



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:02 pm BST

PDB ID : 5WMS
Title : Phosphotriesterase variant S7
Authors : Miton, C.M.; Campbell, E.C.; Jackson, C.J.; Tokuriki, N.
Deposited on : 2017-07-31
Resolution : 1.60 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	:	2.11
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)	:	2.11

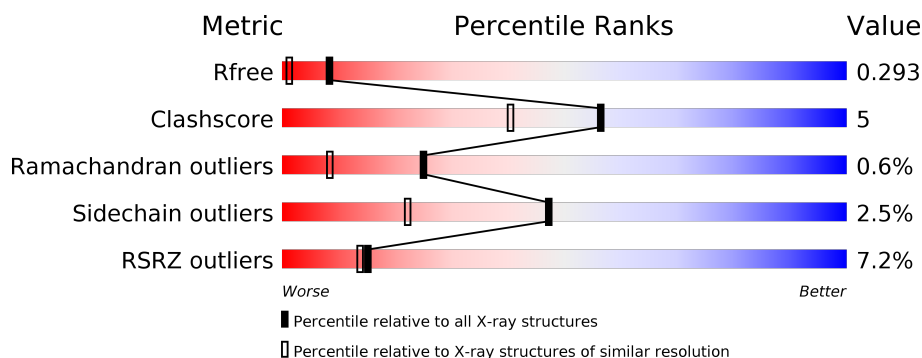
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	333	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	G	333	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>5%</div> </div> </div>
1	Q	333	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>
1	S	333	<div> <div>12%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>6%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	G	2404	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10306 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 Phosphotriesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	5	0
			2434	1537	436	455	6			
1	G	315	Total	C	N	O	S	0	6	0
			2444	1545	435	458	6			
1	Q	316	Total	C	N	O	S	0	4	0
			2439	1539	442	452	6			
1	S	314	Total	C	N	O	S	0	4	0
			2423	1528	435	454	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	LEU	PHE	conflict	UNP A0A060GYS1
A	233	ALA	ASP	conflict	UNP A0A060GYS1
A	234	ALA	THR	conflict	UNP A0A060GYS1
A	254	SER	HIS	conflict	UNP A0A060GYS1
A	260	VAL	ILE	conflict	UNP A0A060GYS1
A	263	GLY	GLU	conflict	UNP A0A060GYS1
A	271	HIS	LEU	conflict	UNP A0A060GYS1
A	293	THR	MET	conflict	UNP A0A060GYS1
A	306	ILE	PHE	conflict	UNP A0A060GYS1
A	320	GLY	VAL	conflict	UNP A0A060GYS1
G	216	LEU	PHE	conflict	UNP A0A060GYS1
G	233	ALA	ASP	conflict	UNP A0A060GYS1
G	234	ALA	THR	conflict	UNP A0A060GYS1
G	254	SER	HIS	conflict	UNP A0A060GYS1
G	260	VAL	ILE	conflict	UNP A0A060GYS1
G	263	GLY	GLU	conflict	UNP A0A060GYS1
G	271	HIS	LEU	conflict	UNP A0A060GYS1
G	293	THR	MET	conflict	UNP A0A060GYS1
G	306	ILE	PHE	conflict	UNP A0A060GYS1
G	320	GLY	VAL	conflict	UNP A0A060GYS1
Q	216	LEU	PHE	conflict	UNP A0A060GYS1

