



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2020 – 04:24 PM EDT

PDB ID : 6XR5
Title : Crystal Structure of Diphosphomevalonate decarboxylase (MVD1) *Cryptococcus neoformans* var. *grubii* serotype A
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2020-07-11
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4

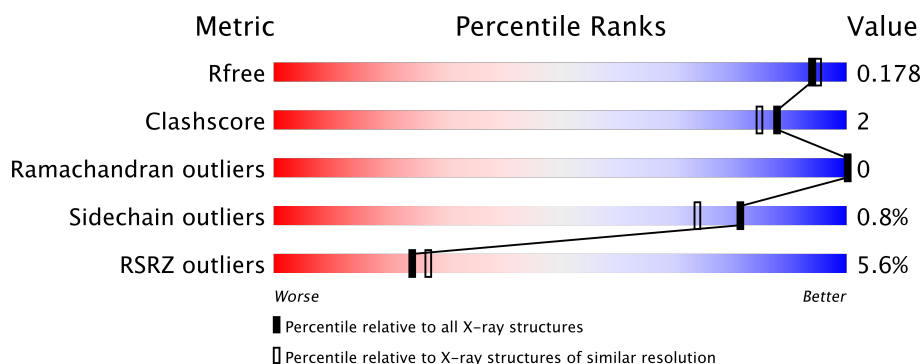
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	403	<div> <div>3%</div> <div>94%</div> <div>6%</div> <div>• •</div> </div>
1	B	403	<div> <div>3%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	C	403	<div> <div>4%</div> <div>92%</div> <div>• •</div> </div>
1	D	403	<div> <div>3%</div> <div>94%</div> <div>• •</div> </div>
1	E	403	<div> <div>3%</div> <div>91%</div> <div>• •</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	403	<div><div></div><div>9%</div><div></div><div>92%</div><div></div><div>5%</div><div></div></div>
1	G	403	<div><div></div><div>14%</div><div></div><div>92%</div><div></div><div>5%</div><div></div></div>
1	H	403	<div><div></div><div>3%</div><div></div><div>94%</div><div></div><div></div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28006 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 Diphosphomevalonate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	16	0
			3047	1927	529	578	13			
1	B	391	Total	C	N	O	S	0	28	0
			3104	1967	537	587	13			
1	C	386	Total	C	N	O	S	0	23	0
			3031	1922	519	577	13			
1	D	393	Total	C	N	O	S	0	18	0
			3059	1939	531	576	13			
1	E	386	Total	C	N	O	S	0	27	0
			3038	1920	523	582	13			
1	F	387	Total	C	N	O	S	0	17	0
			2971	1882	515	563	11			
1	G	393	Total	C	N	O	S	0	16	0
			3002	1901	526	563	12			
1	H	392	Total	C	N	O	S	0	18	0
			3042	1926	529	574	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP J9VRT5
A	-6	ALA	-	expression tag	UNP J9VRT5
A	-5	HIS	-	expression tag	UNP J9VRT5
A	-4	HIS	-	expression tag	UNP J9VRT5
A	-3	HIS	-	expression tag	UNP J9VRT5
A	-2	HIS	-	expression tag	UNP J9VRT5
A	-1	HIS	-	expression tag	UNP J9VRT5
A	0	HIS	-	expression tag	UNP J9VRT5
B	-7	MET	-	initiating methionine	UNP J9VRT5
B	-6	ALA	-	expression tag	UNP J9VRT5
B	-5	HIS	-	expression tag	UNP J9VRT5
B	-4	HIS	-	expression tag	UNP J9VRT5
B	-3	HIS	-	expression tag	UNP J9VRT5

Continued on next page...

Continued from previous page...

