



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:31 PM UTC

PDB ID : 3MF3 / pdb_00003mf3
Title : Cobalt(II)-Substituted Haemophilus influenzae B-Carbonic Anhydrase
Authors : Hoffmann, K.M.; Rowlett, R.S.
Deposited on : 2010-04-01
Resolution : 2.50 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

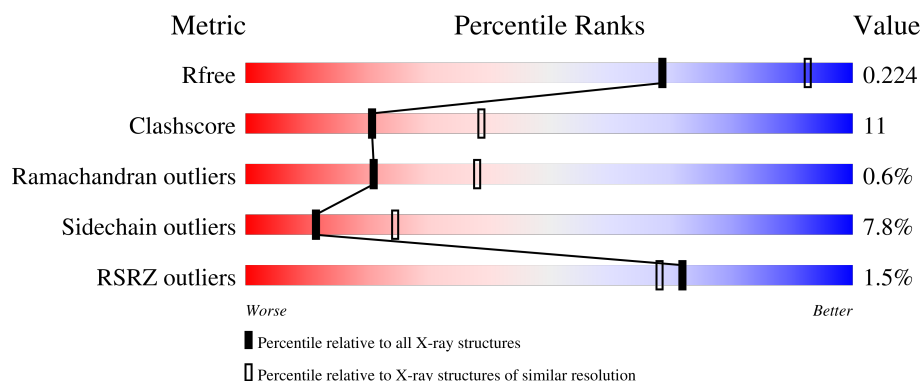
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	221	% 73% 23% .
1	B	221	2% 71% 25% .
1	C	221	79% 17% ..
1	D	221	2% 69% 24% ..
1	E	221	% 71% 25% ..

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Mol	Chain	Length	Quality of chain
1	F	221	% 69% 26%

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	ACT	D	222	-	-	X	-
3	ACT	E	222	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10709 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	220	Total	C	N	O	S	0	0	0
			1772	1125	314	325	8			
1	B	221	Total	C	N	O	S	0	0	0
			1772	1126	315	322	9			
1	C	217	Total	C	N	O	S	0	0	0
			1747	1109	310	319	9			
1	D	214	Total	C	N	O	S	0	0	0
			1719	1094	306	311	8			
1	E	215	Total	C	N	O	S	0	0	0
			1726	1097	308	313	8			
1	F	217	Total	C	N	O	S	0	0	0
			1747	1109	310	319	9			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		
2	B	1	Total	Co	0	0
			1	1		
2	C	1	Total	Co	0	0
			1	1		
2	D	1	Total	Co	0	0
			1	1		
2	E	1	Total	Co	0	0
			1	1		
2	F	1	Total	Co	0	0
			1	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

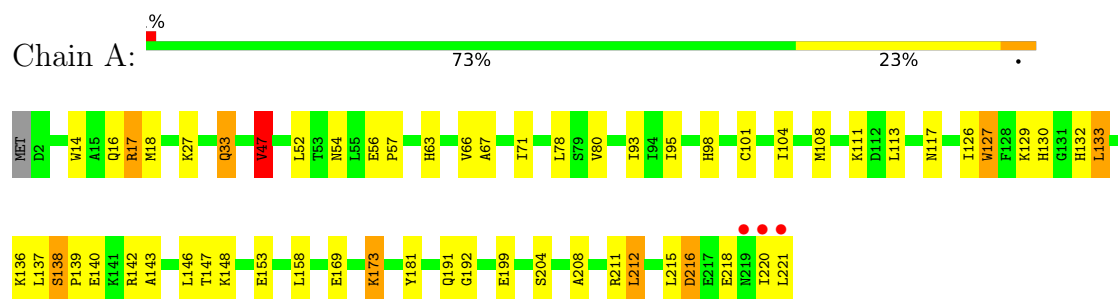
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	40	Total	O	0	0
			40	40		
4	C	33	Total	O	0	0
			33	33		
4	D	33	Total	O	0	0
			33	33		
4	E	30	Total	O	0	0
			30	30		
4	F	30	Total	O	0	0
			30	30		

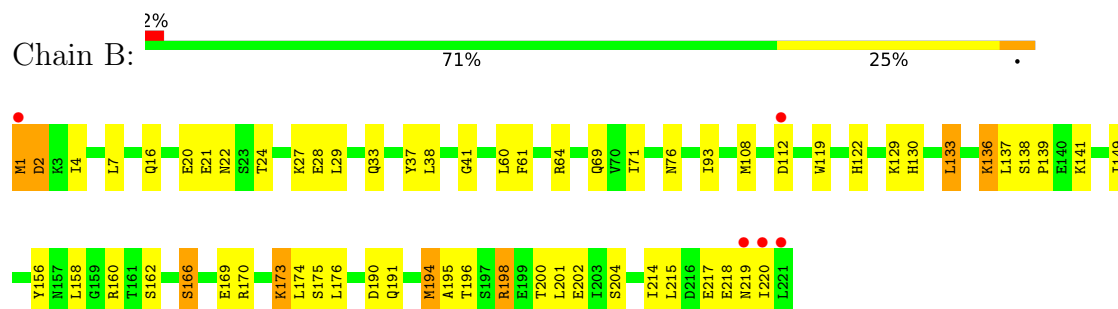
3 Residue-property plots [i](#)

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.

