



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:24 PM UTC

PDB ID : 4E5I / pdb_00004e5i
Title : Crystal structure of avian influenza virus PAn bound to compound 4
Authors : DuBois, R.M.; Slavish, P.J.; Webb, T.R.; White, S.W.
Deposited on : 2012-03-14
Resolution : 2.94 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

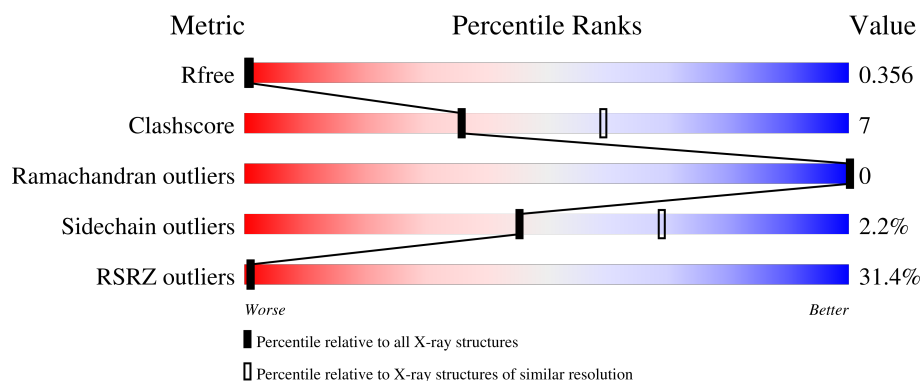
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	187	35% 84% 11% ..
1	B	187	32% 81% 14% ..
1	C	187	28% 84% 12% ..
1	D	187	27% 85% 12% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6075 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 Polymerase protein PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1480	932	256	281	11			
1	B	180	Total	C	N	O	S	0	0	0
			1480	932	256	281	11			
1	C	182	Total	C	N	O	S	0	0	0
			1497	943	258	285	11			
1	D	183	Total	C	N	O	S	0	0	0
			1502	946	259	286	11			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50A	GLY	-	linker	UNP Q5EP34
A	50B	GLY	-	linker	UNP Q5EP34
A	50C	SER	-	linker	UNP Q5EP34
A	196A	ALA	-	expression tag	UNP Q5EP34
A	196B	ALA	-	expression tag	UNP Q5EP34
A	196C	ALA	-	expression tag	UNP Q5EP34
A	197	GLU	-	expression tag	UNP Q5EP34
A	198	LEU	-	expression tag	UNP Q5EP34
A	199	ALA	-	expression tag	UNP Q5EP34
A	200	LEU	-	expression tag	UNP Q5EP34
A	201	VAL	-	expression tag	UNP Q5EP34
A	202	PRO	-	expression tag	UNP Q5EP34
A	203	ARG	-	expression tag	UNP Q5EP34
B	50A	GLY	-	linker	UNP Q5EP34
B	50B	GLY	-	linker	UNP Q5EP34
B	50C	SER	-	linker	UNP Q5EP34
B	196A	ALA	-	expression tag	UNP Q5EP34
B	196B	ALA	-	expression tag	UNP Q5EP34
B	196C	ALA	-	expression tag	UNP Q5EP34
B	197	GLU	-	expression tag	UNP Q5EP34
B	198	LEU	-	expression tag	UNP Q5EP34

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	ALA	-	expression tag	UNP Q5EP34
B	200	LEU	-	expression tag	UNP Q5EP34
B	201	VAL	-	expression tag	UNP Q5EP34
B	202	PRO	-	expression tag	UNP Q5EP34
B	203	ARG	-	expression tag	UNP Q5EP34
C	50A	GLY	-	linker	UNP Q5EP34
C	50B	GLY	-	linker	UNP Q5EP34
C	50C	SER	-	linker	UNP Q5EP34
C	196A	ALA	-	expression tag	UNP Q5EP34
C	196B	ALA	-	expression tag	UNP Q5EP34
C	196C	ALA	-	expression tag	UNP Q5EP34
C	196D	GLU	-	expression tag	UNP Q5EP34
C	196E	LEU	-	expression tag	UNP Q5EP34
C	197	ALA	-	expression tag	UNP Q5EP34
C	198	LEU	-	expression tag	UNP Q5EP34
C	199	VAL	-	expression tag	UNP Q5EP34
C	200	PRO	-	expression tag	UNP Q5EP34
C	201	ARG	-	expression tag	UNP Q5EP34
D	50A	GLY	-	linker	UNP Q5EP34
D	50B	GLY	-	linker	UNP Q5EP34
D	50C	SER	-	linker	UNP Q5EP34
D	196A	ALA	-	expression tag	UNP Q5EP34
D	196B	ALA	-	expression tag	UNP Q5EP34
D	196C	ALA	-	expression tag	UNP Q5EP34
D	196D	GLU	-	expression tag	UNP Q5EP34
D	196E	LEU	-	expression tag	UNP Q5EP34
D	196F	ALA	-	expression tag	UNP Q5EP34
D	197	LEU	-	expression tag	UNP Q5EP34
D	198	VAL	-	expression tag	UNP Q5EP34
D	199	PRO	-	expression tag	UNP Q5EP34
D	200	ARG	-	expression tag	UNP Q5EP34

