



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:53 AM UTC

PDB ID : 1XX1 / pdb_00001xx1
Title : Structural basis for ion-coordination and the catalytic mechanism of sphingomyelinases D
Authors : Murakami, M.T.; Tambourgi, D.V.; Arni, R.K.
Deposited on : 2004-11-03
Resolution : 1.75 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

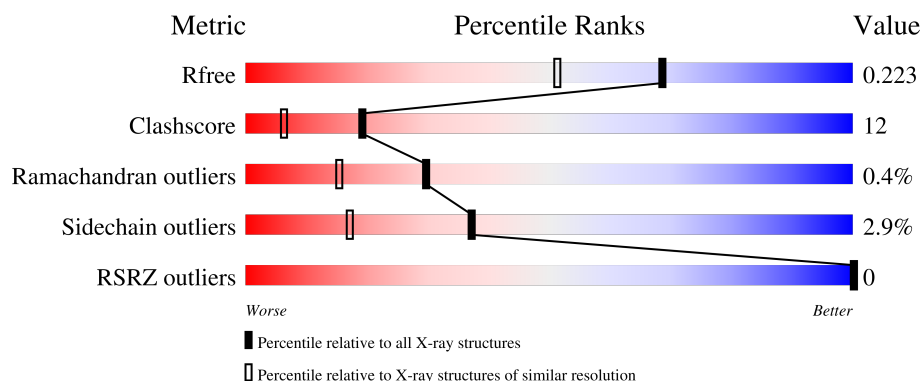
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	285	 81% 18% .
1	B	285	 79% 19% .
1	C	285	 80% 18% .
1	D	285	 80% 17% .

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
2	SO4	B	3002	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10258 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 SpHINGomyelinase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2269	1452	382	430	5			
1	B	285	Total	C	N	O	S	0	0	0
			2269	1452	382	430	5			
1	C	285	Total	C	N	O	S	0	0	0
			2269	1452	382	430	5			
1	D	285	Total	C	N	O	S	0	0	0
			2269	1452	382	430	5			

- 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		

Continued on next page...

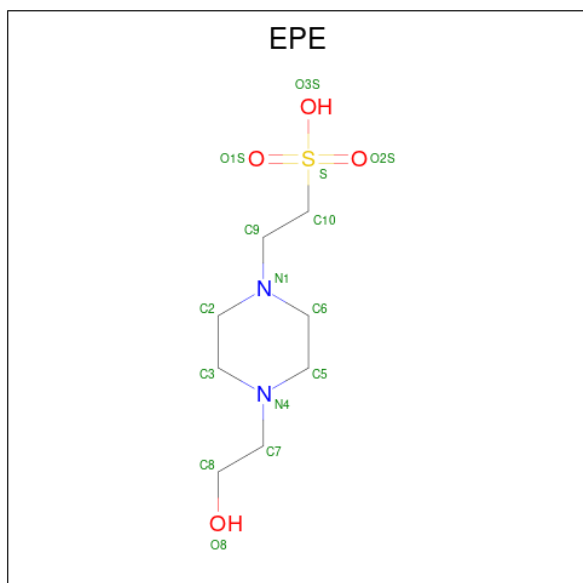
Continued from previous page...

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	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	B	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	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	273	Total	O	0	0
			273	273		

Continued on next page...

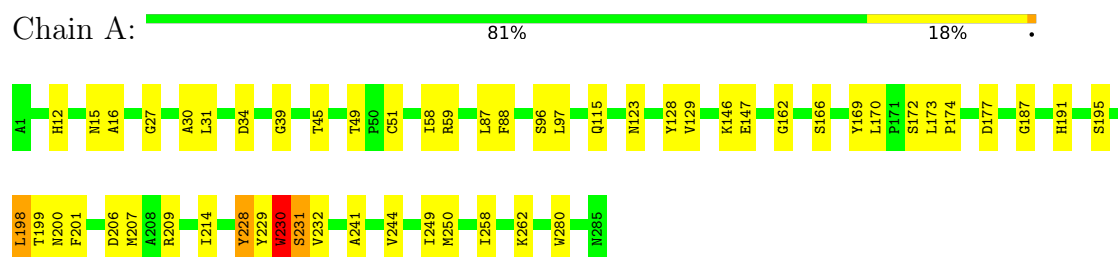
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	283	Total 283	O 283	0	0
5	C	250	Total 250	O 250	0	0
5	D	212	Total 212	O 212	0	0