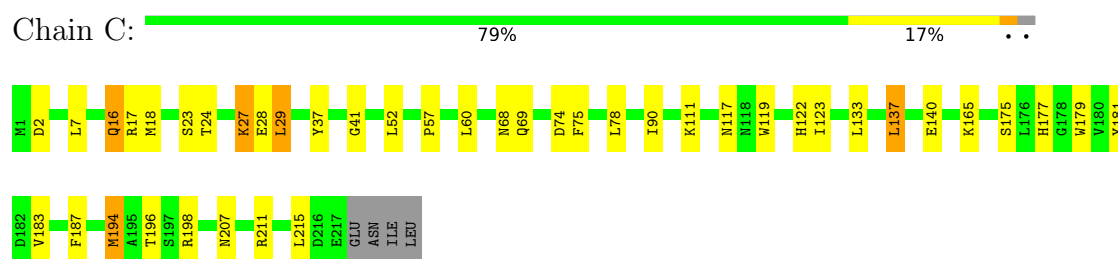
• Molecule 1: Carbonic anhydrase 2



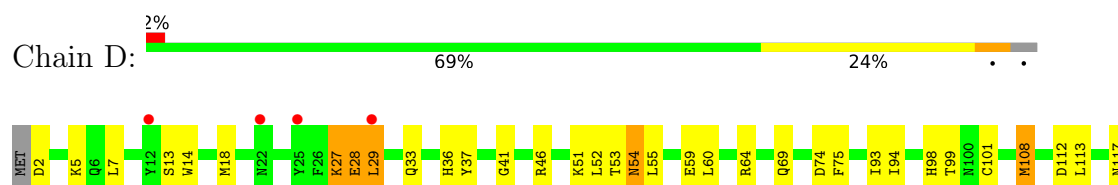
• Molecule 1: Carbonic anhydrase 2

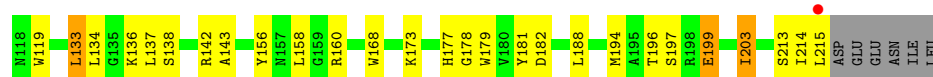


• Molecule 1: Carbonic anhydrase 2



• Molecule 1: Carbonic anhydrase 2

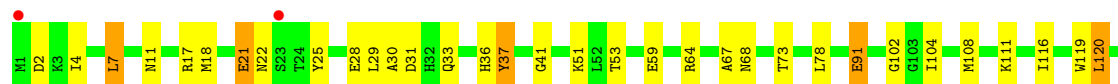




- Molecule 1: Carbonic anhydrase 2



- 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	229.49Å 144.93Å 52.22Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	29.87 – 2.50 29.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.87-2.50) 98.8 (29.87-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.228 0.172 , 0.224	Depositor DCC
R_{free} test set	2941 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10709	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: CO, ACT

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	1.11	1/1811 (0.1%)	1.14	0/2454
1	B	1.11	1/1811 (0.1%)	1.18	5/2454 (0.2%)
1	C	1.07	0/1786	1.12	3/2419 (0.1%)
1	D	1.13	1/1758 (0.1%)	1.15	3/2382 (0.1%)
1	E	1.07	2/1765 (0.1%)	1.12	2/2392 (0.1%)
1	F	1.01	0/1786	1.10	2/2419 (0.1%)
All	All	1.08	5/10717 (0.0%)	1.13	15/14520 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	VAL	CA-CB	8.07	1.64	1.54
1	D	203	ILE	CA-CB	5.77	1.61	1.54
1	E	161	THR	CA-CB	5.29	1.62	1.53
1	E	72	HIS	C-O	-5.26	1.17	1.24
1	B	71	ILE	C-O	-5.08	1.17	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ILE	CB-CA-C	-7.92	102.67	111.23
1	B	136	LYS	N-CA-C	-6.83	104.94	112.72
1	B	119	TRP	N-CA-C	-6.73	104.01	111.82
1	F	2	ASP	N-CA-C	6.28	117.79	111.07
1	B	198	ARG	NE-CZ-NH1	-5.99	115.51	121.50
1	C	123	ILE	CB-CA-C	-5.95	104.01	112.22
1	B	169	GLU	N-CA-C	-5.92	104.76	112.23
1	C	119	TRP	N-CA-C	-5.65	105.20	111.36
1	D	196	THR	N-CA-C	-5.57	105.09	113.89
1	F	194	MET	N-CA-C	-5.37	99.07	107.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	46	ARG	CA-C-N	-5.17	117.65	123.02
1	E	46	ARG	C-N-CA	-5.17	117.65	123.02
1	C	194	MET	N-CA-C	-5.16	99.56	108.69
1	D	138	SER	CA-C-N	-5.11	113.66	119.28
1	D	138	SER	C-N-CA	-5.11	113.66	119.28