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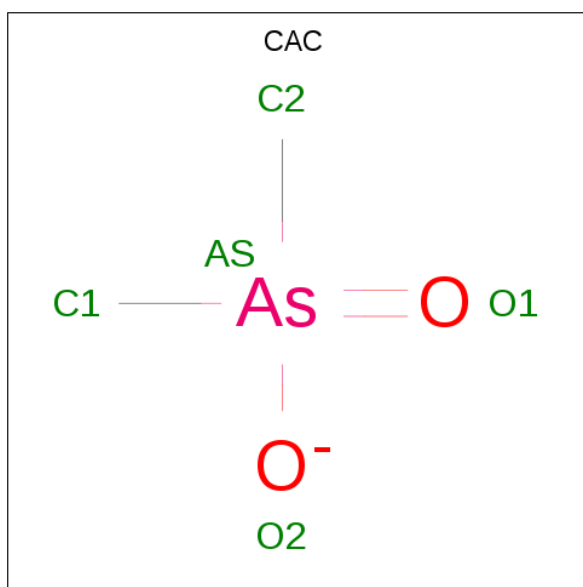
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Chain	Residue	Modelled	Actual	Comment	Reference
Q	233	ALA	ASP	conflict	UNP A0A060GYS1
Q	234	ALA	THR	conflict	UNP A0A060GYS1
Q	254	SER	HIS	conflict	UNP A0A060GYS1
Q	260	VAL	ILE	conflict	UNP A0A060GYS1
Q	263	GLY	GLU	conflict	UNP A0A060GYS1
Q	271	HIS	LEU	conflict	UNP A0A060GYS1
Q	293	THR	MET	conflict	UNP A0A060GYS1
Q	306	ILE	PHE	conflict	UNP A0A060GYS1
Q	320	GLY	VAL	conflict	UNP A0A060GYS1
S	216	LEU	PHE	conflict	UNP A0A060GYS1
S	233	ALA	ASP	conflict	UNP A0A060GYS1
S	234	ALA	THR	conflict	UNP A0A060GYS1
S	254	SER	HIS	conflict	UNP A0A060GYS1
S	260	VAL	ILE	conflict	UNP A0A060GYS1
S	263	GLY	GLU	conflict	UNP A0A060GYS1
S	271	HIS	LEU	conflict	UNP A0A060GYS1
S	293	THR	MET	conflict	UNP A0A060GYS1
S	306	ILE	PHE	conflict	UNP A0A060GYS1
S	320	GLY	VAL	conflict	UNP A0A060GYS1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

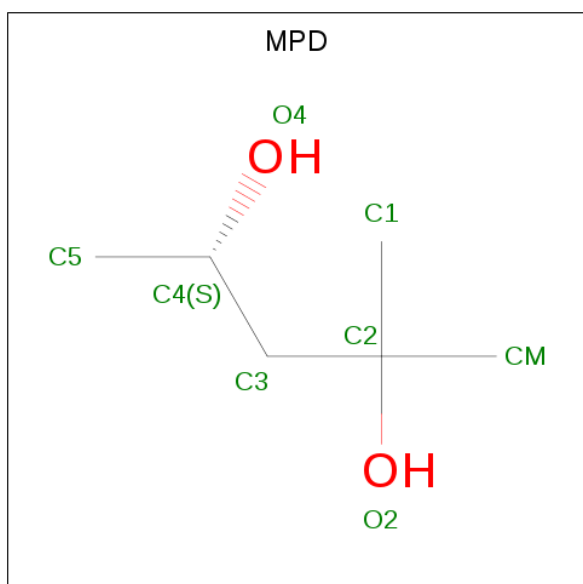
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	Q	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	S	2	Total Zn 2 2	0	0

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	G	1	Total	As	C	O	0	0
			5	1	2	2		
3	Q	1	Total	As	C	O	0	0
			5	1	2	2		
3	S	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	G	1	Total C O 8 6 2	0	0
4	G	1	Total C O 8 6 2	0	0
4	Q	1	Total C O 8 6 2	0	0
4	Q	1	Total C O 8 6 2	0	0
4	Q	1	Total C O 8 6 2	0	0
4	S	1	Total C O 8 6 2	0	0
4	S	1	Total C O 8 6 2	0	0

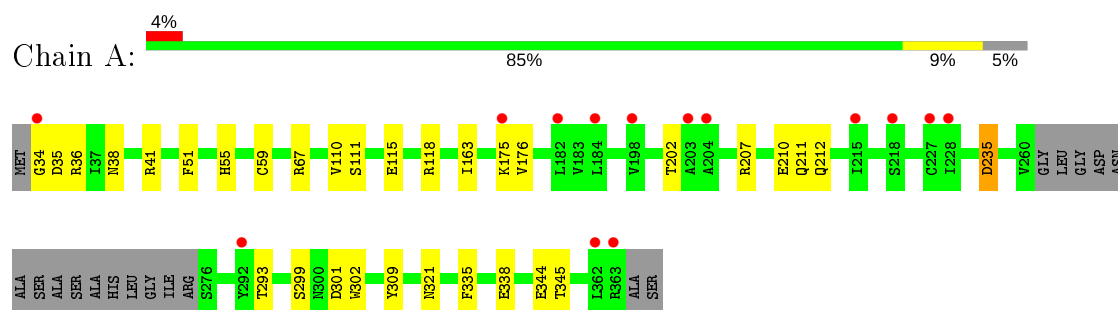
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	131	Total O 131 131	0	0
5	G	107	Total O 107 107	0	0
5	Q	131	Total O 131 131	0	0
5	S	97	Total O 97 97	0	0

