



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:04 AM UTC

PDB ID : 3E3G / pdb_00003e3g
Title : H. influenzae beta-carbonic anhydrase, variant G41A
Authors : Rowlett, R.S.; Failing, H.
Deposited on : 2008-08-07
Resolution : 2.30 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

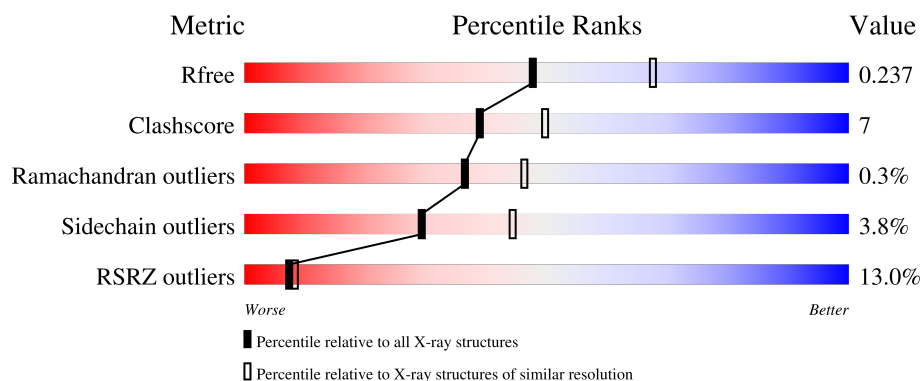
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	229	9% 75% 14% 10%
1	B	229	12% 76% 14% 10%
1	C	229	12% 77% 11% 11%
1	D	229	13% 73% 14% 13%
1	E	229	17% 72% 17% 10%

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Mol	Chain	Length	Quality of chain
1	F	229	

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
3	SO4	A	234	-	-	X	-
3	SO4	B	232	-	-	X	-
3	SO4	D	231	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10130 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 Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	1	0
			1669	1064	296	300	9			
1	B	207	Total	C	N	O	S	0	1	0
			1669	1064	296	300	9			
1	C	204	Total	C	N	O	S	0	1	0
			1644	1047	292	296	9			
1	D	200	Total	C	N	O	S	0	1	0
			1610	1029	287	285	9			
1	E	207	Total	C	N	O	S	0	1	0
			1671	1064	298	300	9			
1	F	206	Total	C	N	O	S	0	1	0
			1663	1058	297	299	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	GLY	engineered mutation	UNP P45148
B	41	ALA	GLY	engineered mutation	UNP P45148
C	41	ALA	GLY	engineered mutation	UNP P45148
D	41	ALA	GLY	engineered mutation	UNP P45148
E	41	ALA	GLY	engineered mutation	UNP P45148
F	41	ALA	GLY	engineered mutation	UNP P45148

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

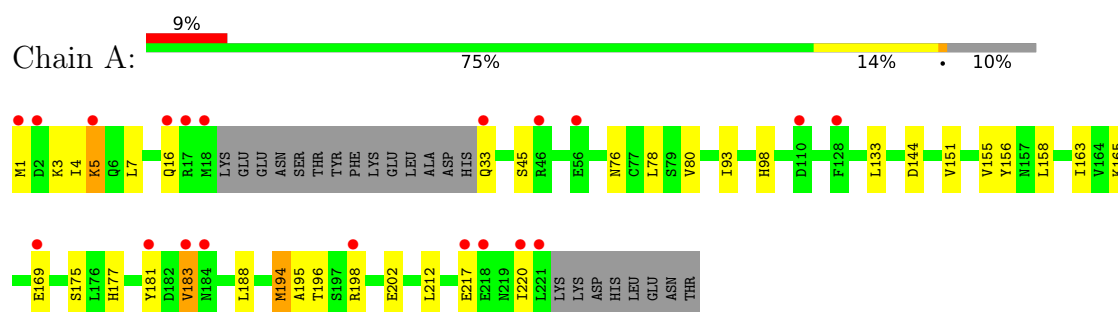
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	22	Total	O	0	0
			22	22		
4	C	21	Total	O	0	0
			21	21		
4	D	24	Total	O	0	0
			24	24		
4	E	15	Total	O	0	0
			15	15		
4	F	17	Total	O	0	0
			17	17		