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	1772	0	1747	52	0
1	B	1772	0	1751	32	0
1	C	1747	0	1725	31	0
1	D	1719	0	1699	46	0
1	E	1726	0	1703	42	0
1	F	1747	0	1725	39	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	4	0	3	0	0
3	B	4	0	3	0	0
3	D	4	0	3	10	0
3	E	4	0	3	9	0
4	A	38	0	0	2	0
4	B	40	0	0	5	0
4	C	33	0	0	3	0
4	D	33	0	0	5	0
4	E	30	0	0	2	0
4	F	30	0	0	5	0
All	All	10709	0	10362	232	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 11.

All (232) 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:C:165:LYS:HD3	1:C:198:ARG:NH1	1.76	1.00
1:D:69:GLN:HG2	4:D:253:HOH:O	1.65	0.96
1:B:173:LYS:HD2	1:B:174:LEU:N	1.81	0.95
1:A:113:LEU:H	1:A:117:ASN:HD21	0.93	0.93
1:A:113:LEU:H	1:A:117:ASN:ND2	1.66	0.93
1:D:113:LEU:H	1:D:117:ASN:ND2	1.68	0.91
1:F:91:GLU:CG	4:F:249:HOH:O	2.19	0.90
1:B:173:LYS:HD2	1:B:173:LYS:C	1.98	0.88
1:D:113:LEU:H	1:D:117:ASN:HD21	1.23	0.86
1:A:173:LYS:C	1:A:173:LYS:HD2	2.03	0.84
1:A:108:MET:SD	1:A:127:TRP:HZ3	2.01	0.84
1:D:75:PHE:H	3:D:222:ACT:H3	1.43	0.84
1:F:91:GLU:HG3	4:F:249:HOH:O	1.76	0.83
1:A:113:LEU:N	1:A:117:ASN:HD21	1.75	0.83
1:D:75:PHE:H	3:D:222:ACT:CH3	1.96	0.78
1:C:75:PHE:H	3:E:222:ACT:H3	1.48	0.77
1:C:165:LYS:CD	1:C:198:ARG:NH1	2.48	0.77
1:C:75:PHE:H	3:E:222:ACT:CH3	1.98	0.76
1:A:132:HIS:CD2	1:A:133:LEU:H	2.03	0.76
1:F:91:GLU:HG2	4:F:249:HOH:O	1.82	0.76
1:C:165:LYS:HD3	1:C:198:ARG:HH11	1.50	0.75
1:E:78:LEU:HD13	1:E:163:ILE:HD12	1.68	0.75
1:C:27:LYS:H	1:C:27:LYS:HD2	1.52	0.75
1:D:136:LYS:O	1:D:137:LEU:HD12	1.87	0.75
1:E:90:ILE:CD1	1:E:92:HIS:O	2.36	0.74
3:D:222:ACT:OXT	3:E:222:ACT:H1	1.89	0.73
1:C:75:PHE:HB2	3:E:222:ACT:H3	1.71	0.73
1:E:90:ILE:HD11	1:E:92:HIS:O	1.88	0.73
1:B:112:ASP:HB3	4:B:257:HOH:O	1.89	0.71
1:A:129:LYS:O	1:A:132:HIS:HE1	1.74	0.70
1:D:69:GLN:CG	4:D:253:HOH:O	2.32	0.70
1:E:211:ARG:HD2	4:E:227:HOH:O	1.92	0.70
1:A:137:LEU:HD13	1:A:215:LEU:HD22	1.74	0.69
1:F:30:ALA:O	1:F:33:GLN:HG2	1.92	0.69
1:B:41:GLY:O	1:B:64:ARG:HA	1.93	0.68
1:A:138:SER:HB3	1:A:140:GLU:OE2	1.93	0.67
1:E:78:LEU:HD13	1:E:163:ILE:CD1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:LYS:HD2	1:D:5:LYS:H	1.60	0.66
1:A:129:LYS:O	1:A:132:HIS:CE1	2.50	0.65
3:D:222:ACT:H1	3:E:222:ACT:OXT	1.97	0.65
1:A:93:ILE:HG21	1:A:158:LEU:HD21	1.78	0.64
1:C:18:MET:HG3	1:C:23:SER:HB3	1.78	0.64
1:E:104:ILE:HG22	1:E:108:MET:HE2	1.80	0.64
1:C:37:TYR:HB2	1:C:60:LEU:HD23	1.79	0.64
1:E:165:LYS:HE3	4:E:248:HOH:O	1.98	0.63
1:A:208:ALA:O	1:A:212:LEU:HD22	1.98	0.63
1:C:16:GLN:C	1:C:18:MET:H	2.07	0.63
1:E:72:HIS:NE2	1:F:125:ASP:OD2	2.29	0.62
1:A:127:TRP:C	1:A:127:TRP:CD1	2.76	0.62
1:A:127:TRP:HE3	1:A:146:LEU:HD22	1.63	0.62
1:B:141:LYS:HE3	4:B:243:HOH:O	1.99	0.62
1:F:18:MET:HE1	1:F:25:TYR:HB3	1.81	0.62
1:D:75:PHE:HB2	3:D:222:ACT:H3	1.82	0.62
1:C:7:LEU:HD21	1:E:53:THR:HG22	1.82	0.61