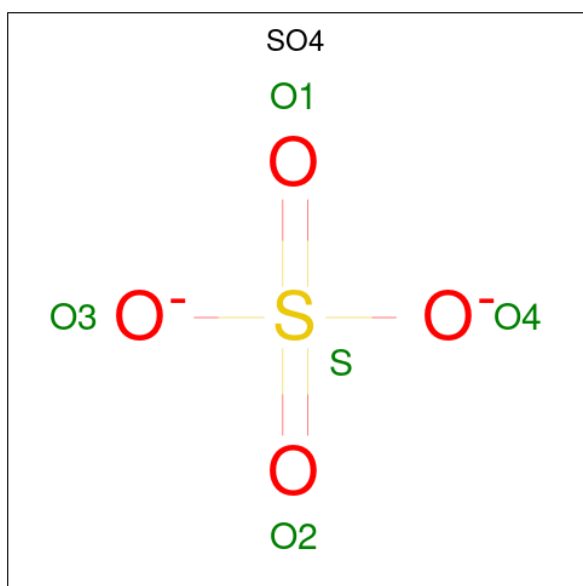
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP J9VRT5
B	-1	HIS	-	expression tag	UNP J9VRT5
B	0	HIS	-	expression tag	UNP J9VRT5
C	-7	MET	-	initiating methionine	UNP J9VRT5
C	-6	ALA	-	expression tag	UNP J9VRT5
C	-5	HIS	-	expression tag	UNP J9VRT5
C	-4	HIS	-	expression tag	UNP J9VRT5
C	-3	HIS	-	expression tag	UNP J9VRT5
C	-2	HIS	-	expression tag	UNP J9VRT5
C	-1	HIS	-	expression tag	UNP J9VRT5
C	0	HIS	-	expression tag	UNP J9VRT5
D	-7	MET	-	initiating methionine	UNP J9VRT5
D	-6	ALA	-	expression tag	UNP J9VRT5
D	-5	HIS	-	expression tag	UNP J9VRT5
D	-4	HIS	-	expression tag	UNP J9VRT5
D	-3	HIS	-	expression tag	UNP J9VRT5
D	-2	HIS	-	expression tag	UNP J9VRT5
D	-1	HIS	-	expression tag	UNP J9VRT5
D	0	HIS	-	expression tag	UNP J9VRT5
E	-7	MET	-	initiating methionine	UNP J9VRT5
E	-6	ALA	-	expression tag	UNP J9VRT5
E	-5	HIS	-	expression tag	UNP J9VRT5
E	-4	HIS	-	expression tag	UNP J9VRT5
E	-3	HIS	-	expression tag	UNP J9VRT5
E	-2	HIS	-	expression tag	UNP J9VRT5
E	-1	HIS	-	expression tag	UNP J9VRT5
E	0	HIS	-	expression tag	UNP J9VRT5
F	-7	MET	-	initiating methionine	UNP J9VRT5
F	-6	ALA	-	expression tag	UNP J9VRT5
F	-5	HIS	-	expression tag	UNP J9VRT5
F	-4	HIS	-	expression tag	UNP J9VRT5
F	-3	HIS	-	expression tag	UNP J9VRT5
F	-2	HIS	-	expression tag	UNP J9VRT5
F	-1	HIS	-	expression tag	UNP J9VRT5
F	0	HIS	-	expression tag	UNP J9VRT5
G	-7	MET	-	initiating methionine	UNP J9VRT5
G	-6	ALA	-	expression tag	UNP J9VRT5
G	-5	HIS	-	expression tag	UNP J9VRT5
G	-4	HIS	-	expression tag	UNP J9VRT5
G	-3	HIS	-	expression tag	UNP J9VRT5
G	-2	HIS	-	expression tag	UNP J9VRT5
G	-1	HIS	-	expression tag	UNP J9VRT5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP J9VRT5
H	-7	MET	-	initiating methionine	UNP J9VRT5
H	-6	ALA	-	expression tag	UNP J9VRT5
H	-5	HIS	-	expression tag	UNP J9VRT5
H	-4	HIS	-	expression tag	UNP J9VRT5
H	-3	HIS	-	expression tag	UNP J9VRT5
H	-2	HIS	-	expression tag	UNP J9VRT5
H	-1	HIS	-	expression tag	UNP J9VRT5
H	0	HIS	-	expression tag	UNP J9VRT5

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



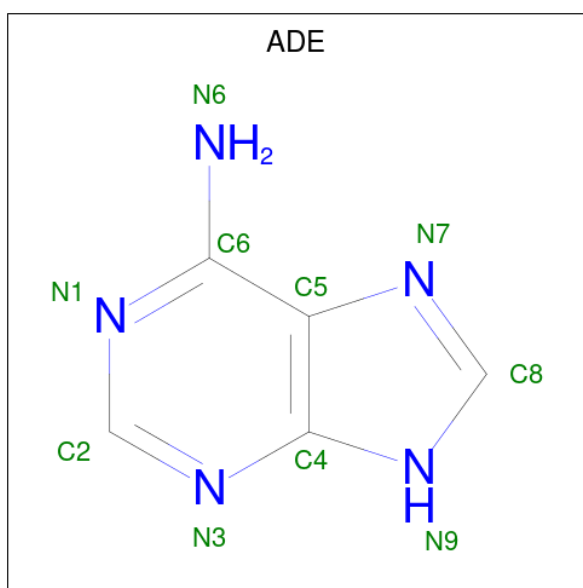
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	5	5		
3	B	1	Total	C	N	0	0
			10	5	5		
3	D	1	Total	C	N	0	0
			10	5	5		
3	E	1	Total	C	N	0	0
			10	5	5		
3	H	1	Total	C	N	0	0
			10	5	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	516	Total	O	0	9
			523	523		
5	B	516	Total	O	0	10
			521	521		
5	C	427	Total	O	0	7
			432	432		
5	D	540	Total	O	0	9
			548	548		
5	E	422	Total	O	0	11
			428	428		
5	F	330	Total	O	0	9
			339	339		
5	G	294	Total	O	0	3
			296	296		
5	H	504	Total	O	0	4
			507	507		