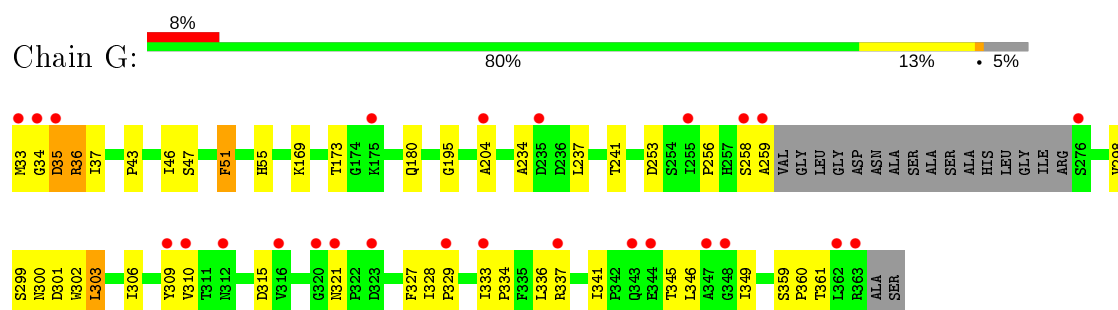
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

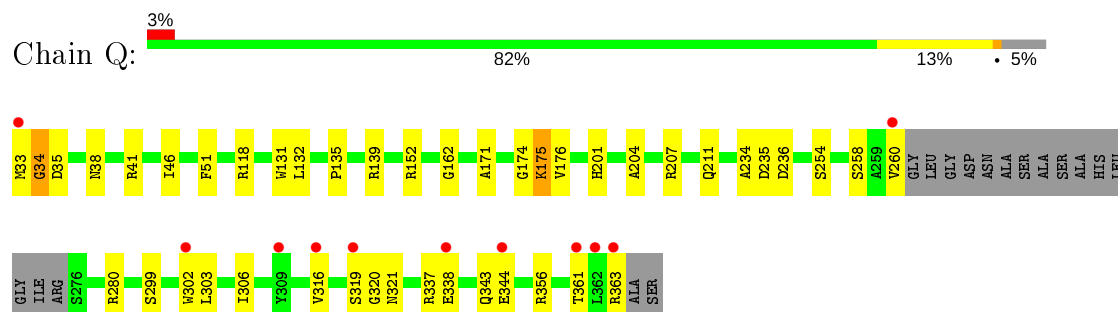
• Molecule 1: Phosphotriesterase



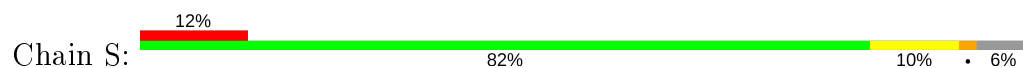
• Molecule 1: Phosphotriesterase

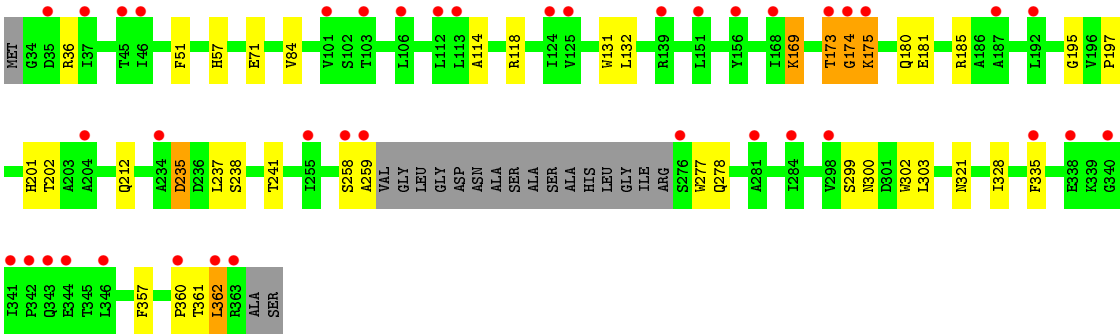


• Molecule 1: Phosphotriesterase



• Molecule 1: Phosphotriesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.66Å 86.12Å 176.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.06 – 1.60 43.06 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.06-1.60) 99.8 (43.06-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.264 , 0.292 0.264 , 0.293	Depositor DCC
R_{free} test set	8643 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10306	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 89.64 % 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 3.1526e-08. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, ZN, MPD, KCX