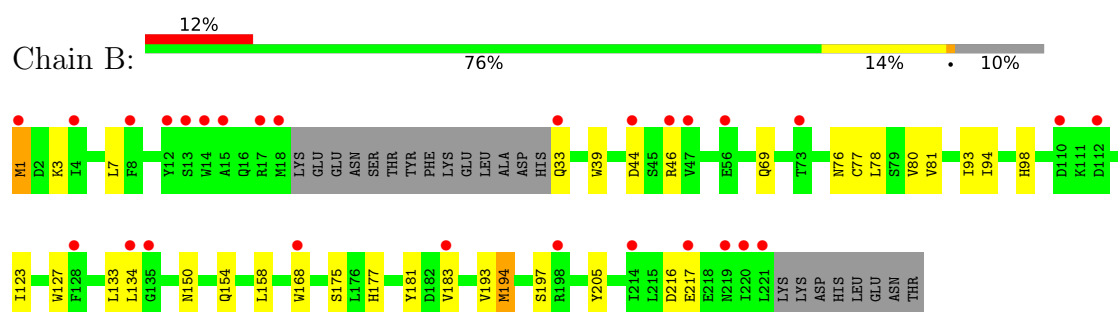
3 Residue-property plots [i](#)

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.

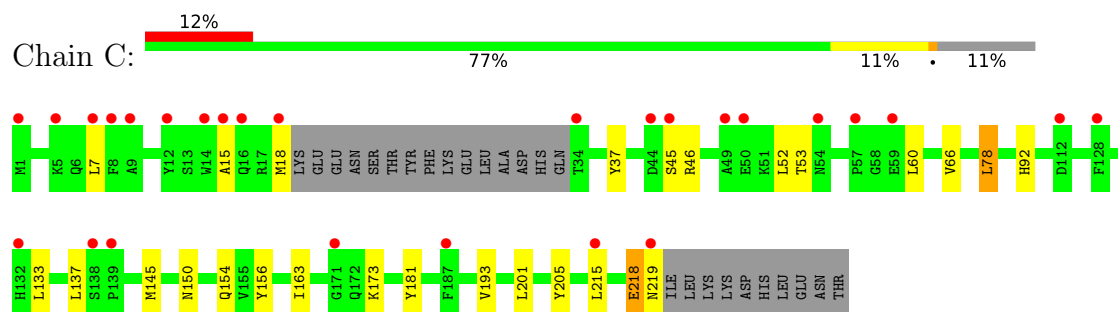
• Molecule 1: Carbonic anhydrase 2



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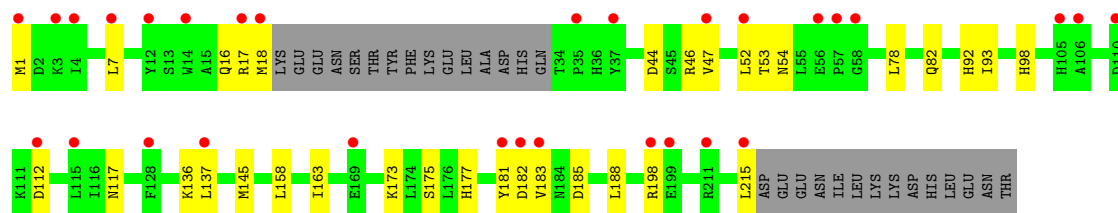


• Molecule 1: Carbonic anhydrase 2

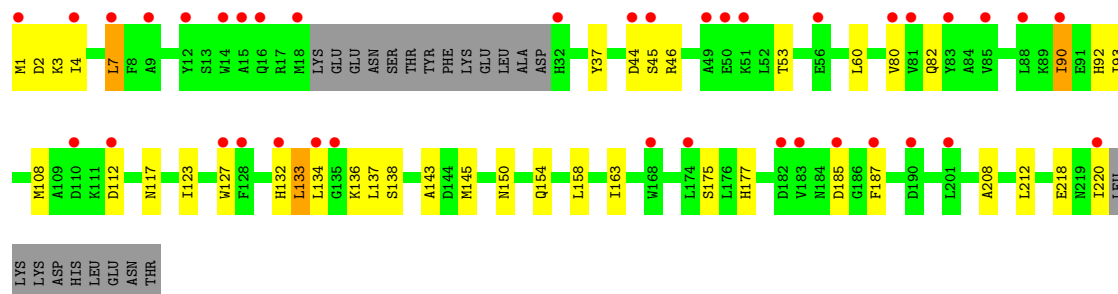
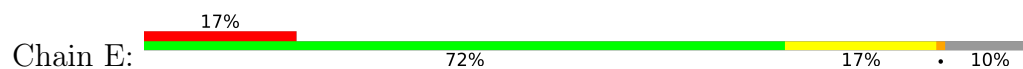