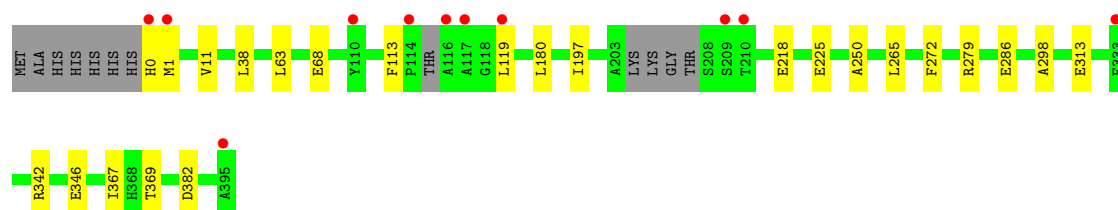
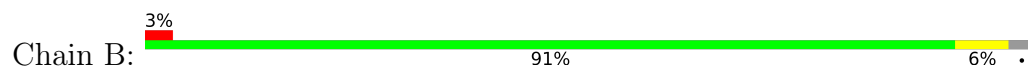
3 Residue-property plots [i](#)

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.

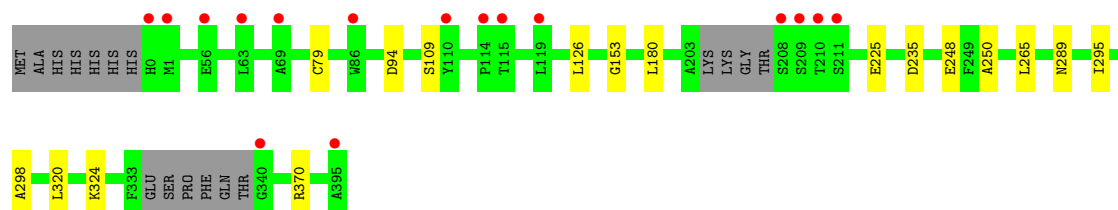
- Molecule 1: Diphosphomevalonate decarboxylase



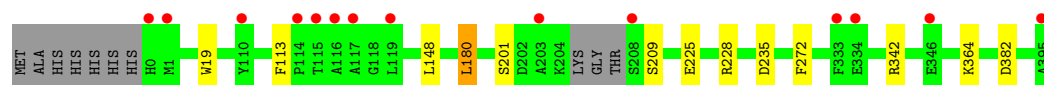
- Molecule 1: Diphosphomevalonate decarboxylase