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	0.35	0/2464	0.56	0/3346
1	G	0.32	0/2475	0.56	0/3362
1	Q	0.34	0/2469	0.56	0/3351
1	S	0.32	0/2453	0.56	0/3330
All	All	0.33	0/9861	0.56	0/13389

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	169	KCX	Mainchain

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	2434	0	2465	22	0
1	G	2444	0	2466	31	0
1	Q	2439	0	2474	23	0
1	S	2423	0	2449	23	0
2	A	2	0	0	0	0
2	G	2	0	0	0	0
2	Q	2	0	0	0	0
2	S	2	0	0	0	0
3	A	5	0	0	0	0
3	G	5	0	0	1	0
3	Q	5	0	0	0	0
3	S	5	0	0	2	0
4	A	16	0	28	2	0
4	G	16	0	28	0	0
4	Q	24	0	42	2	0
4	S	16	0	28	1	0
5	A	131	0	0	5	0
5	G	107	0	0	0	1
5	Q	131	0	0	4	0
5	S	97	0	0	0	0
All	All	10306	0	9980	99	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 5.

All (99) 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:Q:33:MET:O	1:Q:35:ASP:N	2.04	0.90
1:A:34:GLY:O	1:A:36:ARG:N	2.16	0.78
1:S:173:THR:HG22	1:S:180:GLN:HE22	1.50	0.75
1:Q:207:ARG:NH1	1:Q:236:ASP:OD2	2.19	0.74
1:S:258:SER:H	1:S:259:ALA:HB3	1.55	0.71
1:G:35:ASP:N	1:G:35:ASP:OD1	2.24	0.71
1:Q:41:ARG:HD3	1:Q:118:ARG:HG2	1.70	0.71
1:A:235:ASP:HB2	4:Q:2405:MPD:H31	1.74	0.70
1:Q:260:VAL:HA	1:Q:320:GLY:HA3	1.76	0.68
1:Q:38:ASN:ND2	5:Q:2503:HOH:O	2.25	0.68
1:G:55:HIS:CD2	1:G:301:ASP:OD1	2.49	0.65
1:G:258:SER:HB2	1:G:259:ALA:HA	1.79	0.65
1:G:237:LEU:O	1:G:241:THR:HG23	1.99	0.63
1:S:71[B]:GLU:H	1:S:71[B]:GLU:CD	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:131:TRP:HE1	3:S:2403:CAC:C1	2.15	0.58
1:A:202:THR:HB	1:A:212:GLN:NE2	2.19	0.58
1:G:33:MET:HA	1:G:360:PRO:HG2	1.86	0.58
1:A:309:TYR:HB2	4:A:2405:MPD:C1	2.34	0.57
1:S:278:GLN:HG2	1:S:335:PHE:CE1	2.40	0.57
1:A:41[B]:ARG:NH1	1:A:118:ARG:HD3	2.20	0.57
1:S:84:VAL:HG11	4:S:2404:MPD:H53	1.87	0.56
1:S:197:PRO:HB2	1:S:357:PHE:CZ	2.41	0.55
1:S:235:ASP:N	1:S:235:ASP:OD1	2.37	0.55
1:G:298:VAL:HG23	1:G:349[B]:ILE:HD11	1.89	0.55
1:Q:135:PRO:O	1:Q:139[A]:ARG:HG3	2.08	0.54
1:Q:302:TRP:CH2	1:Q:321:ASN:HB3	2.43	0.54
1:A:110[B]:VAL:HG23	5:A:2568:HOH:O	2.08	0.53
1:Q:174:GLY:O	5:Q:2501:HOH:O	2.18	0.53
1:A:38:ASN:OD1	5:A:2502:HOH:O	2.18	0.52
1:Q:361:THR:HG22	1:Q:363:ARG:H	1.74	0.52
1:G:33:MET:O	1:G:35:ASP:N	2.42	0.52
1:G:33:MET:N	1:G:36:ARG:O	2.42	0.52
1:S:237:LEU:O	1:S:241:THR:HG23	2.09	0.52
1:A:202:THR:HG23	5:A:2505:HOH:O	2.09	0.51
1:G:337:ARG:HG3	1:G:346:LEU:HD12	1.93	0.51
1:G:258:SER:N	1:G:259:ALA:HB2	2.27	0.50
1:Q:204:ALA:HB1	1:Q:234:ALA:HB2	1.93	0.50
1:Q:34:GLY:N	5:Q:2507:HOH:O	2.43	0.50
1:S:302:TRP:CH2	1:S:321:ASN:HB3	2.46	0.50
1:G:51:PHE:CE2	1:G:329:PRO:HB3	2.47	0.49
1:G:302:TRP:CH2	1:G:321:ASN:HB3	2.47	0.49
1:S:361:THR:O	1:S:362:LEU:HB2	2.10	0.49