• Molecule 1: Carbonic anhydrase 2

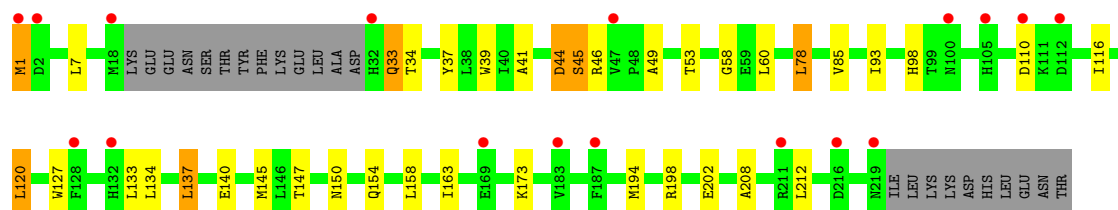
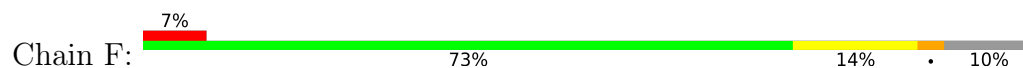




● Molecule 1: Carbonic anhydrase 2



● Molecule 1: Carbonic anhydrase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.93Å 145.23Å 52.97Å 90.00° 93.82° 90.00°	Depositor
Resolution (Å)	39.41 – 2.30 39.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.41-2.30) 98.1 (39.41-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.234 0.201 , 0.237	Depositor DCC
R_{free} test set	3804 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10130	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: SO4, ZN

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	0.70	0/1708	0.82	0/2314
1	B	0.65	0/1708	0.85	1/2314 (0.0%)
1	C	0.62	0/1683	0.79	0/2280
1	D	0.66	0/1649	0.83	1/2234 (0.0%)
1	E	0.62	0/1711	0.85	0/2318
1	F	0.65	0/1703	0.86	2/2307 (0.1%)
All	All	0.65	0/10162	0.83	4/13767 (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	D	44	ASP	CB-CA-C	-6.77	95.83	109.99
1	F	44	ASP	CB-CA-C	-6.54	100.61	110.88
1	B	44	ASP	CB-CA-C	-6.43	99.92	110.85
1	F	85	VAL	N-CA-C	5.18	115.40	110.53

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	1669	0	1662	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1669	0	1662	27	0
1	C	1644	0	1632	16	0
1	D	1610	0	1610	29	0
1	E	1671	0	1658	28	0
1	F	1663	0	1647	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	20	0	0	3	1
3	B	10	0	0	7	0
3	C	10	0	0	0	0
3	D	5	0	0	4	0
3	E	15	0	0	0	0
3	F	5	0	0	0	0
4	A	34	0	0	0	1
4	B	22	0	0	0	0
4	C	21	0	0	0	0
4	D	24	0	0	0	0
4	E	15	0	0	0	0
4	F	17	0	0	1	0
All	All	10130	0	9871	135	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 7.