- Molecule 1: Diphosphomevalonate decarboxylase



- Molecule 1: Diphosphomevalonate decarboxylase



- Molecule 1: Diphosphomevalonate decarboxylase

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.51Å 168.05Å 101.21Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	48.32 – 1.70 48.32 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.32-1.70) 99.7 (48.32-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.156 , 0.182 0.153 , 0.178	Depositor DCC
R_{free} test set	1941 reflections (0.56%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.127 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28006	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% 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: ADE, SO4, 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	0.49	0/3149	0.65	2/4266 (0.0%)
1	B	0.48	0/3245	0.64	1/4399 (0.0%)
1	C	0.47	0/3156	0.62	0/4277
1	D	0.51	0/3173	0.66	1/4303 (0.0%)
1	E	0.45	0/3166	0.62	0/4294
1	F	0.42	0/3080	0.59	1/4187 (0.0%)
1	G	0.42	0/3110	0.62	4/4230 (0.1%)
1	H	0.49	0/3153	0.65	1/4272 (0.0%)
All	All	0.47	0/25232	0.63	10/34228 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	244[A]	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	G	244[B]	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	G	244[A]	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	G	244[B]	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	F	233	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	H	159	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	342	ARG	CG-CD-NE	-5.13	101.03	111.80
1	B	342	ARG	CG-CD-NE	-5.10	101.09	111.80
1	A	159	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	159	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3047	0	3065	9	0
1	B	3104	0	3129	17	0
1	C	3031	0	3070	11	0
1	D	3059	0	3087	9	0
1	E	3038	0	3046	14	0
1	F	2971	0	2929	13	0
1	G	3002	0	2956	13	0
1	H	3042	0	3064	13	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	1	0
2	D	10	0	0	0	0
2	E	10	0	0	1	0
2	F	5	0	0	0	0
2	H	10	0	0	1	0
3	A	10	0	4	1	0
3	B	10	0	4	1	0
3	D	10	0	4	0	0
3	E	10	0	4	0	0
3	H	10	0	4	0	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
5	A	523	0	0	4	0
5	B	521	0	0	7	0
5	C	432	0	0	7	0
5	D	548	0	0	2	0
5	E	428	0	0	9	0
5	F	339	0	0	5	0
5	G	296	0	0	0	0
5	H	507	0	0	8	0
All	All	28006	0	24378	96	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 2.