1:G:37:ILE:HG22	1:G:360:PRO:HD3	1.94	0.49
1:S:202[B]:THR:HG23	1:S:212:GLN:NE2	2.26	0.49
1:A:175:LYS:HA	1:A:211:GLN:HE21	1.77	0.49
1:Q:171:ALA:HA	1:Q:201:HIS:HB3	1.95	0.49
1:A:110[B]:VAL:HG11	1:A:163:ILE:HG21	1.94	0.48
1:A:293:THR:HG21	1:A:345:THR:HG23	1.95	0.48
1:Q:337:ARG:NH1	1:Q:343:GLN:OE1	2.45	0.48
1:Q:316:VAL:O	1:Q:319:SER:OG	2.31	0.47
1:A:344:GLU:H	1:A:344:GLU:CD	2.18	0.47
1:G:336:LEU:HB3	1:G:341:ILE:HD12	1.96	0.47
1:A:309:TYR:HB2	4:A:2405:MPD:H11	1.96	0.47
1:S:201:HIS:CE1	3:S:2403:CAC:C1	2.98	0.46
1:G:204:ALA:HB1	1:G:234:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:259:ALA:HB2	1:S:277:TRP:HB3	1.96	0.46
1:S:57:HIS:CE1	1:S:169:KCX:OQ2	2.69	0.45
1:Q:303:LEU:HD22	1:Q:306:ILE:HG12	1.98	0.45
1:Q:235:ASP:OD1	5:Q:2502:HOH:O	2.21	0.45
1:Q:254:SER:O	1:Q:280:ARG:NH1	2.50	0.45
1:S:174:GLY:HA2	1:S:175:LYS:C	2.36	0.45
1:Q:303:LEU:HD13	1:Q:306:ILE:HD11	1.98	0.44
1:G:258:SER:HB2	1:G:259:ALA:CA	2.46	0.44
1:A:67:ARG:HG3	5:A:2612:HOH:O	2.18	0.43
1:G:359[B]:SER:O	1:G:361:THR:OG1	2.31	0.43
1:Q:258:SER:OG	1:Q:280:ARG:NE	2.51	0.43
1:S:258:SER:N	1:S:259:ALA:HB3	2.28	0.43
1:A:111:SER:O	1:A:115:GLU:HG3	2.18	0.43
1:S:195:GLY:O	1:S:360:PRO:HA	2.19	0.42
1:A:59:CYS:HB3	5:A:2563:HOH:O	2.19	0.42
1:G:169:KCX:OQ1	3:G:2403:CAC:O1	2.37	0.42
1:Q:344:GLU:H	1:Q:344:GLU:CD	2.22	0.42
1:G:173:THR:HG23	1:G:180:GLN:HE22	1.85	0.42
1:G:256:PRO:HB3	1:G:327:PHE:CD2	2.55	0.42
1:G:333:ILE:HB	1:G:334:PRO:HD3	2.02	0.42
1:A:335:PHE:O	1:A:338:GLU:HG2	2.20	0.42
1:G:298:VAL:CG2	1:G:349[B]:ILE:HD11	2.49	0.42
1:Q:175:LYS:HA	1:Q:211:GLN:HE21	1.84	0.42
1:S:175:LYS:HG3	1:S:175:LYS:H	1.50	0.42
1:Q:162:GLY:O	4:Q:2405:MPD:O4	2.38	0.41
1:S:131:TRP:CG	1:S:132:LEU:N	2.87	0.41
1:S:300:ASN:OD1	1:S:328:ILE:HG12	2.21	0.41
1:Q:131:TRP:CG	1:Q:132:LEU:N	2.88	0.41
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.56	0.41
1:G:195:GLY:O	1:G:360:PRO:HA	2.20	0.41
1:G:55:HIS:HB3	1:G:253:ASP:HB2	2.01	0.41
1:S:114:ALA:O	1:S:118:ARG:HG3	2.21	0.41
1:G:258:SER:H	1:G:259:ALA:HB2	1.86	0.41
1:G:46:ILE:HD12	1:G:46:ILE:HA	1.89	0.41
1:G:345:THR:O	1:G:349[B]:ILE:HG22	2.20	0.41
1:S:181:GLU:O	1:S:185:ARG:HG3	2.21	0.41
1:G:303:LEU:HD13	1:G:306:ILE:HD11	2.03	0.41
1:A:207:ARG:NH2	1:A:210:GLU:OE2	2.44	0.41
1:A:55:HIS:CD2	1:A:301:ASP:OD1	2.74	0.41
1:G:36:ARG:HE	1:G:43:PRO:HB2	1.86	0.40
1:G:309:TYR:CD2	1:G:310:VAL:HG22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110[B]:VAL:HG12	1:A:163:ILE:HD13	2.03	0.40
1:A:110[B]:VAL:CG1	1:A:163:ILE:HG21	2.51	0.40
1:G:300:ASN:OD1	1:G:328:ILE:HG12	2.21	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)
5:G:2560:HOH:O	5:G:2597:HOH:O[4_556]	2.13	0.07