All (135) 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:69:GLN:NE2	1:B:123:ILE:HD11	1.77	1.00
1:D:183:VAL:HG12	3:D:231:SO4:O4	1.77	0.85
1:D:112:ASP:HA	1:D:117:ASN:HD21	1.40	0.84
1:D:181:TYR:OH	3:D:231:SO4:O2	1.95	0.83
1:C:92:HIS:NE2	1:E:1:MET:HE3	1.95	0.82
1:D:53:THR:HG22	1:F:7:LEU:HD21	1.61	0.82
1:D:98:HIS:HB3	1:D:181:TYR:CE2	2.16	0.80
1:E:90:ILE:HD12	1:E:92:HIS:H	1.48	0.79
1:B:183:VAL:HG12	3:B:232:SO4:O4	1.84	0.76
1:B:46:ARG:N	3:B:232:SO4:O3	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:SER:HB2	1:B:194:MET:HE1	1.68	0.76
1:C:133:LEU:HD21	1:C:145:MET:HE3	1.68	0.75
1:F:78:LEU:HD13	1:F:163:ILE:HD12	1.71	0.73
1:B:69:GLN:HE22	1:B:123:ILE:HD11	1.51	0.73
1:B:69:GLN:HE22	1:B:123:ILE:CD1	2.03	0.72
1:A:194:MET:HE1	1:A:196:THR:HG23	1.72	0.71
1:D:136:LYS:O	1:D:137:LEU:HD12	1.92	0.70
1:A:181:TYR:OH	3:A:234:SO4:O2	2.06	0.69
1:C:78:LEU:HD13	1:C:163:ILE:HD12	1.73	0.69
1:E:108:MET:HE1	1:E:143:ALA:HB2	1.74	0.68
1:D:112:ASP:HA	1:D:117:ASN:ND2	2.08	0.67
1:A:217:GLU:HA	1:A:220:ILE:HD12	1.77	0.67
1:C:53:THR:HG22	1:E:7:LEU:HD21	1.75	0.67
1:D:78:LEU:HD22	1:D:163:ILE:HD12	1.77	0.66
1:B:1:MET:HE2	1:B:3:LYS:H	1.61	0.66
1:F:116:ILE:HG13	1:F:120:LEU:HD22	1.81	0.62
1:D:145:MET:HE3	1:D:215:LEU:HD11	1.81	0.62
1:C:7:LEU:HD21	1:E:53:THR:HG22	1.82	0.61
1:F:208:ALA:O	1:F:212:LEU:HD23	2.00	0.60
1:A:194:MET:HE2	1:A:195:ALA:N	2.17	0.60
1:F:110:ASP:OD1	1:F:110:ASP:C	2.45	0.58
1:C:53:THR:CG2	1:E:7:LEU:HD21	2.32	0.58
1:D:78:LEU:HD22	1:D:163:ILE:CD1	2.32	0.58
1:E:137:LEU:HD21	1:E:145:MET:HE2	1.85	0.58
1:F:37:TYR:HB2	1:F:60:LEU:HD23	1.85	0.58
1:B:93:ILE:HG21	1:B:158:LEU:HD21	1.85	0.57
1:D:93:ILE:HG21	1:D:158:LEU:HD21	1.86	0.57
1:D:136:LYS:C	1:D:137:LEU:HD12	2.28	0.57
1:E:1:MET:O	1:E:4:ILE:N	2.27	0.57
1:D:92:HIS:NE2	1:F:1:MET:HE3	2.20	0.57
1:D:181:TYR:OH	3:D:231:SO4:S	2.59	0.57
1:E:133:LEU:C	1:E:133:LEU:HD23	2.30	0.57
1:E:112:ASP:HA	1:E:117:ASN:OD1	2.05	0.56
1:A:78:LEU:HD22	1:A:163:ILE:HD12	1.86	0.56
1:A:78:LEU:CD2	1:A:163:ILE:HD12	2.35	0.56
1:A:1:MET:O	1:A:5:LYS:NZ	2.38	0.56
1:C:37:TYR:HB2	1:C:60:LEU:HD23	1.86	0.56
1:F:33:GLN:HG3	1:F:34:THR:N	2.21	0.56
1:D:7:LEU:HD21	1:F:53:THR:HG22	1.88	0.55
1:B:98:HIS:ND1	3:B:232:SO4:O1	2.40	0.55
1:E:93:ILE:HG21	1:E:158:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:HIS:CE1	1:B:194:MET:HE3	2.42	0.55
1:A:183:VAL:HG12	3:A:234:SO4:O4	2.06	0.54
1:A:194:MET:HE1	1:A:196:THR:CG2	2.37	0.54
1:B:76:ASN:O	1:B:80:VAL:HG23	2.09	0.53
1:F:78:LEU:HD13	1:F:163:ILE:CD1	2.39	0.53
1:C:137:LEU:CD1	1:C:215:LEU:HD22	2.39	0.52
1:C:150:ASN:O	1:C:154:GLN:HG2	2.09	0.52
1:E:208:ALA:O	1:E:212:LEU:HD23	2.09	0.52
1:D:175:SER:OG	1:D:177:HIS:NE2	2.41	0.52
1:F:93:ILE:HG21	1:F:158:LEU:HD21	1.91	0.52
1:E:138:SER:N	1:E:220:ILE:HG22	2.24	0.51
1:B:69:GLN:NE2	1:B:123:ILE:CD1	2.56	0.51
1:F:127:TRP:HD1	1:F:134:LEU:HD13	1.75	0.51
1:D:173:LYS:NZ	1:F:1:MET:HE2	2.26	0.51
1:B:193:VAL:HG22	1:B:205:TYR:HA	1.92	0.50
1:A:1:MET:H2	1:A:4:ILE:HB	1.77	0.50