1:A:139:PRO:HB3	1:A:142:ARG:NH1	2.16	0.61
1:E:182:ASP:HB3	1:E:185:ASP:OD2	2.02	0.60
1:A:216:ASP:OD1	1:A:216:ASP:N	2.30	0.60
1:F:181:TYR:HB3	1:F:188:LEU:HD23	1.83	0.59
1:D:53:THR:HG22	1:F:7:LEU:HD21	1.84	0.59
1:E:90:ILE:HD12	1:E:92:HIS:H	1.67	0.59
1:A:139:PRO:HA	1:A:142:ARG:HD2	1.84	0.58
1:A:56:GLU:HG3	1:A:57:PRO:HD2	1.85	0.58
1:E:99:THR:OG1	1:E:182:ASP:HA	2.03	0.58
1:D:99:THR:OG1	1:D:182:ASP:HA	2.04	0.57
1:D:14:TRP:O	1:D:18:MET:HG2	2.04	0.57
1:C:165:LYS:CD	1:C:198:ARG:HH11	2.14	0.57
1:A:108:MET:SD	1:A:127:TRP:CZ3	2.90	0.57
1:D:7:LEU:HD21	1:F:53:THR:HG22	1.87	0.56
1:D:113:LEU:N	1:D:117:ASN:ND2	2.49	0.56
1:B:162:SER:O	1:B:166:SER:HB3	2.06	0.56
1:D:181:TYR:HB3	1:D:188:LEU:HD23	1.88	0.55
1:D:108:MET:HE1	1:D:143:ALA:HB2	1.90	0.54
1:A:146:LEU:O	1:A:147:THR:C	2.50	0.54
1:B:198:ARG:HD2	1:B:198:ARG:O	2.07	0.54
1:C:16:GLN:O	1:C:18:MET:N	2.36	0.54
1:A:47:VAL:HG13	1:A:181:TYR:CE1	2.43	0.54
1:F:108:MET:HE3	1:F:146:LEU:HD22	1.90	0.54
1:B:37:TYR:HB2	1:B:60:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ILE:HG21	1:D:158:LEU:HD21	1.90	0.53
1:D:113:LEU:N	1:D:117:ASN:HD21	2.00	0.53
1:F:18:MET:HE1	1:F:25:TYR:CB	2.37	0.53
1:A:98:HIS:O	1:A:147:THR:HG21	2.09	0.53
1:E:119:TRP:HA	1:F:73:THR:CG2	2.39	0.53
1:E:156:TYR:O	1:E:160:ARG:HD3	2.08	0.53
1:E:38:LEU:N	1:E:90:ILE:HD13	2.23	0.52
1:F:28:GLU:HA	1:F:31:ASP:OD1	2.09	0.52
1:F:116:ILE:HG13	1:F:120:LEU:HD22	1.91	0.52
1:A:117:ASN:ND2	4:A:229:HOH:O	2.38	0.52
1:A:215:LEU:HB2	1:A:220:ILE:HG12	1.91	0.52
1:B:156:TYR:O	1:B:160:ARG:HD3	2.10	0.52
1:D:136:LYS:C	1:D:137:LEU:HD12	2.34	0.52
1:A:215:LEU:O	1:A:220:ILE:HD11	2.10	0.52
1:C:137:LEU:HD13	1:C:215:LEU:HD13	1.90	0.52
1:E:145:MET:HG3	1:E:149:ILE:HD12	1.92	0.52
1:F:37:TYR:N	1:F:37:TYR:CD2	2.78	0.51
1:A:108:MET:HE1	1:A:143:ALA:HB2	1.92	0.51
1:B:137:LEU:HD11	1:B:219:ASN:HB3	1.92	0.51
1:A:132:HIS:CD2	1:A:133:LEU:N	2.75	0.51
1:E:93:ILE:HG21	1:E:158:LEU:HD21	1.93	0.51
1:E:14:TRP:O	1:E:18:MET:HG2	2.10	0.51
1:A:211:ARG:HD3	4:A:223:HOH:O	2.11	0.51
1:A:130:HIS:HA	1:A:132:HIS:CE1	2.45	0.51
1:A:14:TRP:O	1:A:18:MET:HG2	2.11	0.51
1:A:192:GLY:O	1:A:204:SER:HB2	2.11	0.51
1:A:139:PRO:HA	1:A:142:ARG:CD	2.40	0.50
1:C:207:ASN:O	1:C:211:ARG:HG3	2.11	0.50
1:D:112:ASP:HA	1:D:117:ASN:HD21	1.75	0.50
1:F:41:GLY:O	1:F:64:ARG:HA	2.10	0.50
1:B:195:ALA:HB2	1:B:201:LEU:HA	1.94	0.50
1:C:75:PHE:CB	3:E:222:ACT:H3	2.41	0.50
1:D:178:GLY:C	1:D:179:TRP:CD1	2.90	0.49
1:A:148:LYS:HB3	1:A:191:GLN:OE1	2.12	0.49
1:C:117:ASN:HB3	4:D:252:HOH:O	2.12	0.49
1:D:178:GLY:O	1:D:179:TRP:HD1	1.96	0.49
1:B:24:THR:O	1:B:28:GLU:HG2	2.12	0.49
1:E:81:VAL:HG12	1:E:163:ILE:HG21	1.94	0.49
1:F:202:GLU:HG2	4:F:223:HOH:O	2.13	0.48
1:B:190:ASP:OD1	1:B:191:GLN:N	2.46	0.48
1:E:133:LEU:C	1:E:133:LEU:HD23	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:HG3	1:B:218:GLU:O	2.12	0.48