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	315/333 (95%)	306 (97%)	7 (2%)	2 (1%)	25	8
1	G	316/333 (95%)	305 (96%)	10 (3%)	1 (0%)	41	21
1	Q	315/333 (95%)	304 (96%)	9 (3%)	2 (1%)	25	8
1	S	313/333 (94%)	305 (97%)	6 (2%)	2 (1%)	25	8
All	All	1259/1332 (94%)	1220 (97%)	32 (2%)	7 (1%)	25	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	Q	34	GLY
1	A	176	VAL
1	G	34	GLY
1	S	174	GLY
1	Q	176	VAL
1	S	362	LEU

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	256/262 (98%)	253 (99%)	3 (1%)	71	54
1	G	256/262 (98%)	249 (97%)	7 (3%)	44	20
1	Q	255/262 (97%)	247 (97%)	8 (3%)	40	15
1	S	254/262 (97%)	246 (97%)	8 (3%)	40	15
All	All	1021/1048 (97%)	995 (98%)	26 (2%)	47	22

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	235	ASP
1	A	299	SER
1	G	35	ASP
1	G	36	ARG
1	G	47	SER
1	G	51	PHE
1	G	299	SER
1	G	303	LEU
1	G	315	ASP
1	Q	46	ILE
1	Q	51	PHE
1	Q	152	ARG
1	Q	175	LYS
1	Q	299	SER
1	Q	338	GLU
1	Q	356[A]	ARG
1	Q	356[B]	ARG
1	S	36	ARG
1	S	51	PHE
1	S	173	THR
1	S	175	LYS
1	S	235	ASP
1	S	238	SER