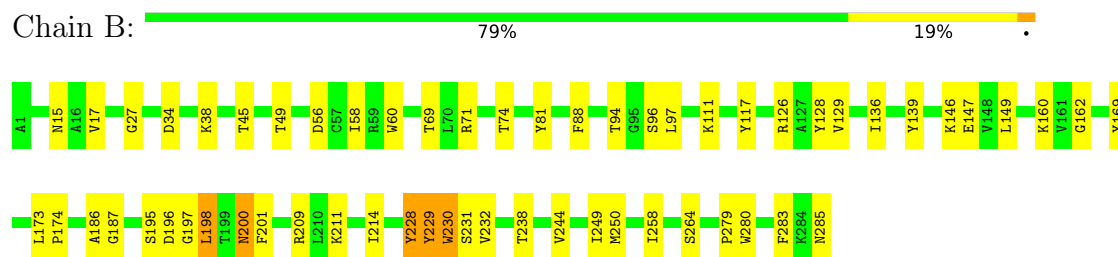
3 Residue-property plots

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.

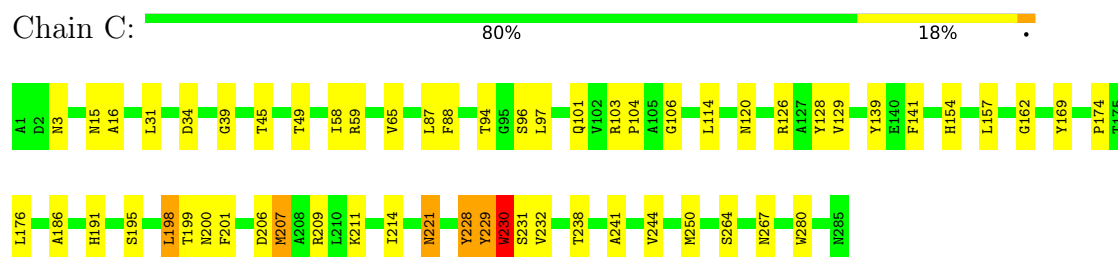
• Molecule 1: Sphingomyelinase I



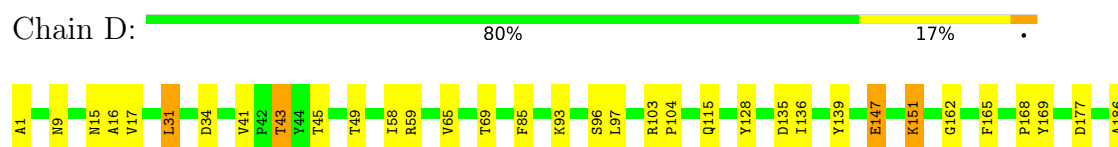
• Molecule 1: Sphingomyelinase I



• Molecule 1: Sphingomyelinase I



• Molecule 1: Sphingomyelinase I





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	139.82Å 139.82Å 113.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.75 30.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-1.75) 99.5 (30.00-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.225 0.184 , 0.223	Depositor DCC
R_{free} test set	6315 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.082 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10258	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: SO4, EPE, 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	0.81	0/2329	0.96	3/3164 (0.1%)
1	B	0.81	0/2329	0.97	3/3164 (0.1%)
1	C	0.73	0/2329	0.94	3/3164 (0.1%)
1	D	0.71	0/2329	0.96	1/3164 (0.0%)
All	All	0.77	0/9316	0.96	10/12656 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	TRP	N-CA-C	8.98	124.22	109.95
1	C	230	TRP	N-CA-C	8.57	122.30	109.95
1	B	230	TRP	N-CA-C	8.51	123.33	110.14
1	A	230	TRP	N-CA-C	6.47	120.07	109.85
1	B	229	TYR	CA-C-N	-5.44	113.34	122.92
1	B	229	TYR	C-N-CA	-5.44	113.34	122.92
1	C	229	TYR	CA-C-N	-5.19	113.66	123.27
1	C	229	TYR	C-N-CA	-5.19	113.66	123.27
1	A	229	TYR	CA-C-N	-5.18	114.11	122.81
1	A	229	TYR	C-N-CA	-5.18	114.11	122.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	TRP	Peptide
1	C	230	TRP	Peptide

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	2269	0	2190	53	0
1	B	2269	0	2190	63	1
1	C	2269	0	2190	56	1
1	D	2269	0	2190	61	1
2	A	30	0	0	0	0
2	B	30	0	0	4	0
2	C	30	0	0	1	0
2	D	25	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	17	0	0
4	C	15	0	17	1	0
4	D	15	0	17	1	0
5	A	273	0	0	10	1
5	B	283	0	0	8	2
5	C	250	0	0	9	1
5	D	212	0	0	5	1
All	All	10258	0	8811	212	4

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 12.