1:E:127:TRP:HD1	1:E:134:LEU:HD13	1.77	0.48
1:C:179:TRP:CH2	1:E:7:LEU:HD22	2.49	0.48
1:D:27:LYS:C	1:D:29:LEU:H	2.21	0.48
1:E:123:ILE:HD12	1:E:150:ASN:OD1	2.14	0.48
1:A:47:VAL:HG22	1:A:52:LEU:HG	1.96	0.48
1:E:85:VAL:O	1:E:89:LYS:HA	2.14	0.47
1:A:140:GLU:CD	1:A:140:GLU:H	2.21	0.47
1:D:2:ASP:HA	1:D:5:LYS:HD3	1.96	0.47
1:D:156:TYR:O	1:D:160:ARG:HD3	2.15	0.47
1:D:52:LEU:O	1:F:11:ASN:ND2	2.43	0.47
1:D:168:TRP:CD2	1:D:197:SER:HA	2.50	0.47
1:E:190:ASP:OD1	1:E:190:ASP:C	2.57	0.47
1:E:181:TYR:HB3	1:E:188:LEU:HD23	1.97	0.47
1:D:75:PHE:N	3:D:222:ACT:H3	2.21	0.47
1:A:93:ILE:CG2	1:A:158:LEU:HD21	2.45	0.46
1:C:175:SER:HB3	1:C:196:THR:HG22	1.97	0.46
1:E:127:TRP:CD1	1:E:134:LEU:HD13	2.50	0.46
1:F:102:GLY:HA3	4:F:237:HOH:O	2.16	0.46
1:B:76:ASN:OD1	1:B:76:ASN:C	2.57	0.46
1:C:177:HIS:CE1	1:E:4:ILE:HG13	2.51	0.46
1:B:136:LYS:O	1:B:136:LYS:HG2	2.15	0.46
1:B:190:ASP:OD1	1:B:190:ASP:C	2.57	0.46
1:C:29:LEU:HD23	1:C:57:PRO:HB2	1.97	0.46
1:B:1:MET:H2	1:B:4:ILE:H	1.64	0.46
1:B:93:ILE:HG21	1:B:158:LEU:HD21	1.97	0.46
1:B:133:LEU:HD21	1:B:215:LEU:HD21	1.98	0.46
1:C:75:PHE:H	3:E:222:ACT:H2	1.79	0.46
1:D:53:THR:HB	1:D:55:LEU:HG	1.97	0.46
1:F:104:ILE:O	1:F:108:MET:HG3	2.16	0.46
1:F:148:LYS:HB3	1:F:191:GLN:OE1	2.15	0.46
1:B:138:SER:O	1:B:139:PRO:C	2.58	0.45
1:D:69:GLN:CD	4:D:253:HOH:O	2.55	0.45
1:C:52:LEU:HD11	1:C:181:TYR:CE2	2.51	0.45
1:A:133:LEU:HD23	1:A:215:LEU:HD11	1.98	0.45
1:D:133:LEU:HD13	1:D:213:SER:HA	1.98	0.45
1:A:127:TRP:C	1:A:127:TRP:HD1	2.22	0.45
1:A:127:TRP:CE3	1:A:146:LEU:HD22	2.48	0.45
1:F:31:ASP:OD1	1:F:31:ASP:N	2.50	0.45
1:B:129:LYS:HG3	4:B:244:HOH:O	2.17	0.44
1:C:27:LYS:HD2	1:C:27:LYS:N	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ASP:O	1:E:89:LYS:HE2	2.18	0.44
1:A:16:GLN:C	1:A:18:MET:N	2.75	0.44
1:B:69:GLN:HE22	1:B:122:HIS:HB2	1.82	0.44
1:D:75:PHE:H	3:D:222:ACT:H2	1.80	0.44
3:D:222:ACT:C	3:E:222:ACT:H1	2.46	0.44
1:A:63:HIS:HB2	1:A:80:VAL:HG11	1.98	0.44
1:B:141:LYS:HA	4:B:262:HOH:O	2.17	0.44
1:D:98:HIS:CE1	1:D:101:CYS:HA	2.53	0.44
1:D:112:ASP:HA	1:D:117:ASN:ND2	2.32	0.44
1:A:66:VAL:O	1:A:67:ALA:HB3	2.15	0.44
1:D:179:TRP:CZ3	1:F:7:LEU:HD22	2.52	0.44
1:C:69:GLN:NE2	4:C:253:HOH:O	2.51	0.44
1:D:177:HIS:CE1	1:F:4:ILE:HG13	2.53	0.44
1:E:108:MET:HE1	1:E:143:ALA:CB	2.47	0.44
1:F:151:VAL:O	1:F:155:VAL:HG23	2.18	0.44
1:F:156:TYR:O	1:F:160:ARG:HD3	2.17	0.44
1:D:75:PHE:CB	3:D:222:ACT:H3	2.46	0.43
1:E:37:TYR:HB2	1:E:60:LEU:HD23	2.00	0.43
1:F:132:HIS:CE1	1:F:136:LYS:HD2	2.53	0.43
1:E:73:THR:CG2	1:F:119:TRP:HA	2.48	0.43
1:C:194:MET:HG3	4:C:237:HOH:O	2.16	0.43
1:E:119:TRP:HA	1:F:73:THR:HG21	1.99	0.43
1:C:165:LYS:NZ	4:C:246:HOH:O	2.51	0.43
1:A:98:HIS:CE1	1:A:101:CYS:HA	2.54	0.43
1:D:36:HIS:HD2	1:D:59:GLU:OE1	2.01	0.43
1:E:199:GLU:CD	1:E:199:GLU:H	2.27	0.43
1:A:126:ILE:HG12	1:A:153:GLU:HG3	1.99	0.43