All (96) 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:H:401:SO4:O3	5:H:501:HOH:O	2.00	0.79
1:C:248[A]:GLU:OE2	5:C:502:HOH:O	2.05	0.74
1:H:239:GLN:OE1	5:H:502:HOH:O	2.06	0.72
2:C:401:SO4:O2	5:C:503:HOH:O	2.06	0.72
1:H:218[B]:GLU:OE2	5:H:503:HOH:O	2.09	0.71
1:B:313:GLU:OE1	5:B:501:HOH:O	2.08	0.70
1:C:235[A]:ASP:OD1	5:C:504:HOH:O	2.08	0.70
1:D:382:ASP:OD2	5:D:501:HOH:O	2.11	0.68
1:D:228:ARG:HD3	1:H:239:GLN:HG3	1.77	0.67
1:C:109[A]:SER:OG	5:C:501:HOH:O	1.98	0.67
1:F:279:ARG:NH2	5:F:501[A]:HOH:O	2.06	0.67
1:C:94:ASP:OD2	5:C:505:HOH:O	2.13	0.66
1:E:114:PRO:O	5:E:501:HOH:O	2.14	0.66
1:E:235[B]:ASP:OD1	5:E:502:HOH:O	2.14	0.65
1:A:218[B]:GLU:OE2	5:A:501:HOH:O	2.14	0.65
1:F:114:PRO:O	5:F:502:HOH:O	2.15	0.64
1:B:279[B]:ARG:NH1	5:B:504:HOH:O	2.18	0.62
1:E:187:ARG:NH1	5:E:509:HOH:O	2.34	0.61
1:A:321:GLY:HA2	1:A:341:VAL:HG13	1.83	0.61
1:B:382:ASP:OD2	5:B:503:HOH:O	2.16	0.61
1:H:182:GLU:OE2	5:H:504:HOH:O	2.16	0.60
1:H:232[A]:LYS:HG3	5:H:512:HOH:O	2.01	0.60
1:H:321:GLY:HA2	1:H:341:VAL:HG13	1.82	0.60
1:E:324:LYS:NZ	5:E:506:HOH:O	2.26	0.59
1:G:38:LEU:HD13	1:G:369:THR:HG21	1.85	0.59
1:C:324:LYS:NZ	5:C:511:HOH:O	2.36	0.57
1:A:182:GLU:OE2	5:A:502:HOH:O	2.16	0.57
1:B:279[B]:ARG:HG2	5:B:568:HOH:O	2.04	0.57
1:E:152:GLN:NE2	5:E:505:HOH:O	2.23	0.56
1:G:50[B]:ARG:HD2	1:G:55:PHE:HZ	1.70	0.56
1:A:148:LEU:HG	1:A:180[B]:LEU:HD23	1.88	0.55
1:G:55:PHE:HB2	1:G:104:PRO:HG2	1.88	0.55
1:E:61:LEU:HD23	1:E:68:GLU:HB3	1.90	0.54
1:F:147:SER:HA	1:F:161:LEU:HD12	1.92	0.51
1:G:333:PHE:CG	1:G:365:GLY:HA3	2.46	0.50
1:D:235[A]:ASP:OD1	5:D:502:HOH:O	2.19	0.50
1:A:321:GLY:CA	1:A:341:VAL:HG13	2.42	0.50
1:C:320[B]:LEU:HG	1:C:324:LYS:HD2	1.93	0.49
1:H:232[A]:LYS:HE2	5:H:856:HOH:O	2.12	0.49
1:B:225:GLU:HB2	1:G:225:GLU:HB2	1.94	0.49
1:G:148[A]:LEU:HD21	1:G:180:LEU:HD23	1.94	0.49
1:D:225:GLU:HB2	1:F:225:GLU:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:232[A]:LYS:HE3	5:H:512:HOH:O	2.14	0.48
1:B:346[B]:GLU:OE1	5:B:505:HOH:O	2.20	0.48
1:A:201:SER:HA	1:A:364[B]:LYS:HE3	1.96	0.47
1:H:321:GLY:CA	1:H:341:VAL:HG13	2.43	0.47
1:B:63[B]:LEU:HD21	3:B:403:ADE:C2	2.50	0.47