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

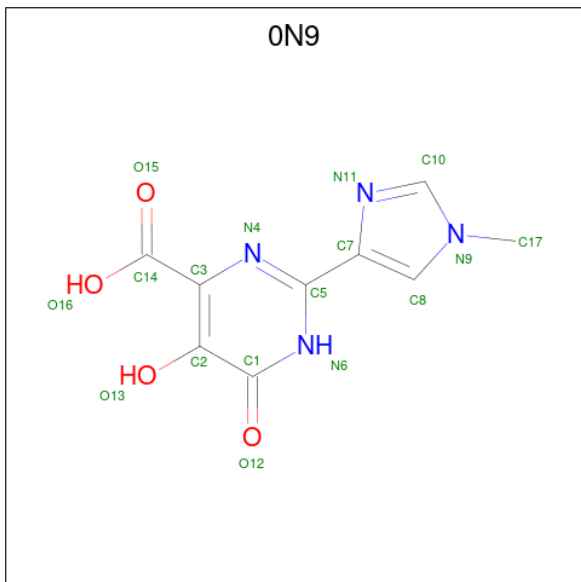


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		
3	C	2	Total	Mn	0	0
			2	2		
3	D	2	Total	Mn	0	0
			2	2		

- Molecule 4 is 5-hydroxy-2-(1-methyl-1H-imidazol-4-yl)-6-oxo-1,6-dihydropyrimidine-4-carboxylic acid (CCD ID: 0N9) (formula: C₉H₈N₄O₄).

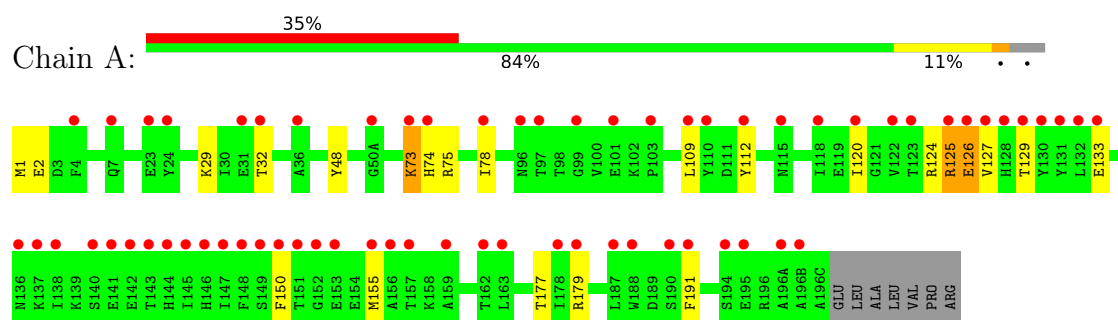


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	4	4		
4	B	1	Total	C	N	O	0	0
			17	9	4	4		
4	C	1	Total	C	N	O	0	0
			17	9	4	4		
4	D	1	Total	C	N	O	0	0
			17	9	4	4		

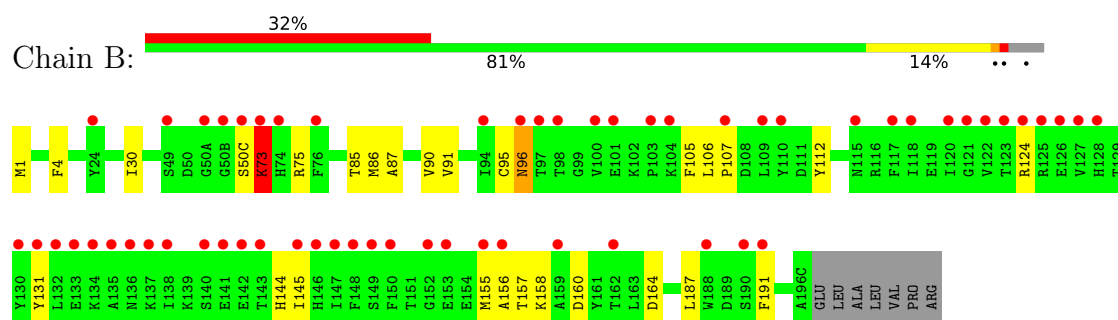
3 Residue-property plots

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.