1:C:187:PHE:HE2	1:E:12:TYR:HA	1.83	0.43
1:F:193:VAL:HA	1:F:204:SER:OG	2.19	0.43
1:F:198:ARG:HE	1:F:198:ARG:HB2	1.63	0.43
1:A:133:LEU:HD21	1:A:215:LEU:HD21	2.01	0.43
1:F:150:ASN:O	1:F:154:GLN:HG2	2.19	0.42
1:B:2:ASP:OD1	1:B:2:ASP:N	2.51	0.42
1:E:137:LEU:HD23	1:E:141:LYS:HB3	2.00	0.42
1:C:41:GLY:C	1:C:68:ASN:HB3	2.45	0.42
1:E:108:MET:HE1	1:E:143:ALA:HB2	2.00	0.42
1:E:175:SER:OG	1:E:177:HIS:NE2	2.52	0.42
1:E:98:HIS:HD2	1:E:99:THR:O	2.03	0.42
1:A:104:ILE:HD13	1:A:104:ILE:HA	1.83	0.42
1:A:16:GLN:O	1:A:17:ARG:C	2.61	0.42
1:A:108:MET:HG2	1:A:127:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:SER:HB3	1:B:196:THR:HG22	2.02	0.42
1:A:33:GLN:H	1:A:33:GLN:HG2	1.74	0.41
1:B:156:TYR:O	1:B:160:ARG:CD	2.67	0.41
1:E:190:ASP:OD1	1:E:191:GLN:N	2.53	0.41
1:F:216:ASP:OD1	1:F:216:ASP:N	2.42	0.41
1:D:41:GLY:O	1:D:64:ARG:HA	2.20	0.41
1:D:134:LEU:HD22	1:D:142:ARG:HG3	2.03	0.41
1:E:108:MET:HE1	1:E:143:ALA:HA	2.03	0.41
1:F:36:HIS:HD2	1:F:59:GLU:OE1	2.04	0.41
1:A:199:GLU:CD	1:A:199:GLU:H	2.29	0.41
1:F:145:MET:HG3	1:F:149:ILE:HD12	2.03	0.41
1:F:178:GLY:C	1:F:179:TRP:CD1	2.99	0.41
1:D:69:GLN:HE21	1:D:119:TRP:NE1	2.19	0.41
1:A:173:LYS:C	1:A:173:LYS:CD	2.83	0.41
1:B:69:GLN:NE2	4:B:263:HOH:O	2.54	0.41
1:C:69:GLN:HE22	1:C:122:HIS:HB2	1.85	0.41
1:D:54:ASN:HD22	1:D:54:ASN:HA	1.65	0.41
1:D:74:ASP:HA	3:D:222:ACT:H2	2.03	0.41
1:F:17:ARG:O	1:F:21:GLU:HB2	2.20	0.41
1:D:199:GLU:HB2	4:D:255:HOH:O	2.20	0.41
1:B:38:LEU:HD12	1:B:61:PHE:O	2.22	0.40
1:A:54:ASN:O	1:A:54:ASN:CG	2.64	0.40
1:D:46:ARG:HA	1:D:46:ARG:HD2	1.84	0.40
1:B:176:LEU:O	1:B:194:MET:HA	2.21	0.40
1:C:74:ASP:HA	3:E:222:ACT:H2	2.03	0.40
1:D:37:TYR:HB2	1:D:60:LEU:HD23	2.03	0.40
1:E:195:ALA:HB2	1:E:201:LEU:HA	2.03	0.40
1:F:67:ALA:C	1:F:68:ASN:CG	2.89	0.40
1:B:130:HIS:CD2	1:B:149:ILE:HG21	2.56	0.40
1:B:200:THR:O	1:B:204:SER:CB	2.69	0.40
1:F:207:ASN:O	1:F:211:ARG:HB3	2.22	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	218/221 (99%)	208 (95%)	9 (4%)	1 (0%)	24	43
1	B	219/221 (99%)	208 (95%)	8 (4%)	3 (1%)	9	17
1	C	215/221 (97%)	207 (96%)	6 (3%)	2 (1%)	14	27
1	D	212/221 (96%)	201 (95%)	10 (5%)	1 (0%)	24	43
1	E	213/221 (96%)	202 (95%)	11 (5%)	0	100	100
1	F	215/221 (97%)	205 (95%)	9 (4%)	1 (0%)	24	43
All	All	1292/1326 (97%)	1231 (95%)	53 (4%)	8 (1%)	21	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	GLU
1	C	17	ARG
1	C	24	THR
1	F	185	ASP
1	B	20	GLU
1	B	22	ASN
1	D	28	GLU
1	A	17	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	192/193 (100%)	175 (91%)	17 (9%)	9	20
1	B	191/193 (99%)	175 (92%)	16 (8%)	10	22
1	C	189/193 (98%)	177 (94%)	12 (6%)	16	34
1	D	185/193 (96%)	169 (91%)	16 (9%)	10	21
1	E	186/193 (96%)	177 (95%)	9 (5%)	23	46
1	F	189/193 (98%)	171 (90%)	18 (10%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1132/1158 (98%)	1044 (92%)	88 (8%)	11	24