1:C:218:GLU:O	1:C:219:ASN:C	2.55	0.49
1:E:127:TRP:CD1	1:E:134:LEU:HD13	2.48	0.49
1:D:16:GLN:C	1:D:18:MET:H	2.21	0.49
1:E:175:SER:OG	1:E:177:HIS:NE2	2.43	0.49
1:F:127:TRP:CD1	1:F:134:LEU:HD13	2.48	0.48
1:B:183:VAL:HG12	3:B:232:SO4:S	2.53	0.48
1:B:127:TRP:CD1	1:B:134:LEU:HD13	2.49	0.48
1:E:136:LYS:O	1:E:220:ILE:HG23	2.13	0.48
1:D:182:ASP:OD1	1:D:183:VAL:N	2.47	0.48
1:B:183:VAL:CG1	3:B:232:SO4:O4	2.57	0.48
1:D:78:LEU:CD2	1:D:163:ILE:HD12	2.44	0.48
1:F:44:ASP:O	1:F:45:SER:C	2.55	0.48
1:E:127:TRP:HD1	1:E:134:LEU:HD13	1.79	0.47
1:A:76:ASN:O	1:A:80:VAL:HG23	2.15	0.47
1:A:156:TYR:OH	1:A:202:GLU:OE2	2.25	0.47
1:B:46:ARG:HG2	3:B:232:SO4:O2	2.15	0.47
1:A:198:ARG:NH2	3:A:232:SO4:O1	2.48	0.47
1:A:7:LEU:C	1:A:7:LEU:HD23	2.41	0.46
1:F:49:ALA:CB	1:F:60:LEU:HD13	2.45	0.46
1:D:183:VAL:CG1	3:D:231:SO4:O4	2.58	0.46
1:D:181:TYR:HB3	1:D:188:LEU:HD23	1.97	0.46
1:F:145:MET:SD	1:F:212:LEU:HD12	2.56	0.46
1:F:150:ASN:O	1:F:154:GLN:HG2	2.15	0.46
1:D:47:VAL:HG12	1:D:52:LEU:HG	1.98	0.46
1:A:78:LEU:HD22	1:A:163:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:O	1:B:154:GLN:HG2	2.16	0.45
1:D:1:MET:HE3	1:F:173:LYS:NZ	2.31	0.45
1:D:137:LEU:HD11	1:D:215:LEU:HD12	1.98	0.45
1:F:49:ALA:HB3	1:F:60:LEU:HD13	1.99	0.45
1:D:173:LYS:HZ1	1:F:1:MET:HE2	1.81	0.45
1:A:1:MET:HE3	1:A:3:LYS:HG3	1.98	0.45
1:A:93:ILE:HG21	1:A:158:LEU:HD21	1.99	0.45
1:E:1:MET:O	1:E:3:LYS:N	2.50	0.44
1:E:90:ILE:CD1	1:E:92:HIS:O	2.65	0.44
1:B:69:GLN:CD	1:B:123:ILE:HD11	2.40	0.44
1:B:181:TYR:OH	3:B:232:SO4:O3	2.25	0.44
1:B:175:SER:HB2	1:B:194:MET:CE	2.45	0.44
1:A:45:SER:HB3	1:A:98:HIS:CD2	2.53	0.44
1:E:37:TYR:HB2	1:E:60:LEU:HD23	2.00	0.44
1:A:1:MET:HE3	1:A:3:LYS:CG	2.48	0.43
1:C:52:LEU:HD11	1:C:181:TYR:CE2	2.54	0.43
1:E:90:ILE:HD11	1:E:92:HIS:O	2.18	0.43
1:E:150:ASN:O	1:E:154:GLN:HG2	2.19	0.43
1:B:7:LEU:HD12	1:B:7:LEU:HA	1.81	0.43
1:B:216:ASP:O	1:B:217:GLU:HB3	2.18	0.43
1:A:175:SER:OG	1:A:177:HIS:NE2	2.50	0.43
1:C:173:LYS:NZ	1:E:1:MET:HE2	2.33	0.43
1:D:82:GLN:HA	1:D:163:ILE:HG21	2.01	0.42
1:F:39:TRP:NE1	1:F:41:ALA:HB2	2.34	0.42
1:D:93:ILE:CG2	1:D:158:LEU:HD21	2.50	0.42
1:C:156:TYR:HA	1:C:201:LEU:HD11	2.02	0.42
1:B:77:CYS:O	1:B:81:VAL:HG23	2.20	0.42
1:E:123:ILE:CD1	1:E:150:ASN:OD1	2.67	0.42
1:C:193:VAL:HG22	1:C:205:TYR:HA	2.01	0.42
1:B:1:MET:HE3	1:B:1:MET:HB2	1.95	0.42
1:C:15:ALA:HB3	1:E:187:PHE:CE2	2.55	0.41
1:A:151:VAL:O	1:A:155:VAL:HG23	2.21	0.41
1:A:181:TYR:HB3	1:A:188:LEU:HD23	2.02	0.41
1:C:66:VAL:HG23	1:E:80:VAL:HG22	2.02	0.41
1:F:98:HIS:O	1:F:147:THR:HG21	2.21	0.41
1:E:82:GLN:HA	1:E:163:ILE:HG21	2.03	0.41
1:E:123:ILE:HD12	1:E:150:ASN:OD1	2.21	0.41
1:A:175:SER:HB2	1:A:194:MET:CE	2.51	0.41
1:F:46:ARG:HG2	4:F:237:HOH:O	2.19	0.40
1:B:168:TRP:CD2	1:B:197:SER:HA	2.56	0.40
1:F:137:LEU:HD12	1:F:137:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:TRP:CZ3	1:B:94:ILE:HD13	2.57	0.40
1:D:46:ARG:HG2	1:F:58:GLY:N	2.37	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)
3:A:233:SO4:O4	4:A:267:HOH:O[2_556]	1.94	0.26