All (212) 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:B:198:LEU:HG	1:B:230:TRP:CZ2	1.63	1.34
1:C:198:LEU:HG	1:C:230:TRP:CZ2	1.75	1.21
1:A:198:LEU:HG	1:A:230:TRP:CZ2	1.74	1.20
1:D:198:LEU:HG	1:D:230:TRP:CZ2	1.80	1.17
1:D:198:LEU:HG	1:D:230:TRP:HZ2	0.96	1.11
1:B:169:TYR:HD2	1:B:173:LEU:HD21	1.17	1.04
1:B:169:TYR:CD2	1:B:173:LEU:HD21	1.93	1.03
1:A:199:THR:HG22	1:B:49:THR:HG21	1.43	1.00
1:B:198:LEU:CG	1:B:230:TRP:HZ2	1.75	0.98
1:B:198:LEU:HG	1:B:230:TRP:HZ2	0.81	0.97
1:C:198:LEU:HG	1:C:230:TRP:HZ2	1.22	0.97
1:B:111:LYS:HD2	5:B:9249:HOH:O	1.66	0.93
1:C:15:ASN:HD21	1:C:34:ASP:H	1.19	0.90
1:D:15:ASN:HD21	1:D:34:ASP:H	1.18	0.90
1:A:199:THR:HG22	1:B:49:THR:CG2	2.01	0.89
1:A:231:SER:HB2	5:A:9103:HOH:O	1.70	0.88
1:A:15:ASN:HD21	1:A:34:ASP:H	1.17	0.88
1:C:3:ASN:HA	5:C:9089:HOH:O	1.74	0.87
1:C:49:THR:OG1	1:D:198:LEU:HD22	1.74	0.87
1:B:15:ASN:HD21	1:B:34:ASP:H	1.20	0.87
1:A:230:TRP:HB2	1:A:250:MET:HB3	1.56	0.85
1:A:198:LEU:HG	1:A:230:TRP:HZ2	1.42	0.85
2:B:5002:SO4:O1	5:B:9181:HOH:O	1.97	0.82
1:B:56:ASP:HB3	5:B:9188:HOH:O	1.79	0.82
1:A:262:LYS:HE3	5:A:9226:HOH:O	1.79	0.81
1:A:200:ASN:HA	1:A:206:ASP:OD2	1.81	0.81
1:C:198:LEU:HD22	1:D:49:THR:OG1	1.81	0.80
1:B:198:LEU:HD21	2:B:3002:SO4:O2	1.81	0.80
1:A:262:LYS:CE	5:A:9226:HOH:O	2.30	0.79
1:B:198:LEU:CD2	2:B:3002:SO4:O2	2.31	0.79
1:C:230:TRP:HB2	1:C:250:MET:HG2	1.64	0.78
1:B:169:TYR:OH	1:B:198:LEU:HB2	1.84	0.77
1:D:115:GLN:HG3	5:D:9082:HOH:O	1.85	0.76
1:C:97:LEU:HD22	1:C:101:GLN:HB3	1.68	0.75
1:B:126:ARG:HG3	5:B:9263:HOH:O	1.87	0.74
1:D:115:GLN:HG2	5:D:9161:HOH:O	1.86	0.73
1:C:201:PHE:CG	1:D:58:ILE:HD11	2.25	0.70
1:C:230:TRP:CB	1:C:250:MET:HB3	2.21	0.70
1:B:230:TRP:HB2	1:B:250:MET:HB3	1.73	0.69
1:A:49:THR:OG1	1:B:198:LEU:HD22	1.93	0.67
5:C:9140:HOH:O	1:D:97:LEU:CD2	2.43	0.67
1:B:230:TRP:CB	1:B:250:MET:HB3	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:THR:HB	1:C:97:LEU:HD12	1.77	0.66
1:C:199:THR:HG22	1:D:49:THR:CG2	2.25	0.66
1:B:169:TYR:HD2	1:B:173:LEU:CD2	1.99	0.66
1:D:31:LEU:HD13	1:D:85:PHE:CZ	2.30	0.66
1:A:230:TRP:HB2	1:A:250:MET:CB	2.26	0.65
1:A:231:SER:OG	5:A:9104:HOH:O	2.14	0.65
1:C:200:ASN:HA	1:C:206:ASP:OD2	1.97	0.64
1:B:15:ASN:ND2	1:B:34:ASP:H	1.94	0.64
1:D:229:TYR:HD2	1:D:232:VAL:CG2	2.11	0.64
1:A:230:TRP:CB	1:A:250:MET:HB3	2.28	0.64