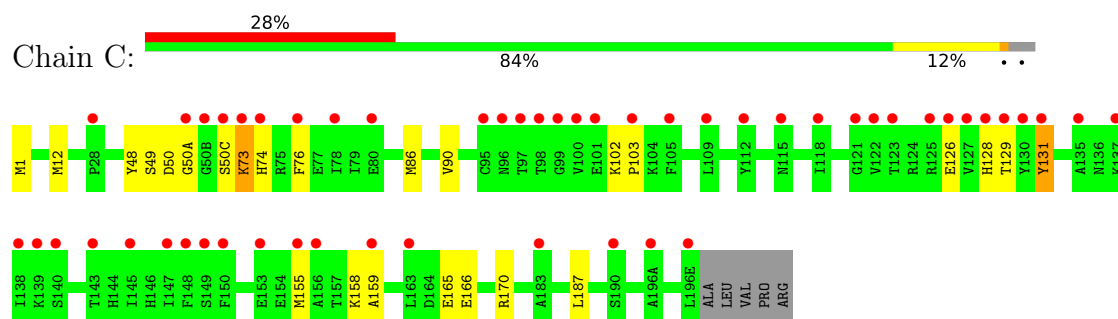
• Molecule 1: Polymerase protein PA



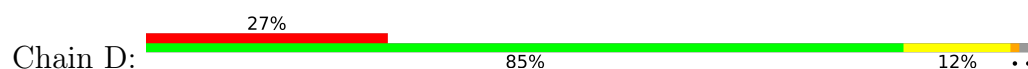
• Molecule 1: Polymerase protein PA

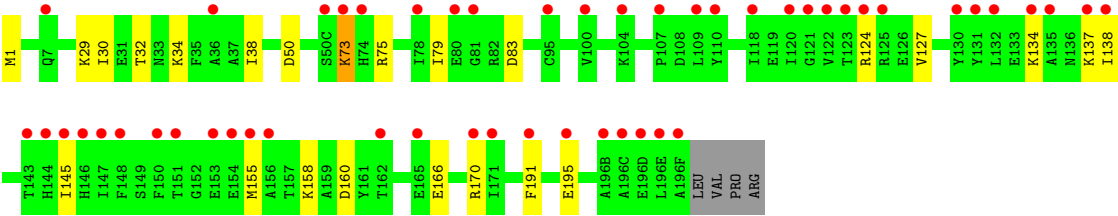


• Molecule 1: Polymerase protein PA



• Molecule 1: Polymerase protein PA





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	126.33Å 134.83Å 126.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.13 – 2.94 46.13 – 2.94	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.13-2.94) 96.5 (46.13-2.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.96Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.320 , 0.368 0.318 , 0.356	Depositor DCC
R_{free} test set	1143 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6075	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9230e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MN, SO4, ON9

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	0.42	0/1510	0.86	3/2028 (0.1%)
1	B	0.42	0/1510	0.88	4/2028 (0.2%)
1	C	0.42	0/1527	0.84	1/2051 (0.0%)
1	D	0.44	0/1532	0.86	0/2058
All	All	0.42	0/6079	0.86	8/8165 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	N-CA-C	-10.17	95.02	108.34
1	C	165	GLU	N-CA-C	7.72	119.77	111.36
1	B	73	LYS	N-CA-C	6.38	118.77	111.11
1	A	126	GLU	N-CA-C	5.87	118.74	110.23
1	B	50(C)	SER	N-CA-C	-5.50	103.23	110.33
1	B	106	LEU	CA-C-N	5.24	125.71	120.52
1	B	106	LEU	C-N-CA	5.24	125.71	120.52
1	A	125	ARG	CB-CA-C	-5.18	100.92	113.19