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	204/229 (89%)	201 (98%)	3 (2%)	0	100	100
1	B	204/229 (89%)	198 (97%)	6 (3%)	0	100	100
1	C	201/229 (88%)	193 (96%)	7 (4%)	1 (0%)	24	31
1	D	197/229 (86%)	190 (96%)	6 (3%)	1 (0%)	24	31
1	E	204/229 (89%)	197 (97%)	5 (2%)	2 (1%)	12	15
1	F	203/229 (89%)	199 (98%)	4 (2%)	0	100	100
All	All	1213/1374 (88%)	1178 (97%)	31 (3%)	4 (0%)	36	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	ASP
1	E	45	SER
1	D	17	ARG
1	C	46	ARG

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	181/201 (90%)	171 (94%)	10 (6%)	19	28
1	B	181/201 (90%)	176 (97%)	5 (3%)	38	56
1	C	178/201 (89%)	174 (98%)	4 (2%)	45	65
1	D	174/201 (87%)	171 (98%)	3 (2%)	53	72
1	E	181/201 (90%)	173 (96%)	8 (4%)	25	38
1	F	180/201 (90%)	169 (94%)	11 (6%)	17	24
All	All	1075/1206 (89%)	1034 (96%)	41 (4%)	29	44

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	16	GLN
1	A	33	GLN
1	A	133	LEU
1	A	144	ASP
1	A	165	LYS
1	A	169	GLU
1	A	183	VAL
1	A	194	MET
1	A	212	LEU
1	B	1	MET
1	B	33	GLN
1	B	78	LEU
1	B	133	LEU
1	B	194	MET
1	C	18	MET
1	C	45	SER
1	C	78	LEU
1	C	218	GLU
1	D	54	ASN
1	D	185	ASP
1	D	198	ARG

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Mol	Chain	Res	Type
1	E	7	LEU
1	E	44	ASP
1	E	46	ARG
1	E	90	ILE
1	E	132	HIS
1	E	133	LEU
1	E	185	ASP
1	E	218	GLU
1	F	1	MET
1	F	33	GLN
1	F	45	SER
1	F	78	LEU
1	F	120	LEU
1	F	133	LEU
1	F	137	LEU
1	F	140	GLU
1	F	194	MET
1	F	198	ARG
1	F	202	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	10	ASN
1	A	16	GLN
1	A	33	GLN
1	A	36	HIS
1	A	54	ASN
1	A	117	ASN
1	A	132	HIS
1	B	33	GLN
1	B	54	ASN
1	B	69	GLN
1	B	132	HIS
1	C	16	GLN
1	C	54	ASN
1	C	219	ASN
1	D	6	GLN
1	D	117	ASN
1	D	132	HIS
1	D	191	GLN