1:B:174:PRO:HA	5:B:9222:HOH:O	1.97	0.64
1:B:283:PHE:CZ	1:B:285:ASN:HB2	2.33	0.64
1:D:198:LEU:CG	1:D:230:TRP:CZ2	2.70	0.64
1:A:170:LEU:HD22	1:B:60:TRP:CD1	2.32	0.63
1:B:139:TYR:HB2	1:B:186:ALA:HB2	1.80	0.63
1:A:15:ASN:ND2	1:A:34:ASP:H	1.95	0.62
1:D:230:TRP:CB	1:D:250:MET:HB3	2.29	0.62
1:A:166:SER:HA	5:A:9194:HOH:O	1.99	0.62
5:C:9140:HOH:O	1:D:97:LEU:HD21	1.99	0.61
1:B:174:PRO:O	1:B:209:ARG:NH1	2.32	0.61
1:D:15:ASN:ND2	1:D:34:ASP:H	1.97	0.60
1:A:199:THR:CG2	1:B:49:THR:HG21	2.27	0.60
1:C:230:TRP:HB2	1:C:250:MET:CG	2.32	0.59
1:D:41:VAL:O	1:D:43:THR:HG22	2.03	0.59
1:A:58:ILE:HD11	1:B:201:PHE:CG	2.39	0.58
1:A:201:PHE:CG	1:B:58:ILE:HD11	2.38	0.58
1:C:230:TRP:HB2	1:C:250:MET:HB3	1.86	0.58
1:C:15:ASN:ND2	1:C:34:ASP:H	1.98	0.58
1:C:39:GLY:O	1:C:97:LEU:HD21	2.04	0.57
1:A:198:LEU:HD22	1:B:49:THR:OG1	2.03	0.57
1:B:198:LEU:HD23	2:B:3002:SO4:O2	2.04	0.57
1:D:93:LYS:HE3	5:D:9075:HOH:O	2.05	0.57
1:A:49:THR:OG1	1:B:198:LEU:HB3	2.06	0.56
1:D:221:ASN:H	1:D:221:ASN:HD22	1.54	0.56
1:C:195:SER:HB3	1:C:228:TYR:CZ	2.41	0.56
1:C:96:SER:HB3	5:C:9140:HOH:O	2.05	0.56
1:A:232:VAL:HB	1:A:249:ILE:HG23	1.88	0.55
1:D:229:TYR:HD2	1:D:232:VAL:HG22	1.71	0.55
1:B:231:SER:HB2	5:B:9126:HOH:O	2.05	0.55
1:C:199:THR:HG22	1:D:49:THR:HG21	1.88	0.55
1:C:199:THR:HG22	1:D:49:THR:HG23	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:CB	1:B:198:LEU:HD22	2.37	0.55
1:B:88:PHE:CZ	1:B:129:VAL:HG22	2.41	0.55
1:D:203:PRO:O	1:D:207:MET:HG2	2.08	0.54
1:A:169:TYR:OH	1:A:198:LEU:HB3	2.08	0.54
1:D:195:SER:HB3	1:D:228:TYR:CZ	2.42	0.54
1:D:196:ASP:OD1	1:D:197:GLY:N	2.40	0.53
1:C:201:PHE:CB	1:D:58:ILE:HD11	2.38	0.53
1:D:135:ASP:OD1	1:D:168:PRO:HD3	2.09	0.53
1:C:65:VAL:HG11	4:C:2003:EPE:H82	1.91	0.52
1:B:195:SER:HB3	1:B:228:TYR:CZ	2.44	0.52
1:B:198:LEU:CG	1:B:230:TRP:CZ2	2.60	0.52
1:C:241:ALA:O	1:C:244:VAL:HG22	2.09	0.52
1:D:17:VAL:HB	1:D:69:THR:HG21	1.91	0.52
1:D:34:ASP:O	1:D:45:THR:HA	2.08	0.52
1:C:162:GLY:HA3	1:C:280:TRP:CH2	2.45	0.51
1:A:262:LYS:HE2	5:A:9226:HOH:O	2.04	0.51
1:C:232:VAL:HG11	1:C:238:THR:HA	1.92	0.51
1:C:34:ASP:O	1:C:45:THR:HA	2.10	0.51
1:B:195:SER:HB3	1:B:228:TYR:CE2	2.45	0.51
1:C:195:SER:HB3	1:C:228:TYR:CE2	2.46	0.50
1:C:88:PHE:CE1	1:C:129:VAL:HG13	2.45	0.50
1:C:221:ASN:HA	5:C:9203:HOH:O	2.11	0.50
1:D:229:TYR:CD2	1:D:232:VAL:HG22	2.46	0.50