2:E:401:SO4:O2	5:E:503:HOH:O	2.20	0.47
1:C:289:ASN:HB3	1:C:295[B]:ILE:HD13	1.96	0.46
1:G:331:GLU:HA	1:G:334:GLU:HB2	1.98	0.46
1:B:250:ALA:HB1	1:B:298:ALA:HB2	1.98	0.46
1:D:201:SER:HA	1:D:364:LYS:HE3	1.97	0.46
1:F:26:LEU:HD23	1:F:152:GLN:HE22	1.80	0.46
1:B:286[B]:GLU:OE2	1:G:270:PRO:HD2	2.16	0.45
1:D:148[B]:LEU:HB2	1:D:180[B]:LEU:CD2	2.47	0.45
1:F:161:LEU:HD23	1:F:161:LEU:HA	1.80	0.45
1:H:117:ALA:HA	1:H:199:VAL:HG11	1.99	0.45
1:F:63[B]:LEU:HD23	1:F:109:SER:HB2	1.98	0.45
1:G:110[B]:TYR:CZ	1:G:384:LEU:HD21	2.51	0.45
1:B:11[B]:VAL:HG13	5:B:824:HOH:O	2.17	0.45
1:B:113:PHE:N	1:B:113:PHE:CD1	2.83	0.45
5:B:820:HOH:O	1:H:81:LYS:HE3	2.17	0.44
1:B:218[B]:GLU:HG3	5:H:887:HOH:O	2.16	0.44
1:F:294[B]:GLU:HG3	1:F:296:ILE:HG23	1.98	0.44
1:A:88:LYS:NZ	5:A:512:HOH:O	2.51	0.44
1:H:250:ALA:HB1	1:H:298:ALA:HB2	1.99	0.44
3:A:403:ADE:N1	5:A:505:HOH:O	2.36	0.43
1:G:194:HIS:HA	1:G:370:ARG:HA	2.00	0.43
1:A:148:LEU:HG	1:A:180[B]:LEU:CD2	2.48	0.43
1:G:4:GLU:OE1	1:G:50[B]:ARG:NE	2.48	0.43
1:D:272:PHE:CD2	1:F:279:ARG:HG3	2.54	0.43
1:C:225:GLU:HB2	1:H:225:GLU:HB2	2.00	0.43
1:G:113:PHE:CD1	1:G:113:PHE:N	2.86	0.43
1:C:370:ARG:NH2	5:C:518:HOH:O	2.48	0.42
1:B:113:PHE:HB3	1:B:119:LEU:HD12	2.02	0.42
1:E:235[A]:ASP:OD1	5:E:504:HOH:O	2.21	0.42
1:G:147:SER:HB2	1:G:158:CYS:HB2	2.02	0.42
1:E:75[B]:ARG:HD3	1:E:153[B]:GLY:O	2.19	0.42
1:B:0:HIS:CG	1:B:1:MET:N	2.87	0.41
1:A:225:GLU:HB2	1:E:225:GLU:HB2	2.02	0.41
1:F:39:ASP:OD2	5:F:503:HOH:O	2.22	0.41
1:E:38:LEU:HD13	1:E:369:THR:HG21	2.01	0.41
1:D:113:PHE:CD1	1:D:113:PHE:N	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD13	1:B:369:THR:HG21	2.02	0.41
1:F:279:ARG:NH1	5:F:509:HOH:O	2.37	0.41
1:E:370:ARG:NH2	5:E:516:HOH:O	2.48	0.41
1:B:265[A]:LEU:HD13	1:B:272:PHE:CE1	2.56	0.41
1:C:79[B]:CYS:SG	1:C:153:GLY:HA3	2.61	0.41
1:F:114:PRO:HB2	1:F:117:ALA:HB2	2.03	0.41
1:F:279:ARG:HG2	5:F:609:HOH:O	2.21	0.41
1:C:250:ALA:HB1	1:C:298:ALA:HB2	2.02	0.41
1:D:19:TRP:CZ3	1:D:209:SER:HB2	2.56	0.41
1:B:197:ILE:HB	1:B:367:ILE:HB	2.02	0.40
1:E:61:LEU:HD21	1:E:63[B]:LEU:HD21	2.03	0.40
1:E:279[B]:ARG:NH1	5:E:526:HOH:O	2.54	0.40