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	1480	0	1444	27	0
1	B	1480	0	1444	18	0
1	C	1497	0	1461	29	0
1	D	1502	0	1466	24	0
2	A	10	0	0	1	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	17	0	6	0	0
4	B	17	0	6	0	0
4	C	17	0	6	0	0
4	D	17	0	6	1	0
All	All	6075	0	5839	87	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 7.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LYS:H	1:D:73:LYS:CD	1.57	1.17
1:B:73:LYS:HE3	1:B:73:LYS:H	1.13	1.12
1:C:73:LYS:CE	1:C:73:LYS:H	1.64	1.09
1:A:73:LYS:H	1:A:73:LYS:HE3	0.90	1.06
1:A:73:LYS:HE3	1:A:73:LYS:N	1.73	1.03
1:C:73:LYS:H	1:C:73:LYS:HE2	1.14	1.03
1:D:73:LYS:HD3	1:D:73:LYS:N	1.67	1.03
1:B:73:LYS:HE3	1:B:73:LYS:N	1.77	1.00
1:D:73:LYS:H	1:D:73:LYS:HD3	0.82	0.98
1:D:73:LYS:CD	1:D:73:LYS:N	2.30	0.85
1:A:73:LYS:H	1:A:73:LYS:CE	1.84	0.84
1:C:73:LYS:HE2	1:C:73:LYS:N	1.92	0.84
1:B:105:PHE:O	1:B:107:PRO:HD3	1.89	0.72
1:B:157:THR:HG22	1:B:158:LYS:HG3	1.72	0.71
1:C:74:HIS:HB3	1:D:170:ARG:HD2	1.73	0.70
1:A:75:ARG:O	1:A:112:TYR:HD2	1.75	0.70
1:A:125:ARG:NH2	1:A:133:GLU:OE2	2.26	0.69
1:C:74:HIS:HB3	1:D:170:ARG:CD	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:HIS:HB3	1:C:155:MET:HE1	1.80	0.62
1:C:74:HIS:CG	1:D:170:ARG:HD3	2.36	0.61
1:A:126:GLU:H	1:A:126:GLU:CD	2.08	0.61
1:B:144:HIS:CE1	1:B:160:ASP:HB3	2.36	0.60
1:A:74:HIS:HB3	1:C:170:ARG:HD3	1.83	0.60
1:B:73:LYS:H	1:B:73:LYS:CE	2.02	0.60
1:B:96:ASN:HD22	1:B:96:ASN:N	1.99	0.60
1:A:1:MET:HG3	1:A:32:THR:HB	1.83	0.59
1:A:125:ARG:HH22	1:A:133:GLU:CD	2.13	0.57
1:A:74:HIS:O	1:C:170:ARG:HD2	2.04	0.57
1:D:1:MET:HG3	1:D:32:THR:HB	1.86	0.56
1:C:73:LYS:CE	1:C:73:LYS:N	2.50	0.55
1:C:73:LYS:H	1:C:73:LYS:HE3	1.63	0.54
1:C:74:HIS:CB	1:D:170:ARG:HD2	2.37	0.54
1:C:50(C):SER:HB2	1:C:73:LYS:HE3	1.89	0.54
1:C:131:TYR:CD2	1:C:131:TYR:C	2.87	0.53
1:A:127:VAL:HG12	1:A:155:MET:CB	2.39	0.53
1:A:125:ARG:NH2	1:A:133:GLU:CD	2.67	0.52
1:C:74:HIS:NE2	1:D:170:ARG:NH1	2.57	0.52
1:D:124:ARG:HD3	1:D:191:PHE:CE2	2.44	0.52
1:A:127:VAL:CG1	1:A:155:MET:HB2	2.40	0.52
1:C:1:MET:HE2	1:C:187:LEU:HB3	1.92	0.51
1:A:74:HIS:HB3	1:C:170:ARG:CD	2.41	0.51
1:D:127:VAL:HG22	1:D:155:MET:SD	2.50	0.51
1:C:74:HIS:CD2	1:D:170:ARG:NH1	2.79	0.50
1:A:127:VAL:CG1	1:A:155:MET:CB	2.89	0.50
1:D:50:ASP:O	1:D:50:ASP:OD1	2.30	0.50