1:C:198:LEU:CG	1:C:230:TRP:CZ2	2.69	0.50
1:D:103:ARG:HB3	1:D:104:PRO:HD3	1.94	0.49
1:C:16:ALA:HB2	1:C:59:ARG:HB3	1.94	0.49
1:D:16:ALA:HB2	1:D:59:ARG:HB3	1.93	0.49
1:C:198:LEU:HG	1:C:230:TRP:CH2	2.40	0.49
1:D:230:TRP:HB2	1:D:250:MET:HB3	1.94	0.49
1:B:94:THR:HB	1:B:97:LEU:HD12	1.94	0.49
1:D:162:GLY:HA3	1:D:280:TRP:CH2	2.48	0.49
1:D:195:SER:HB2	1:D:230:TRP:CZ3	2.48	0.48
1:A:174:PRO:HG2	5:A:9194:HOH:O	2.13	0.48
1:C:58:ILE:HD11	1:D:201:PHE:HB2	1.95	0.48
1:B:229:TYR:HD2	1:B:232:VAL:CG2	2.26	0.48
1:C:230:TRP:HB3	1:C:250:MET:HB3	1.94	0.48
1:D:1:ALA:HA	5:D:9180:HOH:O	2.13	0.48
1:D:169:TYR:CE2	1:D:199:THR:HG21	2.48	0.48
1:C:230:TRP:HB2	1:C:250:MET:CB	2.45	0.47
1:A:201:PHE:CD2	1:B:58:ILE:HD11	2.49	0.47
1:D:190:GLY:O	1:D:191:HIS:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASP:O	1:B:45:THR:HA	2.14	0.47
1:B:214:ILE:HD13	1:B:244:VAL:O	2.14	0.47
1:A:230:TRP:HB2	1:A:250:MET:HG2	1.97	0.47
1:A:214:ILE:HD13	1:A:244:VAL:O	2.15	0.46
1:A:241:ALA:O	1:A:244:VAL:HG12	2.15	0.46
1:D:198:LEU:HD23	2:D:3004:SO4:O1	2.14	0.46
1:A:39:GLY:O	1:A:97:LEU:HD21	2.16	0.46
1:B:74:THR:O	1:B:126:ARG:HG2	2.15	0.46
1:C:106:GLY:HA3	1:C:141:PHE:O	2.15	0.46
1:A:27:GLY:HA3	1:A:258:ILE:HG13	1.98	0.46
1:C:174:PRO:O	1:C:209:ARG:NH2	2.48	0.46
1:A:88:PHE:CZ	1:A:129:VAL:HG22	2.50	0.46
1:A:195:SER:HB3	1:A:228:TYR:CZ	2.51	0.46
1:B:96:SER:HB3	5:B:9195:HOH:O	2.16	0.46
1:D:214:ILE:HD13	1:D:244:VAL:O	2.16	0.46
1:B:160:LYS:HA	1:B:160:LYS:HD2	1.75	0.45
1:C:162:GLY:HA2	1:C:191:HIS:HB3	1.99	0.45
1:C:229:TYR:HD2	1:C:232:VAL:CG2	2.29	0.45
1:A:199:THR:HG22	1:B:49:THR:HG23	1.89	0.45
1:D:230:TRP:HB3	1:D:250:MET:HB3	1.98	0.45
1:B:17:VAL:HB	1:B:69:THR:HG21	1.98	0.45
1:B:169:TYR:HA	1:B:173:LEU:HD23	1.98	0.45
1:B:229:TYR:HD2	1:B:232:VAL:HG23	1.82	0.45
1:D:15:ASN:HD21	1:D:34:ASP:N	1.99	0.44
1:D:195:SER:HB2	1:D:230:TRP:HZ3	1.83	0.44
1:B:15:ASN:HD21	1:B:34:ASP:N	2.01	0.44
2:C:5003:SO4:O2	5:C:9100:HOH:O	2.21	0.44
1:D:9:ASN:HB2	1:D:257:LEU:HD23	1.99	0.44
1:D:96:SER:HB3	5:D:9167:HOH:O	2.17	0.44
1:A:115:GLN:HG3	5:A:9181:HOH:O	2.18	0.44
1:A:34:ASP:O	1:A:45:THR:HA	2.17	0.43
1:D:232:VAL:HG11	1:D:238:THR:HA	2.00	0.43
1:A:195:SER:HA	1:A:228:TYR:O	2.18	0.43
1:B:128:TYR:CG	1:B:279:PRO:HG3	2.53	0.43
1:A:16:ALA:HB2	1:A:59:ARG:HB3	1.99	0.43
1:A:58:ILE:HD11	1:B:201:PHE:CB	2.49	0.43