There are no symmetry-related clashes.

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	402/403 (100%)	395 (98%)	7 (2%)	0	100	100
1	B	413/403 (102%)	405 (98%)	8 (2%)	0	100	100
1	C	403/403 (100%)	395 (98%)	8 (2%)	0	100	100
1	D	407/403 (101%)	400 (98%)	7 (2%)	0	100	100
1	E	407/403 (101%)	398 (98%)	9 (2%)	0	100	100
1	F	398/403 (99%)	391 (98%)	7 (2%)	0	100	100
1	G	405/403 (100%)	398 (98%)	7 (2%)	0	100	100
1	H	404/403 (100%)	396 (98%)	8 (2%)	0	100	100
All	All	3239/3224 (100%)	3178 (98%)	61 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	326/327 (100%)	323 (99%)	3 (1%)	78	70
1	B	336/327 (103%)	333 (99%)	3 (1%)	78	70
1	C	328/327 (100%)	324 (99%)	4 (1%)	71	59
1	D	328/327 (100%)	326 (99%)	2 (1%)	86	80
1	E	326/327 (100%)	322 (99%)	4 (1%)	71	59
1	F	307/327 (94%)	304 (99%)	3 (1%)	76	67
1	G	309/327 (94%)	307 (99%)	2 (1%)	86	80
1	H	325/327 (99%)	322 (99%)	3 (1%)	78	70
All	All	2585/2616 (99%)	2561 (99%)	24 (1%)	81	70

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	TYR
1	A	180[A]	LEU
1	A	180[B]	LEU
1	B	68	GLU
1	B	180[A]	LEU
1	B	180[B]	LEU
1	C	126	LEU
1	C	180[A]	LEU
1	C	180[B]	LEU
1	C	265	LEU
1	D	180[A]	LEU
1	D	180[B]	LEU
1	E	61	LEU
1	E	84	ARG
1	E	180	LEU
1	E	265	LEU
1	F	152	GLN
1	F	180	LEU
1	F	265	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	180	LEU
1	G	209	SER
1	H	110	TYR
1	H	180[A]	LEU
1	H	180[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	152	GLN
1	F	152	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
2	SO4	B	402	-	4,4,4	0.16	0	6,6,6	0.12	0
3	ADE	B	403	-	9,11,11	0.95	0	7,15,15	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	402	-	4,4,4	0.11	0	6,6,6	0.10	0
3	ADE	H	403	-	9,11,11	1.03	1 (11%)	7,15,15	1.12	1 (14%)
2	SO4	H	402	-	4,4,4	0.12	0	6,6,6	0.48	0
4	EDO	G	600	-	3,3,3	0.48	0	2,2,2	0.50	0
2	SO4	E	401	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	E	403	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	H	401	-	4,4,4	0.24	0	6,6,6	0.24	0
3	ADE	D	403	-	9,11,11	0.92	0	7,15,15	1.09	0
2	SO4	A	402	-	4,4,4	0.10	0	6,6,6	0.51	0
3	ADE	A	403	-	9,11,11	0.99	0	7,15,15	1.10	0
2	SO4	C	401	-	4,4,4	0.19	0	6,6,6	0.41	0
2	SO4	D	401	-	4,4,4	0.15	0	6,6,6	0.58	0
2	SO4	A	401	-	4,4,4	0.25	0	6,6,6	0.38	0
2	SO4	B	401	-	4,4,4	0.27	0	6,6,6	0.44	0
4	EDO	F	402	-	3,3,3	0.51	0	2,2,2	0.51	0
2	SO4	F	401	-	4,4,4	0.13	0	6,6,6	0.09	0
3	ADE	E	402	-	9,11,11	0.99	1 (11%)	7,15,15	1.07	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
3	ADE	B	403	-	-	-	0/2/2/2
3	ADE	H	403	-	-	-	0/2/2/2
4	EDO	G	600	-	-	0/1/1/1	-
4	EDO	F	402	-	-	0/1/1/1	-
3	ADE	D	403	-	-	-	0/2/2/2
3	ADE	A	403	-	-	-	0/2/2/2
3	ADE	E	402	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	ADE	C4-N9	2.17	1.38	1.34
3	H	403	ADE	C4-N9	2.03	1.38	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	403	ADE	C5-C6-N6	2.10	123.54	120.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	ADE	1	0
2	E	401	SO4	1	0
2	H	401	SO4	1	0
3	A	403	ADE	1	0
2	C	401	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 ⓘ