1:A:75:ARG:NH1	2:A:301:SO4:O1	2.43	0.49
1:A:126:GLU:OE1	1:A:126:GLU:N	2.30	0.49
1:B:131:TYR:CD1	1:B:155:MET:HG2	2.47	0.49
1:D:138:ILE:HD11	1:D:145:ILE:HD11	1.95	0.49
1:C:50:ASP:OD1	1:C:50:ASP:O	2.30	0.48
1:A:126:GLU:CD	1:A:126:GLU:N	2.70	0.48
1:A:127:VAL:HG12	1:A:155:MET:HB3	1.95	0.48
1:C:166:GLU:OE1	1:C:166:GLU:N	2.30	0.48
1:B:75:ARG:NH1	2:B:301:SO4:O3	2.46	0.48
1:A:150:PHE:HD2	1:A:179:ARG:HB2	1.78	0.47
1:C:74:HIS:CB	1:D:170:ARG:CD	2.93	0.46
1:D:75:ARG:HD2	2:D:301:SO4:O2	2.15	0.46
1:B:1:MET:HE2	1:B:187:LEU:HB3	1.97	0.46
1:B:95:CYS:HB2	1:B:96:ASN:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LYS:HZ2	4:D:305:ON9:H8	1.79	0.46
1:C:74:HIS:CG	1:D:170:ARG:CD	2.98	0.46
1:D:29:LYS:C	1:D:30:ILE:HD12	2.41	0.46
1:B:75:ARG:O	1:B:112:TYR:HD2	1.98	0.46
1:C:131:TYR:C	1:C:131:TYR:HD2	2.25	0.45
1:C:158:LYS:O	1:C:159:ALA:HB3	2.17	0.45
1:A:2:GLU:OE2	1:A:29:LYS:HE3	2.17	0.45
1:A:78:ILE:HA	1:A:109:LEU:HD23	1.99	0.44
1:B:96:ASN:HD22	1:B:96:ASN:H	1.63	0.44
1:A:127:VAL:HG12	1:A:155:MET:HB2	1.99	0.43
1:C:86:MET:O	1:C:90:VAL:HG23	2.18	0.43
1:A:124:ARG:HD3	1:A:191:PHE:CD2	2.54	0.43
1:B:124:ARG:HD3	1:B:191:PHE:CE2	2.54	0.43
1:A:48:TYR:CG	1:A:120:ILE:HD11	2.55	0.42
1:D:158:LYS:C	1:D:160:ASP:N	2.77	0.42
1:A:126:GLU:HB2	1:A:129:THR:OG1	2.19	0.42
1:C:48:TYR:C	1:C:50(A):GLY:H	2.27	0.42
1:D:134:LYS:O	1:D:138:ILE:HG12	2.21	0.41
1:C:49:SER:HA	1:C:76:PHE:CD1	2.55	0.41
1:C:126:GLU:HB2	1:C:129:THR:OG1	2.21	0.41
1:A:127:VAL:HG11	1:A:155:MET:HB2	2.01	0.41
1:B:1:MET:O	1:B:4:PHE:HB3	2.21	0.41
1:B:87:ALA:O	1:B:91:VAL:HG23	2.20	0.41
1:B:86:MET:O	1:B:90:VAL:HG23	2.21	0.40
1:D:124:ARG:CZ	1:D:195:GLU:HB2	2.51	0.40
1:B:145:ILE:O	1:B:156:ALA:HA	2.21	0.40
1:C:102:LYS:HA	1:C:103:PRO:HD2	1.97	0.40
1:D:34:LYS:O	1:D:38:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/187 (95%)	174 (98%)	4 (2%)	0	100	100
1	B	178/187 (95%)	173 (97%)	5 (3%)	0	100	100
1	C	180/187 (96%)	174 (97%)	6 (3%)	0	100	100
1	D	181/187 (97%)	175 (97%)	6 (3%)	0	100	100
All	All	717/748 (96%)	696 (97%)	21 (3%)	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	159/165 (96%)	157 (99%)	2 (1%)	61	77
1	B	159/165 (96%)	154 (97%)	5 (3%)	35	60
1	C	161/165 (98%)	158 (98%)	3 (2%)	50	71
1	D	161/165 (98%)	157 (98%)	4 (2%)	42	66
All	All	640/660 (97%)	626 (98%)	14 (2%)	45	69