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	33	GLN
1	A	47	VAL
1	A	71	ILE
1	A	78	LEU
1	A	95	ILE
1	A	111	LYS
1	A	127	TRP
1	A	133	LEU
1	A	136	LYS
1	A	138	SER
1	A	169	GLU
1	A	173	LYS
1	A	212	LEU
1	A	216	ASP
1	A	218	GLU
1	A	221	LEU
1	B	1	MET
1	B	2	ASP
1	B	7	LEU
1	B	16	GLN
1	B	27	LYS
1	B	29	LEU
1	B	33	GLN
1	B	108	MET
1	B	133	LEU
1	B	166	SER
1	B	170	ARG
1	B	173	LYS
1	B	194	MET
1	B	202	GLU
1	B	217	GLU
1	B	220	ILE
1	C	2	ASP
1	C	16	GLN
1	C	27	LYS
1	C	28	GLU

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Mol	Chain	Res	Type
1	C	29	LEU
1	C	78	LEU
1	C	90	ILE
1	C	111	LYS
1	C	133	LEU
1	C	137	LEU
1	C	140	GLU
1	C	183	VAL
1	D	13	SER
1	D	27	LYS
1	D	28	GLU
1	D	29	LEU
1	D	33	GLN
1	D	51	LYS
1	D	54	ASN
1	D	94	ILE
1	D	108	MET
1	D	133	LEU
1	D	173	LYS
1	D	194	MET
1	D	199	GLU
1	D	203	ILE
1	D	214	ILE
1	D	215	LEU
1	E	2	ASP
1	E	13	SER
1	E	54	ASN
1	E	56	GLU
1	E	78	LEU
1	E	90	ILE
1	E	133	LEU
1	E	204	SER
1	E	212	LEU
1	F	7	LEU
1	F	21	GLU
1	F	22	ASN
1	F	29	LEU
1	F	37	TYR
1	F	51	LYS
1	F	78	LEU
1	F	91	GLU
1	F	111	LYS