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Mol	Chain	Res	Type
1	S	299	SER
1	S	303	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	S	169	1,2	7,11,12	0.73	0	4,12,14	1.29	1 (25%)
1	KCX	G	169	1,2	7,11,12	0.73	0	4,12,14	1.50	1 (25%)
1	KCX	A	169	1,2	7,11,12	0.61	0	4,12,14	1.84	1 (25%)
1	KCX	Q	169	1,2	7,11,12	0.64	0	4,12,14	0.82	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
1	KCX	S	169	1,2	-	1/7/10/12	-
1	KCX	G	169	1,2	-	1/7/10/12	-
1	KCX	A	169	1,2	-	1/7/10/12	-
1	KCX	Q	169	1,2	-	0/7/10/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	KCX	CE-NZ-CX	-2.98	117.90	122.95
1	G	169	KCX	CE-NZ-CX	-2.69	118.39	122.95
1	S	169	KCX	CE-NZ-CX	-2.25	119.13	122.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S	169	KCX	C-CA-CB-CG
1	A	169	KCX	C-CA-CB-CG
1	G	169	KCX	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S	169	KCX	1	0
1	G	169	KCX	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 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	CAC	G	2403	2	0,4,4	0.00	-	0,6,6	0.00	-
4	MPD	G	2404	-	7,7,7	0.60	0	9,10,10	0.72	0
3	CAC	A	2403	2	0,4,4	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	A	2404	-	7,7,7	0.71	0	9,10,10	0.37	0
4	MPD	A	2405	-	7,7,7	0.65	0	9,10,10	0.54	0
4	MPD	G	2405	-	7,7,7	0.66	0	9,10,10	0.38	0
4	MPD	S	2404	-	7,7,7	0.66	0	9,10,10	0.35	0
3	CAC	Q	2403	2	0,4,4	0.00	-	0,6,6	0.00	-
4	MPD	Q	2404	-	7,7,7	0.67	0	9,10,10	0.68	0
3	CAC	S	2403	2	0,4,4	0.00	-	0,6,6	0.00	-
4	MPD	Q	2405	-	7,7,7	0.65	0	9,10,10	0.55	0
4	MPD	S	2405	-	7,7,7	0.74	0	9,10,10	0.38	0
4	MPD	Q	2406	-	7,7,7	0.70	0	9,10,10	0.35	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	MPD	G	2404	-	-	1/5/5/5	-
4	MPD	A	2404	-	-	3/5/5/5	-
4	MPD	A	2405	-	-	0/5/5/5	-
4	MPD	G	2405	-	-	3/5/5/5	-
4	MPD	S	2404	-	-	1/5/5/5	-
4	MPD	Q	2404	-	-	1/5/5/5	-
4	MPD	Q	2405	-	-	3/5/5/5	-
4	MPD	S	2405	-	-	2/5/5/5	-
4	MPD	Q	2406	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2404	MPD	C2-C3-C4-O4
4	Q	2405	MPD	C1-C2-C3-C4
4	Q	2405	MPD	O2-C2-C3-C4
4	A	2404	MPD	O2-C2-C3-C4
4	G	2405	MPD	O2-C2-C3-C4
4	A	2404	MPD	C1-C2-C3-C4
4	G	2405	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	G	2405	MPD	CM-C2-C3-C4
4	S	2405	MPD	C1-C2-C3-C4
4	Q	2405	MPD	CM-C2-C3-C4
4	Q	2406	MPD	C1-C2-C3-C4
4	S	2404	MPD	O2-C2-C3-C4
4	S	2405	MPD	O2-C2-C3-C4
4	G	2404	MPD	C2-C3-C4-C5
4	Q	2404	MPD	C2-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2403	CAC	1	0
4	A	2405	MPD	2	0
4	S	2404	MPD	1	0
3	S	2403	CAC	2	0
4	Q	2405	MPD	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	314/333 (94%)	0.40	14 (4%) 33 30	14, 26, 42, 58	2 (0%)
1	G	314/333 (94%)	0.67	26 (8%) 11 10	18, 33, 48, 59	1 (0%)
1	Q	315/333 (94%)	0.47	11 (3%) 44 41	12, 30, 48, 61	2 (0%)
1	S	313/333 (93%)	1.03	40 (12%) 3 3	22, 39, 49, 58	0