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	392/403 (97%)	0.04	14 (3%)	42	47	12, 19, 42, 77	0
1	B	391/403 (97%)	-0.06	11 (2%)	53	57	12, 19, 38, 80	0
1	C	386/403 (95%)	0.06	16 (4%)	37	41	12, 23, 45, 72	0
1	D	393/403 (97%)	0.04	14 (3%)	42	47	11, 18, 39, 70	0
1	E	386/403 (95%)	0.08	14 (3%)	42	47	13, 24, 48, 81	0
1	F	387/403 (96%)	0.50	37 (9%)	8	9	12, 29, 63, 90	0
1	G	393/403 (97%)	0.69	57 (14%)	2	2	14, 33, 69, 87	0
1	H	392/403 (97%)	-0.00	11 (2%)	53	57	11, 20, 44, 79	0
All	All	3120/3224 (96%)	0.17	174 (5%)	24	27	11, 22, 56, 90	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	116	ALA	11.8
1	G	116	ALA	11.1
1	F	119	LEU	9.8
1	F	53	ALA	8.5
1	F	2	VAL	7.1
1	E	395	ALA	6.6
1	A	395	ALA	6.5
1	G	210	THR	6.4
1	G	211	SER	6.1
1	A	210	THR	6.0
1	D	115	THR	6.0
1	F	395	ALA	6.0
1	G	70	ILE	5.9
1	F	115	THR	5.4
1	G	395	ALA	5.4
1	H	395	ALA	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	211	SER	5.2
1	G	69	ALA	5.1
1	A	119	LEU	4.9
1	C	115	THR	4.9
1	G	119	LEU	4.9
1	B	116	ALA	4.9
1	G	103	TRP	4.9
1	D	395	ALA	4.8
1	G	97	LEU	4.8
1	G	96	ASN	4.8
1	C	208	SER	4.7
1	F	70	ILE	4.7
1	D	114	PRO	4.6
1	B	0	HIS	4.6
1	G	53	ALA	4.5
1	F	394	LEU	4.5
1	G	2	VAL	4.5
1	G	92	THR	4.5
1	G	209	SER	4.4
1	G	73	GLY	4.3
1	G	390	VAL	4.3
1	F	205	LYS	4.3
1	A	211	SER	4.2
1	G	330	SER	4.2
1	G	333	PHE	4.1
1	E	210	THR	4.0
1	F	1	MET	4.0
1	H	211	SER	4.0
1	C	395	ALA	3.9
1	D	0	HIS	3.9
1	A	207	THR	3.9
1	H	207	THR	3.8
1	G	61	LEU	3.8
1	G	394	LEU	3.8
1	C	0	HIS	3.7
1	F	203	ALA	3.7
1	G	3	HIS	3.7
1	E	110	TYR	3.7
1	G	105	LEU	3.6
1	G	86	TRP	3.6
1	D	333	PHE	3.5
1	H	210	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.5
1	G	104	PRO	3.4
1	A	110	TYR	3.4
1	C	210	THR	3.4
1	B	117	ALA	3.4
1	G	332	GLU	3.4
1	B	395	ALA	3.3
1	D	334	GLU	3.3
1	F	110[A]	TYR	3.3
1	D	1	MET	3.3
1	F	104	PRO	3.3
1	C	211	SER	3.3
1	G	384	LEU	3.3
1	G	389	GLY	3.3
1	B	333	PHE	3.2
1	F	120	ALA	3.2
1	F	136	LEU	3.2
1	G	55	PHE	3.2
1	F	207	THR	3.1
1	F	65	GLY	3.1
1	F	54	SER	3.1
1	G	58	GLY	3.0
1	G	102	GLU	3.0
1	C	209	SER	3.0
1	G	65	GLY	3.0
1	F	69	ALA	2.9
1	G	5	ALA	2.9
1	F	114	PRO	2.9
1	F	133	LEU	2.9
1	C	114	PRO	2.9
1	F	52	ASP	2.8
1	G	1	MET	2.8
1	A	120	ALA	2.8
1	G	54	SER	2.8
1	B	210	THR	2.8
1	H	203	ALA	2.8
1	G	382	ASP	2.8
1	G	90	MET	2.7
1	B	114	PRO	2.7
1	D	110[A]	TYR	2.7
1	D	117	ALA	2.7
1	G	203	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	117	ALA	2.6
1	F	97	LEU	2.6
1	H	209	SER	2.6
1	C	340	GLY	2.6
1	A	1	MET	2.6
1	A	63[A]	LEU	2.6
1	G	115	THR	2.6
1	D	116	ALA	2.6
1	F	393	VAL	2.6
1	E	63[A]	LEU	2.6
1	D	346	GLU	2.5
1	E	72	GLU	2.5
1	F	57	ALA	2.5
1	G	139	LEU	2.5
1	E	68	GLU	2.5
1	A	209	SER	2.5
1	G	120	ALA	2.5
1	F	73	GLY	2.5
1	C	119	LEU	2.5
1	H	110	TYR	2.5
1	G	62	TRP	2.5
1	G	110[A]	TYR	2.5
1	C	69	ALA	2.5
1	A	355	GLU	2.5
1	G	204	LYS	2.4
1	E	1	MET	2.4
1	G	52	ASP	2.4
1	E	115	THR	2.4
1	G	63[A]	LEU	2.4
1	H	121	SER	2.4
1	C	110	TYR	2.4
1	G	137	TYR	2.4
1	G	60	ARG	2.4
1	G	85	ALA	2.4
1	B	209	SER	2.3
1	E	339	THR	2.3
1	F	335	SER	2.3
1	F	384	LEU	2.3
1	H	1	MET	2.3
1	A	206	GLY	2.3
1	G	334	GLU	2.3
1	A	393	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	110[A]	TYR	2.3
1	F	137	TYR	2.3
1	G	106	ARG	2.3
1	B	119	LEU	2.3
1	D	119	LEU	2.3
1	E	85	ALA	2.3
1	E	340	GLY	2.3
1	H	93	LYS	2.3
1	C	86	TRP	2.2
1	C	63[A]	LEU	2.2
1	G	101	SER	2.2
1	F	390	VAL	2.2
1	C	1	MET	2.2
1	G	129	LEU	2.2
1	G	89	GLU	2.2
1	F	88	LYS	2.2
1	F	92	THR	2.2
1	F	118	GLY	2.2
1	F	60	ARG	2.2
1	E	209	SER	2.1
1	D	203	ALA	2.1
1	F	42	HIS	2.1
1	F	129	LEU	2.1
1	G	76	LEU	2.1
1	E	208	SER	2.1
1	C	56	GLU	2.1
1	G	72	GLU	2.1
1	A	117	ALA	2.0
1	G	117	ALA	2.0
1	D	208	SER	2.0
1	G	113	PHE	2.0
1	F	103	TRP	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADE	H	403	10/10	0.47	0.37	34,40,43,45	10
3	ADE	E	402	10/10	0.64	0.21	29,34,39,42	10
3	ADE	B	403	10/10	0.67	0.20	38,39,39,39	10
3	ADE	A	403	10/10	0.73	0.19	29,34,36,37	10
3	ADE	D	403	10/10	0.78	0.17	26,27,29,30	10
2	SO4	E	403	5/5	0.84	0.21	37,43,51,52	5
2	SO4	F	401	5/5	0.85	0.16	55,55,60,61	5
2	SO4	B	402	5/5	0.89	0.13	30,32,40,43	5
2	SO4	D	402	5/5	0.90	0.13	30,33,46,46	5
2	SO4	H	402	5/5	0.91	0.14	14,29,32,34	5
2	SO4	A	402	5/5	0.91	0.13	14,26,30,31	5
4	EDO	G	600	4/4	0.93	0.14	24,25,32,32	0
2	SO4	C	401	5/5	0.94	0.15	26,34,38,45	5
2	SO4	E	401	5/5	0.96	0.13	22,36,38,49	5
2	SO4	A	401	5/5	0.98	0.07	23,26,34,43	0
2	SO4	B	401	5/5	0.98	0.07	19,24,28,32	0
2	SO4	H	401	5/5	0.98	0.08	23,25,31,39	0
4	EDO	F	402	4/4	0.98	0.09	22,23,25,29	0
2	SO4	D	401	5/5	0.98	0.07	17,23,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.