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Mol	Chain	Res	Type
1	F	120	LEU
1	F	133	LEU
1	F	140	GLU
1	F	169	GLU
1	F	173	LYS
1	F	198	ARG
1	F	202	GLU
1	F	212	LEU
1	F	216	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	92	HIS
1	A	100	ASN
1	A	117	ASN
1	A	132	HIS
1	B	6	GLN
1	B	16	GLN
1	B	33	GLN
1	B	69	GLN
1	C	6	GLN
1	C	16	GLN
1	C	32	HIS
1	C	33	GLN
1	C	69	GLN
1	C	117	ASN
1	D	16	GLN
1	D	32	HIS
1	D	36	HIS
1	D	54	ASN
1	D	69	GLN
1	D	117	ASN
1	E	16	GLN
1	E	22	ASN
1	E	98	HIS
1	F	22	ASN
1	F	33	GLN
1	F	36	HIS
1	F	54	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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	ACT	E	222	-	3,3,3	0.86	0	3,3,3	1.45	1 (33%)
3	ACT	A	222	-	3,3,3	0.95	0	3,3,3	1.05	0
3	ACT	D	222	-	3,3,3	1.10	0	3,3,3	2.27	1 (33%)
3	ACT	B	222	-	3,3,3	1.21	0	3,3,3	0.93	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	222	ACT	OXT-C-CH3	3.16	128.29	115.05
3	E	222	ACT	OXT-C-CH3	2.03	123.57	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	222	ACT	9	0
3	D	222	ACT	10	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	220/221 (99%)	-0.15	3 (1%) 73 70	38, 61, 103, 114	0
1	B	221/221 (100%)	-0.08	5 (2%) 61 57	39, 62, 111, 129	0
1	C	217/221 (98%)	-0.11	0 100 100	36, 61, 110, 134	0
1	D	214/221 (96%)	-0.03	5 (2%) 61 57	37, 63, 126, 146	0
1	E	215/221 (97%)	-0.05	3 (1%) 73 70	40, 65, 115, 134	0
1	F	217/221 (98%)	-0.02	3 (1%) 73 70	41, 69, 105, 122	0
All	All	1304/1326 (98%)	-0.08	19 (1%) 72 68	36, 64, 112, 146	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	ASN	4.2
1	B	221	LEU	4.0
1	A	220	ILE	3.7
1	B	220	ILE	3.5
1	E	29	LEU	3.4
1	D	29	LEU	3.1
1	D	22	ASN	2.9
1	A	221	LEU	2.6
1	B	1	MET	2.6
1	A	219	ASN	2.5
1	F	1	MET	2.5
1	F	23	SER	2.5
1	F	217	GLU	2.2
1	D	215	LEU	2.1
1	D	12	TYR	2.1
1	B	112	ASP	2.0
1	E	216	ASP	2.0
1	E	30	ALA	2.0
1	D	25	TYR	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($\text{\AA}^2$)	Q<0.9
3	ACT	A	222	4/4	0.89	0.15	43,43,44,44	4
3	ACT	D	222	4/4	0.89	0.13	39,44,44,45	0
3	ACT	E	222	4/4	0.89	0.14	56,56,57,58	0
3	ACT	B	222	4/4	0.92	0.10	37,37,38,39	4
2	CO	E	230	1/1	1.00	0.02	59,59,59,59	0
2	CO	F	230	1/1	1.00	0.01	56,56,56,56	0
2	CO	A	230	1/1	1.00	0.01	52,52,52,52	0
2	CO	B	230	1/1	1.00	0.02	56,56,56,56	0
2	CO	C	230	1/1	1.00	0.03	51,51,51,51	0
2	CO	D	230	1/1	1.00	0.02	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.