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	177	THR
1	B	30	ILE
1	B	73	LYS
1	B	85	THR
1	B	96	ASN
1	B	164	ASP
1	C	12	MET
1	C	73	LYS
1	C	131	TYR
1	D	73	LYS
1	D	79	ILE
1	D	83	ASP

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Mol	Chain	Res	Type
1	D	166	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	A	302	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	301	-	4,4,4	0.23	0	6,6,6	0.05	0
4	0N9	A	305	3	16,18,18	1.48	4 (25%)	14,26,26	3.50	7 (50%)
2	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	301	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	D	302	-	4,4,4	0.24	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	0N9	D	305	3	16,18,18	1.46	3 (18%)	14,26,26	3.49	7 (50%)
2	SO4	C	301	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	B	302	-	4,4,4	0.24	0	6,6,6	0.08	0
4	0N9	B	305	3	16,18,18	1.53	4 (25%)	14,26,26	3.36	7 (50%)
4	0N9	C	305	3	16,18,18	1.57	3 (18%)	14,26,26	3.73	7 (50%)
2	SO4	D	301	-	4,4,4	0.24	0	6,6,6	0.08	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	0N9	B	305	3	-	3/4/8/8	0/2/2/2
4	0N9	C	305	3	-	1/4/8/8	0/2/2/2
4	0N9	D	305	3	-	1/4/8/8	0/2/2/2
4	0N9	A	305	3	-	3/4/8/8	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	305	0N9	C5-N4	2.49	1.37	1.32
4	C	305	0N9	C7-C5	2.44	1.50	1.46
4	C	305	0N9	C1-N6	-2.34	1.34	1.38
4	B	305	0N9	C5-N4	2.33	1.36	1.32
4	A	305	0N9	C1-N6	-2.25	1.34	1.38
4	B	305	0N9	C7-C5	2.24	1.49	1.46
4	B	305	0N9	C1-N6	-2.20	1.34	1.38
4	D	305	0N9	C1-N6	-2.18	1.34	1.38
4	A	305	0N9	C8-N9	-2.15	1.34	1.37
4	D	305	0N9	C5-N4	2.12	1.36	1.32
4	B	305	0N9	C8-N9	-2.09	1.34	1.37
4	D	305	0N9	C7-C5	2.07	1.49	1.46
4	A	305	0N9	C5-N4	2.04	1.36	1.32
4	A	305	0N9	C7-C5	2.01	1.49	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	305	0N9	N9-C10-N11	-9.58	108.99	112.66
4	D	305	0N9	N9-C10-N11	-8.94	109.24	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	305	0N9	N9-C10-N11	-8.88	109.26	112.66
4	B	305	0N9	N9-C10-N11	-8.36	109.46	112.66
4	D	305	0N9	C3-N4-C5	6.90	121.95	114.56
4	C	305	0N9	C3-N4-C5	6.79	121.83	114.56
4	A	305	0N9	C3-N4-C5	6.76	121.80	114.56
4	B	305	0N9	C3-N4-C5	6.62	121.65	114.56
4	C	305	0N9	C8-N9-C10	3.95	108.27	106.71
4	D	305	0N9	C8-N9-C10	3.92	108.26	106.71
4	A	305	0N9	C8-N9-C10	3.61	108.14	106.71
4	A	305	0N9	C5-C7-N11	3.55	127.99	121.40
4	B	305	0N9	C5-C7-N11	3.50	127.90	121.40
4	C	305	0N9	C5-C7-N11	3.44	127.79	121.40
4	B	305	0N9	C8-N9-C10	3.16	107.96	106.71
4	C	305	0N9	C14-C3-N4	3.15	122.43	114.16
4	B	305	0N9	C14-C3-N4	2.88	121.72	114.16
4	C	305	0N9	C10-N11-C7	2.76	107.77	104.92
4	D	305	0N9	C5-C7-N11	2.67	126.36	121.40
4	A	305	0N9	C14-C3-N4	2.61	120.99	114.16
4	A	305	0N9	C10-N11-C7	2.42	107.42	104.92
4	D	305	0N9	C14-C3-N4	2.41	120.47	114.16
4	D	305	0N9	C10-N11-C7	2.36	107.36	104.92
4	C	305	0N9	C8-C7-N11	-2.32	107.17	109.78
4	B	305	0N9	C10-N11-C7	2.25	107.25	104.92
4	B	305	0N9	C8-C7-N11	-2.10	107.42	109.78