1:A:230:TRP:HB2	1:A:250:MET:CG	2.49	0.43
1:B:232:VAL:HG11	1:B:238:THR:HA	2.01	0.43
1:C:154:HIS:HB3	1:C:157:LEU:HD12	1.99	0.43
1:D:195:SER:HA	1:D:228:TYR:O	2.19	0.43
1:C:207:MET:HB2	5:C:9242:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:HIS:HB2	1:A:250:MET:HG3	2.01	0.43
1:C:31:LEU:C	1:C:31:LEU:HD12	2.44	0.42
1:A:15:ASN:HD21	1:A:34:ASP:N	1.99	0.42
1:A:174:PRO:O	1:A:209:ARG:NH2	2.53	0.42
1:C:201:PHE:HB3	1:D:58:ILE:HD11	2.00	0.42
1:D:65:VAL:HG11	4:D:2004:EPE:H82	2.02	0.42
1:B:195:SER:HB2	1:B:230:TRP:CZ3	2.55	0.42
1:C:58:ILE:HD11	1:D:201:PHE:CG	2.53	0.42
1:C:103:ARG:HB3	1:C:104:PRO:HD3	2.01	0.42
1:C:169:TYR:OH	1:C:198:LEU:HB3	2.19	0.42
1:D:147:GLU:O	1:D:151:LYS:HB3	2.20	0.42
1:A:162:GLY:HA3	1:A:280:TRP:CH2	2.55	0.42
1:B:38:LYS:HE3	5:B:9239:HOH:O	2.19	0.42
1:D:162:GLY:HA2	1:D:191:HIS:HB3	2.00	0.42
1:B:196:ASP:O	1:B:229:TYR:HA	2.20	0.42
1:C:126:ARG:HG3	5:C:9094:HOH:O	2.20	0.42
1:C:214:ILE:HD13	1:C:244:VAL:O	2.20	0.42
5:C:9140:HOH:O	1:D:97:LEU:HD23	2.14	0.42
1:B:162:GLY:HA3	1:B:280:TRP:CH2	2.55	0.41
1:D:195:SER:HB3	1:D:228:TYR:CE1	2.55	0.41
1:C:87:LEU:HA	1:C:128:TYR:O	2.20	0.41
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.90	0.41
1:B:81:TYR:OH	1:B:126:ARG:CZ	2.69	0.41
1:C:114:LEU:HG	1:C:120:ASN:ND2	2.35	0.41
1:D:169:TYR:CE2	1:D:199:THR:CG2	3.03	0.41
1:A:51:CYS:HB2	5:A:9102:HOH:O	2.20	0.41
1:D:136:ILE:HG22	1:D:165:PHE:HB3	2.02	0.41
1:C:139:TYR:HB2	1:C:186:ALA:HB2	2.02	0.41
1:D:198:LEU:CB	1:D:230:TRP:CZ2	3.04	0.41
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.60	0.41
1:C:264:SER:HA	1:C:267:ASN:ND2	2.36	0.41
1:A:87:LEU:HA	1:A:128:TYR:O	2.21	0.41
1:D:128:TYR:CG	1:D:279:PRO:HG3	2.56	0.41
1:D:135:ASP:CG	1:D:168:PRO:HD3	2.46	0.41
1:A:30:ALA:HA	1:A:87:LEU:O	2.21	0.41
1:B:232:VAL:HB	1:B:249:ILE:HG23	2.02	0.41
1:C:176:LEU:HD23	1:C:176:LEU:HA	1.88	0.41
1:B:71:ARG:HD2	1:B:117:TYR:O	2.20	0.40
1:C:15:ASN:HD21	1:C:34:ASP:N	2.01	0.40
1:B:27:GLY:HA3	1:B:258:ILE:HG13	2.03	0.40
1:A:146:LYS:NZ	1:A:187:GLY:O	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:HD13	1:B:174:PRO:HB3	2.02	0.40
1:A:96:SER:HB3	5:A:9126:HOH:O	2.21	0.40
1:B:146:LYS:NZ	1:B:187:GLY:O	2.54	0.40
1:A:162:GLY:HA2	1:A:191:HIS:HB3	2.04	0.40
1:C:195:SER:HA	1:C:228:TYR:O	2.21	0.40
1:D:139:TYR:HB2	1:D:186:ALA:HB2	2.03	0.40

