	A	7	ARG	2.4
1	A	146	GLU	2.4
1	A	142	LEU	2.4
1	A	282	LYS	2.4
1	B	248	PRO	2.4
1	B	103	GLU	2.4
1	B	199	GLU	2.4
1	A	125	SER	2.4
1	D	219	ASP	2.4
1	A	82	ARG	2.4
1	C	242	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	269	LYS	2.4
1	A	94	ASP	2.3
1	B	285	ARG	2.3
1	A	86	PHE	2.3
1	A	18	GLU	2.3
1	D	214	ILE	2.3
1	B	164	ASN	2.3
1	A	51	PRO	2.3
1	A	284	PRO	2.3
1	A	200	GLY	2.3
1	A	165	SER	2.3
1	A	203	LEU	2.3
1	A	52	GLY	2.3
1	A	127	GLU	2.3
1	A	279	GLU	2.3
1	D	18	GLU	2.3
1	D	146	GLU	2.3
1	B	233	THR	2.3
1	A	166	ALA	2.3
1	B	208	ALA	2.3
1	D	167	ALA	2.3
1	C	241	ARG	2.3
1	A	17	LYS	2.3
1	A	23	LEU	2.3
1	A	204	LEU	2.2
1	A	262	LEU	2.2
1	B	131	LEU	2.2
1	C	42	LEU	2.2
1	A	266	ALA	2.2
1	D	166	ALA	2.2
1	B	149	ARG	2.2
1	A	11	VAL	2.2
1	C	62	VAL	2.2
1	D	279	GLU	2.2
1	A	50	LEU	2.2
1	A	240	ASP	2.2
1	B	228	GLY	2.2
1	A	211	PRO	2.2
1	B	271	PHE	2.2
1	B	148	LYS	2.2
1	B	206	ARG	2.2
1	C	82	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	199	GLU	2.2
1	B	243	THR	2.2
1	C	6	ASP	2.2
1	D	33	ASP	2.2
1	A	14	SER	2.2
1	C	77	ALA	2.2
1	C	128	ALA	2.2
1	B	70	PHE	2.1
1	A	15	TYR	2.1
1	B	214	ILE	2.1
1	A	236	VAL	2.1
1	B	209	VAL	2.1
1	C	79	THR	2.1
1	B	204	LEU	2.1
1	A	167	ALA	2.1
1	A	230	TRP	2.1
1	B	100	SER	2.1
1	B	196	SER	2.1
1	B	244	LYS	2.1
1	A	103	GLU	2.1
1	A	174	LYS	2.1
1	A	45	VAL	2.1
1	A	56	ASN	2.1
1	B	124	VAL	2.1
1	C	193	VAL	2.1
1	A	276	PRO	2.1
1	D	203	LEU	2.1
1	D	278	ARG	2.1
1	A	172	ALA	2.0
1	D	99	ARG	2.0
1	D	266	ALA	2.0
1	B	163	ASP	2.0
1	B	282	LYS	2.0
1	C	137	THR	2.0
1	A	179	VAL	2.0
1	D	143	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(\AA^2)	Q<0.9
2	SO4	D	506	5/5	0.49	0.16	73,77,77,79	0
2	SO4	D	505	5/5	0.51	0.18	47,48,53,57	0
2	SO4	A	503	5/5	0.57	0.18	72,73,75,78	0
3	PGE	A	504	10/10	0.59	0.26	52,53,55,55	0
5	EDO	C	505	4/4	0.66	0.22	47,49,49,50	0
5	EDO	C	504	4/4	0.68	0.17	41,41,42,42	0
2	SO4	B	502	5/5	0.68	0.16	50,54,56,58	0
2	SO4	D	507	5/5	0.70	0.23	58,62,68,69	0
2	SO4	C	502	5/5	0.71	0.14	68,68,69,71	0
2	SO4	C	503	5/5	0.75	0.14	41,47,48,49	0
2	SO4	A	502	5/5	0.77	0.14	45,51,53,55	0
2	SO4	D	504	5/5	0.81	0.13	51,52,54,55	0
6	EPE	D	508	15/15	0.81	0.16	34,37,44,47	0
2	SO4	A	501	5/5	0.82	0.15	70,72,73,74	0
2	SO4	C	501	5/5	0.84	0.19	83,85,87,88	0
4	CL	D	501	1/1	0.85	0.21	65,65,65,65	0
4	CL	B	501	1/1	0.85	0.20	61,61,61,61	0
2	SO4	B	503	5/5	0.87	0.11	72,73,74,75	0
2	SO4	D	503	5/5	0.88	0.14	36,45,45,46	0
5	EDO	B	504	4/4	0.89	0.12	37,37,38,39	0
4	CL	D	502	1/1	0.93	0.14	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.