4	A	305	0N9	C8-C7-N11	-2.10	107.42	109.78
4	D	305	0N9	C8-C7-N11	-2.01	107.53	109.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	0N9	O16-C14-C3-C2
4	A	305	0N9	O15-C14-C3-C2
4	B	305	0N9	O16-C14-C3-C2
4	B	305	0N9	O15-C14-C3-C2
4	A	305	0N9	O16-C14-C3-N4
4	B	305	0N9	O16-C14-C3-N4
4	D	305	0N9	O16-C14-C3-N4
4	C	305	0N9	O15-C14-C3-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	SO4	1	0
2	A	301	SO4	1	0
4	D	305	0N9	1	0
2	D	301	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	180/187 (96%)	1.84	66 (36%) 1 1	55, 81, 100, 108	0
1	B	180/187 (96%)	1.65	59 (32%) 1 1	57, 81, 101, 104	0
1	C	182/187 (97%)	1.50	52 (28%) 1 1	55, 80, 99, 104	0
1	D	183/187 (97%)	1.54	51 (27%) 1 1	53, 80, 100, 107	0
All	All	725/748 (96%)	1.63	228 (31%) 1 1	53, 80, 100, 108	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	ALA	7.3
1	B	128	HIS	6.9
1	A	74	HIS	6.7
1	A	128	HIS	6.2
1	C	50(B)	GLY	6.2
1	C	74	HIS	6.0
1	A	132	LEU	5.9
1	B	143	THR	5.6
1	D	122	VAL	5.5
1	B	74	HIS	5.2
1	A	127	VAL	5.2
1	C	155	MET	5.1
1	B	152	GLY	5.1
1	C	153	GLU	5.0
1	B	127	VAL	4.9
1	A	152	GLY	4.7
1	A	123	THR	4.6
1	B	123	THR	4.6
1	C	138	ILE	4.6
1	A	190	SER	4.6
1	B	148	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	155	MET	4.5
1	A	138	ILE	4.5
1	D	150	PHE	4.4
1	B	155	MET	4.4
1	A	148	PHE	4.4
1	B	122	VAL	4.4
1	C	115	ASN	4.3
1	D	7	GLN	4.2
1	B	138	ILE	4.2
1	A	143	THR	4.1
1	B	131	TYR	4.0
1	B	136	ASN	4.0
1	B	153	GLU	4.0
1	B	137	LYS	4.0
1	B	147	ILE	3.9
1	C	129	THR	3.9
1	D	151	THR	3.9
1	A	118	ILE	3.8
1	A	145	ILE	3.8
1	C	137	LYS	3.8
1	B	97	THR	3.8
1	A	147	ILE	3.7
1	A	153	GLU	3.7
1	A	115	ASN	3.7
1	D	74	HIS	3.6
1	B	150	PHE	3.6
1	A	136	ASN	3.6
1	C	156	ALA	3.6
1	B	124	ARG	3.6
1	D	125	ARG	3.6
1	D	155	MET	3.6
1	D	148	PHE	3.5
1	D	147	ILE	3.4
1	D	137	LYS	3.4
1	C	126	GLU	3.4
1	B	140	SER	3.4
1	D	131	TYR	3.4
1	A	137	LYS	3.4
1	C	118	ILE	3.4
1	D	138	ILE	3.4
1	C	103	PRO	3.4
1	B	115	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	141	GLU	3.3
1	B	162	THR	3.3
1	C	122	VAL	3.3
1	A	156	ALA	3.3
1	B	50(B)	GLY	3.3
1	B	73	LYS	3.2
1	A	99	GLY	3.2
1	C	139	LYS	3.2
1	D	118	ILE	3.2
1	D	73	LYS	3.2
1	A	149	SER	3.2
1	C	50(A)	GLY	3.2
1	D	153	GLU	3.2
1	B	159	ALA	3.1
1	A	159	ALA	3.1
1	A	4	PHE	3.1
1	C	143	THR	3.1
1	D	36	ALA	3.1
1	D	196(C)	ALA	3.1
1	A	162	THR	3.1
1	B	49	SER	3.0
1	C	140	SER	3.0
1	C	98	THR	3.0
1	C	148	PHE	3.0
1	C	99	GLY	3.0
1	D	132	LEU	3.0
1	C	105	PHE	3.0
1	A	129	THR	3.0
1	C	109	LEU	3.0
1	B	190	SER	3.0
1	D	165	GLU	3.0
1	C	78	ILE	2.9
1	A	188	TRP	2.9
1	C	163	LEU	2.9
1	C	196(E)	LEU	2.9
1	D	196(E)	LEU	2.9
1	A	151	THR	2.9
1	C	73	LYS	2.9
1	B	118	ILE	2.9
1	A	50(A)	GLY	2.9
1	A	112	TYR	2.9
1	C	149	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	147	ILE	2.9
1	C	121	GLY	2.8
1	A	131	TYR	2.8
1	A	150	PHE	2.8
1	A	78	ILE	2.8
1	B	125	ARG	2.8
1	A	187	LEU	2.8
1	A	126	GLU	2.8
1	A	141	GLU	2.8
1	C	112	TYR	2.8
1	C	183	ALA	2.8