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Mol	Chain	Res	Type
1	E	33	GLN
1	E	54	ASN
1	E	191	GLN
1	E	219	ASN
1	F	100	ASN
1	F	105	HIS
1	F	219	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 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	$\# Z > 2$
3	SO4	C	231	-	4,4,4	0.29	0	6,6,6	0.29	0
3	SO4	B	232	-	4,4,4	0.25	0	6,6,6	0.30	0
3	SO4	A	233	-	4,4,4	0.49	0	6,6,6	0.78	0
3	SO4	A	231	-	4,4,4	0.28	0	6,6,6	0.59	0
3	SO4	C	232	-	4,4,4	0.30	0	6,6,6	0.29	0
3	SO4	E	233	-	4,4,4	0.25	0	6,6,6	0.31	0
3	SO4	B	231	-	4,4,4	0.21	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	231	-	4,4,4	0.24	0	6,6,6	0.29	0
3	SO4	F	231	-	4,4,4	0.31	0	6,6,6	0.37	0
3	SO4	E	232	-	4,4,4	0.21	0	6,6,6	0.37	0
3	SO4	E	231	-	4,4,4	0.26	0	6,6,6	0.25	0
3	SO4	A	232	-	4,4,4	0.20	0	6,6,6	0.43	0
3	SO4	A	234	-	4,4,4	0.20	0	6,6,6	0.26	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.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	232	SO4	7	0
3	A	233	SO4	0	1
3	D	231	SO4	4	0
3	A	232	SO4	1	0
3	A	234	SO4	2	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	207/229 (90%)	0.83	20 (9%) 13 15	26, 42, 55, 67	1 (0%)
1	B	207/229 (90%)	1.12	28 (13%) 7 8	27, 46, 66, 81	1 (0%)
1	C	204/229 (89%)	1.02	27 (13%) 7 8	30, 49, 75, 89	1 (0%)
1	D	200/229 (87%)	1.09	30 (15%) 5 6	26, 46, 66, 88	1 (0%)
1	E	207/229 (90%)	1.38	38 (18%) 3 4	31, 51, 71, 90	1 (0%)
1	F	206/229 (89%)	0.85	17 (8%) 17 19	32, 47, 62, 76	1 (0%)
All	All	1231/1374 (89%)	1.05	160 (12%) 7 8	26, 47, 68, 90	6 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	128[A]	PHE	7.0
1	D	181	TYR	5.6
1	E	220	ILE	4.7
1	A	128[A]	PHE	4.7
1	C	128[A]	PHE	4.7
1	B	128[A]	PHE	4.3
1	E	128[A]	PHE	4.3
1	E	18	MET	4.3
1	D	128[A]	PHE	4.3
1	E	1	MET	4.3
1	A	220	ILE	4.2
1	E	32	HIS	4.0
1	E	132	HIS	4.0
1	B	1	MET	4.0
1	D	215	LEU	3.9
1	D	18	MET	3.9
1	D	1	MET	3.8
1	C	18	MET	3.6
1	A	18	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	1	MET	3.6
1	E	15	ALA	3.5
1	C	34	THR	3.4
1	B	110	ASP	3.4
1	D	12	TYR	3.4
1	C	1	MET	3.4
1	E	50	GLU	3.4
1	B	221	LEU	3.4
1	B	13	SER	3.4
1	E	12	TYR	3.4
1	A	1	MET	3.3
1	B	18	MET	3.3
1	D	112	ASP	3.3
1	E	168	TRP	3.2
1	E	90	ILE	3.2
1	B	56	GLU	3.1
1	A	16	GLN	3.1
1	C	50	GLU	3.1
1	B	47	VAL	3.1
1	A	221	LEU	3.1
1	A	110	ASP	3.0
1	D	110	ASP	3.0
1	A	184	ASN	2.9
1	B	112	ASP	2.9
1	B	15	ALA	2.9
1	E	7	LEU	2.9
1	A	183	VAL	2.9
1	F	47	VAL	2.9
1	B	44	ASP	2.9
1	E	44	ASP	2.9
1	A	56	GLU	2.8
1	D	199	GLU	2.8
1	D	4	ILE	2.8
1	C	45	SER	2.8
1	E	16	GLN	2.7
1	A	217	GLU	2.7
1	D	183	VAL	2.7
1	F	183	VAL	2.7
1	F	110	ASP	2.7
1	E	14	TRP	2.7
1	B	219	ASN	2.7