All	All	1256/1332 (94%)	0.64	91 (7%) 15 14	12, 33, 47, 61	5 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	362	LEU	11.1
1	G	33	MET	10.6
1	S	174	GLY	9.3
1	G	363	ARG	9.0
1	A	363	ARG	8.5
1	G	362	LEU	8.3
1	A	34	GLY	6.4
1	S	37	ILE	6.3
1	S	204	ALA	5.7
1	S	259	ALA	5.4
1	S	156	TYR	5.3
1	S	363	ARG	4.9
1	G	34	GLY	4.7
1	Q	362	LEU	4.6
1	S	173	THR	4.5
1	G	258	SER	3.9
1	S	175	LYS	3.9
1	G	235	ASP	3.8
1	Q	344	GLU	3.7
1	A	362	LEU	3.5
1	S	124	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	S	234	ALA	3.5
1	Q	338	GLU	3.4
1	G	337	ARG	3.4
1	G	175	LYS	3.3
1	A	204	ALA	3.3
1	Q	33	MET	3.2
1	Q	363	ARG	3.2
1	G	255	ILE	3.1
1	S	284	ILE	3.0
1	S	258	SER	2.9
1	S	338	GLU	2.9
1	Q	302	TRP	2.8
1	S	45	THR	2.8
1	S	106	LEU	2.8
1	G	329	PRO	2.8
1	Q	309	TYR	2.7
1	G	259	ALA	2.7
1	A	203	ALA	2.7
1	Q	361	THR	2.7
1	S	360	PRO	2.7
1	A	215	ILE	2.7
1	Q	319	SER	2.6
1	S	35	ASP	2.6
1	A	198	VAL	2.6
1	S	125	VAL	2.6
1	S	341	ILE	2.6
1	G	320	GLY	2.5
1	A	175	LYS	2.5
1	S	46	ILE	2.5
1	G	344	GLU	2.4
1	G	316	VAL	2.4
1	G	348	GLY	2.4
1	S	151	LEU	2.4
1	S	192	LEU	2.4
1	G	312	ASN	2.4
1	S	101	VAL	2.4
1	A	184	LEU	2.3
1	A	292	TYR	2.3
1	G	309	TYR	2.3
1	S	139	ARG	2.3
1	G	333	ILE	2.3
1	S	335	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	S	276	SER	2.2
1	A	182	LEU	2.2
1	S	344	GLU	2.2
1	S	113	LEU	2.2
1	S	343	GLN	2.2
1	S	342	PRO	2.1
1	A	227	CYS	2.1
1	G	310	VAL	2.1
1	S	255	ILE	2.1
1	G	347	ALA	2.1
1	A	218	SER	2.1
1	S	346	LEU	2.1
1	A	228	ILE	2.1
1	G	321	ASN	2.1
1	G	35	ASP	2.1
1	G	276	SER	2.1
1	G	323	ASP	2.1
1	S	187	ALA	2.1
1	S	168	ILE	2.1
1	G	204	ALA	2.0
1	S	340	GLY	2.0
1	Q	260	VAL	2.0
1	S	298	VAL	2.0
1	S	112	LEU	2.0
1	S	103	THR	2.0
1	S	281	ALA	2.0
1	G	343	GLN	2.0
1	Q	316	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	S	169	12/13	0.70	0.20	39,40,40,40	0
1	KCX	G	169	12/13	0.85	0.10	18,22,25,26	0
1	KCX	A	169	12/13	0.90	0.10	15,17,19,20	0
1	KCX	Q	169	12/13	0.94	0.09	17,18,21,22	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
4	MPD	G	2404	8/8	0.23	0.42	35,41,44,45	0
4	MPD	S	2404	8/8	0.64	0.29	35,39,45,45	0
4	MPD	A	2405	8/8	0.65	0.28	18,25,28,32	8
4	MPD	Q	2405	8/8	0.67	0.28	34,37,41,44	0
4	MPD	S	2405	8/8	0.72	0.35	42,43,46,48	0
4	MPD	G	2405	8/8	0.77	0.40	41,43,44,47	0
4	MPD	Q	2406	8/8	0.80	0.34	33,38,40,46	0
4	MPD	Q	2404	8/8	0.82	0.29	39,43,44,44	0
4	MPD	A	2404	8/8	0.82	0.21	32,34,40,44	0
2	ZN	G	2402	1/1	0.90	0.10	21,21,21,21	1
2	ZN	G	2401	1/1	0.92	0.10	20,20,20,20	0
2	ZN	S	2401	1/1	0.94	0.08	20,20,20,20	1
3	CAC	S	2403	5/5	0.95	0.15	10,15,20,22	5
2	ZN	S	2402	1/1	0.95	0.08	21,21,21,21	1
3	CAC	G	2403	5/5	0.96	0.17	13,23,25,33	5
3	CAC	Q	2403	5/5	0.98	0.10	15,16,20,22	5
2	ZN	A	2402	1/1	0.99	0.06	14,14,14,14	1
2	ZN	Q	2401	1/1	0.99	0.09	15,15,15,15	1
3	CAC	A	2403	5/5	0.99	0.10	12,13,15,18	5
2	ZN	Q	2402	1/1	0.99	0.07	17,17,17,17	1
2	ZN	A	2401	1/1	1.00	0.04	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.