1	A	157	THR	2.8
1	D	100	VAL	2.8
1	C	131	TYR	2.8
1	A	73	LYS	2.8
1	B	109	LEU	2.7
1	D	134	LYS	2.7
1	B	142	GLU	2.7
1	D	80	GLU	2.7
1	D	145	ILE	2.7
1	A	31	GLU	2.7
1	B	126	GLU	2.7
1	D	146	HIS	2.7
1	C	145	ILE	2.6
1	A	191	PHE	2.6
1	A	146	HIS	2.6
1	A	179	ARG	2.6
1	D	107	PRO	2.6
1	A	196(A)	ALA	2.6
1	A	140	SER	2.6
1	A	103	PRO	2.6
1	B	107	PRO	2.6
1	D	196(D)	GLU	2.6
1	B	110	TYR	2.6
1	C	100	VAL	2.6
1	D	196(F)	ALA	2.6
1	D	123	THR	2.5
1	D	154	GLU	2.5
1	A	109	LEU	2.5
1	D	120	ILE	2.5
1	B	117	PHE	2.5
1	C	125	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	50(A)	GLY	2.5
1	B	121	GLY	2.5
1	D	78	ILE	2.5
1	D	81	GLY	2.5
1	D	156	ALA	2.5
1	A	125	ARG	2.5
1	A	96	ASN	2.5
1	C	95	CYS	2.5
1	B	188	TRP	2.5
1	B	134	LYS	2.5
1	A	163	LEU	2.4
1	B	132	LEU	2.4
1	C	50(C)	SER	2.4
1	D	143	THR	2.4
1	A	178	ILE	2.4
1	B	133	GLU	2.4
1	A	110	TYR	2.4
1	C	97	THR	2.4
1	B	146	HIS	2.4
1	D	171	ILE	2.4
1	B	191	PHE	2.4
1	D	191	PHE	2.4
1	A	36	ALA	2.4
1	B	98	THR	2.4
1	C	96	ASN	2.4
1	B	156	ALA	2.4
1	B	103	PRO	2.4
1	D	195	GLU	2.3
1	C	130	TYR	2.3
1	C	159	ALA	2.3
1	B	145	ILE	2.3
1	B	100	VAL	2.3
1	B	96	ASN	2.3
1	D	95	CYS	2.3
1	B	104	LYS	2.3
1	C	128	HIS	2.3
1	D	144	HIS	2.3
1	D	121	GLY	2.3
1	A	133	GLU	2.2
1	D	130	TYR	2.2
1	A	120	ILE	2.2
1	A	97	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	123	THR	2.2
1	B	149	SER	2.2
1	B	76	PHE	2.2
1	A	101	GLU	2.2
1	C	80	GLU	2.2
1	B	50(C)	SER	2.2
1	C	76	PHE	2.2
1	A	195	GLU	2.2
1	B	101	GLU	2.2
1	A	122	VAL	2.2
1	B	24	TYR	2.2
1	C	135	ALA	2.2
1	C	28	PRO	2.1
1	C	150	PHE	2.1
1	A	194	SER	2.1
1	B	120	ILE	2.1
1	A	7	GLN	2.1
1	A	24	TYR	2.1
1	D	170	ARG	2.1
1	C	127	VAL	2.1
1	D	109	LEU	2.1
1	C	196(A)	ALA	2.1
1	D	196(B)	ALA	2.1
1	A	23	GLU	2.1
1	B	94	ILE	2.1
1	B	130	TYR	2.1
1	C	190	SER	2.1
1	D	50(C)	SER	2.1
1	D	124	ARG	2.1
1	A	196(B)	ALA	2.1
1	D	135	ALA	2.1
1	A	142	GLU	2.1
1	C	101	GLU	2.1
1	D	110	TYR	2.1
1	A	130	TYR	2.0
1	A	144	HIS	2.0
1	A	32	THR	2.0
1	D	162	THR	2.0
1	D	104	LYS	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
2	SO4	C	302	5/5	0.44	0.14	187,188,188,188	0
2	SO4	D	302	5/5	0.44	0.15	183,183,183,183	0
2	SO4	A	302	5/5	0.62	0.12	169,169,169,169	0
4	ON9	C	305	17/17	0.66	0.12	62,64,66,67	0
2	SO4	C	301	5/5	0.67	0.11	113,113,113,113	0
2	SO4	B	301	5/5	0.69	0.13	111,111,111,111	0
4	ON9	B	305	17/17	0.70	0.12	63,65,66,66	0
2	SO4	B	302	5/5	0.70	0.12	247,247,247,247	0
4	ON9	D	305	17/17	0.70	0.12	69,70,71,71	0
2	SO4	D	301	5/5	0.75	0.12	107,107,107,107	0
4	ON9	A	305	17/17	0.79	0.11	65,67,68,68	0
2	SO4	A	301	5/5	0.83	0.09	104,104,105,105	0
3	MN	B	304	1/1	0.91	0.06	96,96,96,96	0
3	MN	A	303	1/1	0.93	0.07	98,98,98,98	0
3	MN	A	304	1/1	0.96	0.05	80,80,80,80	0
3	MN	C	304	1/1	0.96	0.05	93,93,93,93	0
3	MN	C	303	1/1	0.98	0.05	89,89,89,89	0
3	MN	B	303	1/1	0.98	0.08	78,78,78,78	0
3	MN	D	303	1/1	0.98	0.07	89,89,89,89	0
3	MN	D	304	1/1	0.98	0.05	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.