All (4) 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)
1:C:200:ASN:O	5:B:9107:HOH:O[4_654]	1.95	0.25
1:B:200:ASN:O	5:C:9128:HOH:O[4_655]	2.00	0.20
1:D:200:ASN:O	5:A:9163:HOH:O[4_654]	2.08	0.12
5:B:9153:HOH:O	5:D:9215:HOH:O[4_655]	2.19	0.01

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	283/285 (99%)	278 (98%)	4 (1%)	1 (0%)	30	15
1	B	283/285 (99%)	275 (97%)	6 (2%)	2 (1%)	18	7
1	C	283/285 (99%)	275 (97%)	7 (2%)	1 (0%)	30	15
1	D	283/285 (99%)	275 (97%)	8 (3%)	0	100	100
All	All	1132/1140 (99%)	1103 (97%)	25 (2%)	4 (0%)	30	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	198	LEU
1	C	231	SER
1	B	197	GLY

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	240/240 (100%)	231 (96%)	9 (4%)	29	10
1	B	240/240 (100%)	234 (98%)	6 (2%)	42	22
1	C	240/240 (100%)	235 (98%)	5 (2%)	47	27
1	D	240/240 (100%)	232 (97%)	8 (3%)	33	13
All	All	960/960 (100%)	932 (97%)	28 (3%)	37	17