1	F	169	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	45	SER	2.7
1	D	58	GLY	2.6
1	E	9	ALA	2.6
1	E	187	PHE	2.6
1	F	105	HIS	2.6
1	B	135	GLY	2.6
1	F	187	PHE	2.6
1	E	85	VAL	2.6
1	B	12	TYR	2.5
1	C	57	PRO	2.5
1	E	81	VAL	2.5
1	B	134	LEU	2.5
1	A	218	GLU	2.5
1	C	219	ASN	2.5
1	E	185	ASP	2.5
1	F	32	HIS	2.5
1	B	217	GLU	2.4
1	F	132	HIS	2.4
1	A	46	ARG	2.4
1	B	198	ARG	2.4
1	F	211	ARG	2.4
1	D	3	LYS	2.4
1	C	7	LEU	2.4
1	D	52	LEU	2.4
1	C	12	TYR	2.4
1	D	37	TYR	2.4
1	F	216	ASP	2.4
1	E	135	GLY	2.4
1	C	187	PHE	2.4
1	A	2	ASP	2.4
1	A	169	GLU	2.4
1	D	182	ASP	2.4
1	E	182	ASP	2.4
1	F	219	ASN	2.4
1	D	35	PRO	2.4
1	C	49	ALA	2.4
1	C	5	LYS	2.4
1	B	214	ILE	2.4
1	E	4	ILE	2.4
1	A	33	GLN	2.4
1	C	14	TRP	2.4
1	E	183	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	211	ARG	2.3
1	E	134	LEU	2.3
1	F	112	ASP	2.3
1	E	83	TYR	2.3
1	E	127	TRP	2.3
1	C	15	ALA	2.3
1	B	46	ARG	2.3
1	D	105	HIS	2.3
1	C	16	GLN	2.3
1	D	115	LEU	2.3
1	B	17	ARG	2.3
1	D	106	ALA	2.3
1	C	59	GLU	2.3
1	D	169	GLU	2.3
1	C	215	LEU	2.2
1	E	88	LEU	2.2
1	F	18	MET	2.2
1	A	181	TYR	2.2
1	E	49	ALA	2.2
1	C	8	PHE	2.2
1	C	138	SER	2.2
1	A	198	ARG	2.2
1	C	54	ASN	2.2
1	A	17	ARG	2.2
1	E	112	ASP	2.2
1	C	9	ALA	2.2
1	D	7	LEU	2.1
1	A	5	LYS	2.1
1	B	73	THR	2.1
1	D	198	ARG	2.1
1	F	100	ASN	2.1
1	B	14	TRP	2.1
1	C	171	GLY	2.1
1	B	4	ILE	2.1
1	E	174	LEU	2.1
1	C	112	ASP	2.1
1	E	190	ASP	2.1
1	F	2	ASP	2.1
1	B	33	GLN	2.1
1	B	183	VAL	2.1
1	B	8	PHE	2.1
1	D	56	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	132	HIS	2.1
1	E	201	LEU	2.1
1	E	110	ASP	2.1
1	D	57	PRO	2.1
1	E	80	VAL	2.1
1	B	168	TRP	2.1
1	D	14	TRP	2.1
1	C	139	PRO	2.0
1	D	47	VAL	2.0
1	E	51	LYS	2.0
1	E	56	GLU	2.0
1	C	44	ASP	2.0
1	D	137	LEU	2.0
1	B	220	ILE	2.0
1	D	17	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	E	231	5/5	0.74	0.20	88,89,89,90	0
3	SO4	D	231	5/5	0.82	0.21	50,50,51,53	5
3	SO4	B	232	5/5	0.85	0.28	63,64,65,65	5
3	SO4	B	231	5/5	0.87	0.22	64,64,65,65	5
3	SO4	C	232	5/5	0.90	0.21	63,63,64,67	0
3	SO4	C	231	5/5	0.91	0.17	66,67,68,69	0
3	SO4	E	233	5/5	0.91	0.16	63,63,66,66	0
3	SO4	A	234	5/5	0.92	0.21	45,46,46,48	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	E	232	5/5	0.93	0.16	74,74,74,74	0
3	SO4	A	231	5/5	0.95	0.14	59,60,60,61	0
3	SO4	F	231	5/5	0.95	0.17	61,62,63,64	0
3	SO4	A	232	5/5	0.96	0.14	55,55,56,56	0
3	SO4	A	233	5/5	0.96	0.15	44,44,46,47	5
2	ZN	D	230	1/1	0.98	0.11	40,40,40,40	0
2	ZN	F	230	1/1	0.98	0.10	42,42,42,42	0
2	ZN	A	230	1/1	0.98	0.12	38,38,38,38	0
2	ZN	B	230	1/1	0.98	0.12	42,42,42,42	0
2	ZN	C	230	1/1	0.98	0.11	46,46,46,46	0
2	ZN	E	230	1/1	0.99	0.12	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.