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	123	ASN
1	A	147	GLU
1	A	172	SER
1	A	177	ASP
1	A	198	LEU
1	A	207	MET
1	A	228	TYR
1	A	230	TRP
1	B	147	GLU
1	B	149	LEU
1	B	200	ASN
1	B	211	LYS
1	B	228	TYR
1	B	264	SER
1	C	198	LEU
1	C	207	MET
1	C	211	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	221	ASN
1	C	228	TYR
1	D	31	LEU
1	D	43	THR
1	D	147	GLU
1	D	151	LYS
1	D	177	ASP
1	D	198	LEU
1	D	200	ASN
1	D	221	ASN

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	ASN
1	A	99	ASN
1	A	122	ASN
1	B	15	ASN
1	C	15	ASN
1	C	99	ASN
1	C	116	ASN
1	C	120	ASN
1	C	122	ASN
1	C	123	ASN
1	D	15	ASN
1	D	122	ASN
1	D	123	ASN
1	D	200	ASN
1	D	221	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 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	C	7003	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	D	8004	-	4,4,4	0.28	0	6,6,6	0.19	0
4	EPE	C	2003	-	15,15,15	0.73	1 (6%)	19,20,20	1.72	4 (21%)
2	SO4	D	7004	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	C	6003	-	4,4,4	0.28	0	6,6,6	0.46	0
2	SO4	A	5001	-	4,4,4	0.31	0	6,6,6	0.16	0
2	SO4	B	8002	-	4,4,4	0.31	0	6,6,6	0.20	0
2	SO4	C	8003	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	C	5003	-	4,4,4	0.25	0	6,6,6	0.40	0
2	SO4	B	7002	-	4,4,4	0.24	0	6,6,6	0.23	0
4	EPE	D	2004	-	15,15,15	0.79	1 (6%)	19,20,20	1.91	5 (26%)
2	SO4	C	3003	-	4,4,4	0.23	0	6,6,6	0.50	0
2	SO4	D	6004	-	4,4,4	0.25	0	6,6,6	0.49	0
2	SO4	C	4003	-	4,4,4	0.21	0	6,6,6	0.14	0
4	EPE	A	2001	-	15,15,15	0.69	1 (6%)	19,20,20	1.69	3 (15%)
2	SO4	A	3001	-	4,4,4	0.35	0	6,6,6	0.48	0
2	SO4	A	4001	-	4,4,4	0.28	0	6,6,6	0.31	0
2	SO4	B	3002	-	4,4,4	0.30	0	6,6,6	0.38	0
2	SO4	D	5004	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	B	5002	-	4,4,4	0.27	0	6,6,6	0.25	0
2	SO4	A	6001	-	4,4,4	0.22	0	6,6,6	0.57	0
2	SO4	A	8001	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	D	3004	-	4,4,4	0.28	0	6,6,6	0.37	0
2	SO4	A	7001	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	B	4002	-	4,4,4	0.36	0	6,6,6	0.33	0
2	SO4	B	6002	-	4,4,4	0.32	0	6,6,6	0.63	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	EPE	A	2001	-	-	1/9/19/19	0/1/1/1
4	EPE	D	2004	-	-	0/9/19/19	0/1/1/1
4	EPE	C	2003	-	-	1/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2004	EPE	C10-S	2.58	1.81	1.77
4	C	2003	EPE	C10-S	2.15	1.80	1.77
4	A	2001	EPE	C10-S	2.02	1.80	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2004	EPE	C5-N4-C3	4.94	119.48	108.84
4	C	2003	EPE	C5-N4-C3	4.65	118.86	108.84
4	A	2001	EPE	C5-N4-C3	4.57	118.69	108.84
4	D	2004	EPE	O1S-S-C10	4.29	113.21	106.73
4	A	2001	EPE	C9-N1-C6	-3.54	101.80	111.24
4	D	2004	EPE	O2S-S-C10	-3.08	102.07	106.73
4	C	2003	EPE	C3-C2-N1	-3.06	104.49	110.65
4	A	2001	EPE	C5-C6-N1	-2.78	105.03	110.65
4	C	2003	EPE	O3S-S-C10	2.28	110.46	106.00
4	C	2003	EPE	C7-N4-C5	2.24	117.20	111.24
4	D	2004	EPE	C5-C6-N1	-2.22	106.18	110.65
4	D	2004	EPE	C3-C2-N1	-2.14	106.34	110.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2003	EPE	C10-C9-N1-C2
4	A	2001	EPE	C8-C7-N4-C3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2003	EPE	1	0
2	C	5003	SO4	1	0
4	D	2004	EPE	1	0
2	B	3002	SO4	3	0
2	B	5002	SO4	1	0
2	D	3004	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	285/285 (100%)	-1.35	0 100 100	11, 18, 35, 59	0
1	B	285/285 (100%)	-1.32	0 100 100	12, 19, 35, 60	0
1	C	285/285 (100%)	-1.26	0 100 100	13, 22, 42, 58	0
1	D	285/285 (100%)	-1.18	0 100 100	13, 25, 49, 72	0
All	All	1140/1140 (100%)	-1.28	0 100 100	11, 21, 42, 72	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	3001	5/5	0.98	0.04	35,35,36,39	0
2	SO4	C	3003	5/5	0.98	0.05	29,30,31,32	0
2	SO4	C	7003	5/5	0.98	0.04	51,52,53,53	0
2	SO4	D	5004	5/5	0.98	0.05	52,53,54,54	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	SO4	D	7004	5/5	0.98	0.04	63,64,64,64	0
2	SO4	D	8004	5/5	0.98	0.04	50,51,51,52	0
2	SO4	B	4002	5/5	0.99	0.06	29,34,35,36	0
2	SO4	B	5002	5/5	0.99	0.04	45,47,48,48	0
2	SO4	B	6002	5/5	0.99	0.06	29,31,31,33	0
2	SO4	B	7002	5/5	0.99	0.03	46,48,49,49	0
2	SO4	B	8002	5/5	0.99	0.04	55,55,56,56	0
2	SO4	A	4001	5/5	0.99	0.07	23,30,32,33	0
2	SO4	C	4003	5/5	0.99	0.04	48,48,49,49	0
2	SO4	C	5003	5/5	0.99	0.03	48,48,49,51	0
2	SO4	A	5001	5/5	0.99	0.05	60,63,63,64	0
2	SO4	C	8003	5/5	0.99	0.04	51,51,53,53	0
2	SO4	D	3004	5/5	0.99	0.05	28,28,28,30	0
2	SO4	A	7001	5/5	0.99	0.03	44,45,47,47	0
2	SO4	A	8001	5/5	0.99	0.03	46,47,48,49	0
2	SO4	B	3002	5/5	0.99	0.05	29,34,34,36	0
2	SO4	D	6004	5/5	1.00	0.02	19,20,20,22	0
2	SO4	A	6001	5/5	1.00	0.02	20,21,23,23	0
2	SO4	C	6003	5/5	1.00	0.02	17,18,19,19	0
3	MG	A	9001	1/1	1.00	0.02	7,7,7,7	0
3	MG	B	9002	1/1	1.00	0.01	6,6,6,6	0
3	MG	C	9003	1/1	1.00	0.02	7,7,7,7	0
3	MG	D	9004	1/1	1.00	0.02	8,8,8,8	0
4	EPE	A	2001	15/15	1.00	0.02	17,18,21,23	0
4	EPE	C	2003	15/15	1.00	0.02	17,18,24,28	0
4	EPE	D	2004	15/15	1.00	0.02	18,20,24,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.