



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:33 pm BST

PDB ID : 3FLO
Title : Crystal structure of the carboxyl-terminal domain of yeast DNA polymerase alpha in complex with its B subunit
Authors : Klinge, S.N.; Pellegrini, L.
Deposited on : 2008-12-19
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 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

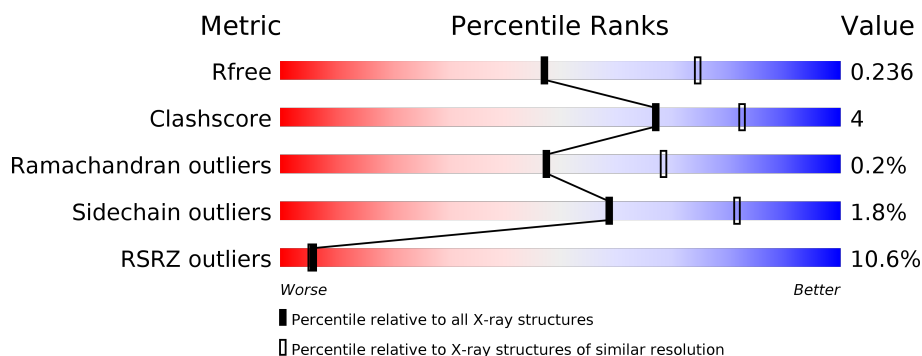
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	460	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	C	460	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
1	E	460	<div> <div>16%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
1	G	460	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
2	I	3	<div> <div></div> <div>100%</div> </div>
2	J	3	<div> <div></div> <div>100%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	3	 100%
2	L	3	 100%
3	B	206	 4% 78% 9% 13%
3	D	206	 17% 79% 8% 13%
3	F	206	 25% 75% 11% 13%
3	H	206	 7% 74% 13% 13%

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
4	SO4	A	32	-	-	-	X
4	SO4	A	34	-	-	-	X
4	SO4	A	35	-	-	-	X
4	SO4	A	47	-	-	-	X
4	SO4	B	38	-	-	-	X
4	SO4	B	59	-	-	-	X
4	SO4	B	68	-	-	-	X
4	SO4	C	53	-	-	-	X
4	SO4	D	39	-	-	-	X
4	SO4	D	67	-	-	-	X
4	SO4	E	22	-	-	-	X
4	SO4	E	45	-	-	-	X
4	SO4	E	54	-	-	-	X
4	SO4	G	17	-	-	-	X
4	SO4	G	42	-	-	-	X
4	SO4	G	56	-	-	-	X
4	SO4	H	65	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20656 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 DNA polymerase alpha subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	3	0
			3458	2208	589	651	10			
1	C	433	Total	C	N	O	S	0	3	0
			3458	2208	589	651	10			
1	E	433	Total	C	N	O	S	0	3	0
			3458	2208	589	651	10			
1	G	433	Total	C	N	O	S	0	3	0
			3458	2208	589	651	10			

- Molecule 2 is a protein called DNA polymerase alpha catalytic subunit A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	J	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	K	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	L	3	Total	C	N	O	0	0	0
			15	9	3	3			

- Molecule 3 is a protein called DNA polymerase alpha catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	180	Total	C	N	O	S	0	1	0
			1471	925	247	287	12			
3	D	180	Total	C	N	O	S	0	0	0
			1463	921	246	284	12			
3	F	180	Total	C	N	O	S	0	0	0
			1463	921	246	284	12			
3	H	180	Total	C	N	O	S	0	0	0
			1463	921	246	284	12			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0
5	D	2	Total Zn 2 2	0	0
5	F	2	Total Zn 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	135	Total O 135 135	0	0
6	B	79	Total O 79 79	0	0
6	C	106	Total O 106 106	0	0

Continued on next page...

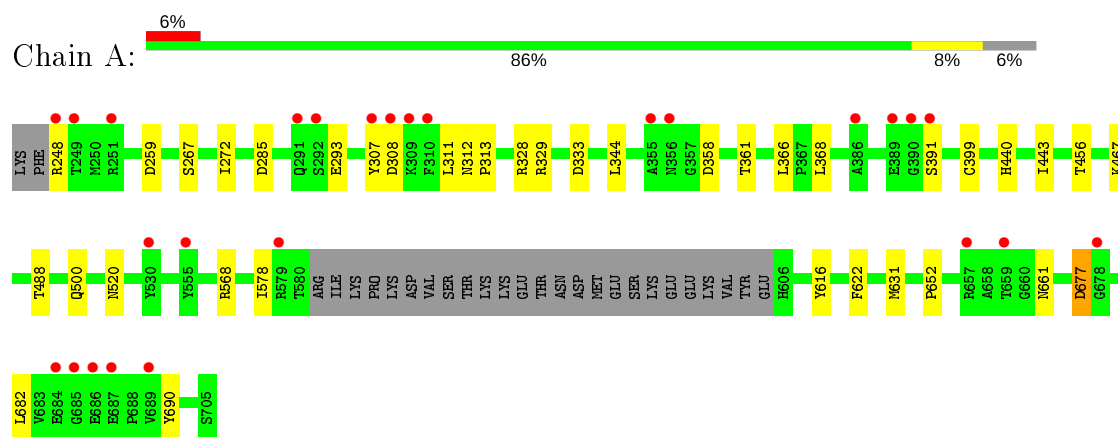
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	13	Total 13	O 13	0	0
6	E	65	Total 65	O 65	0	0
6	F	8	Total 8	O 8	0	0
6	G	138	Total 138	O 138	0	0
6	H	27	Total 27	O 27	0	0

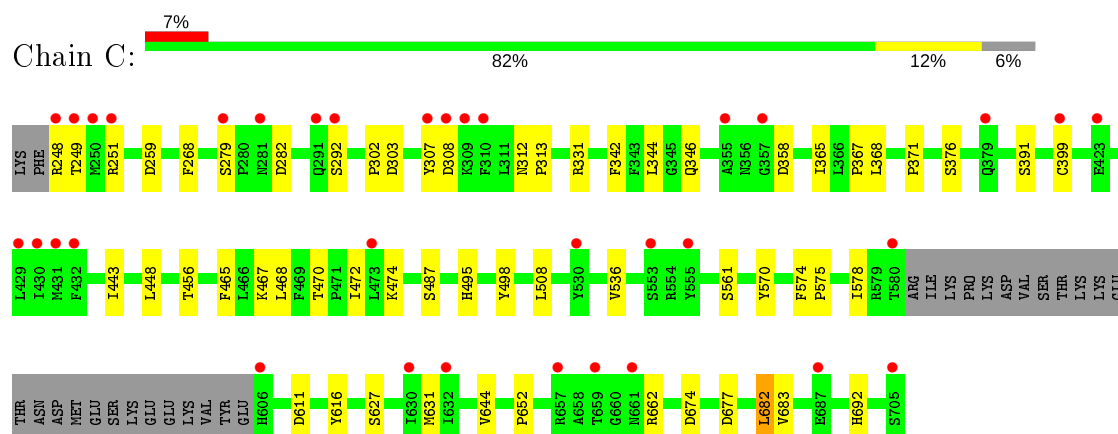
3 Residue-property plots [i](#)

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.

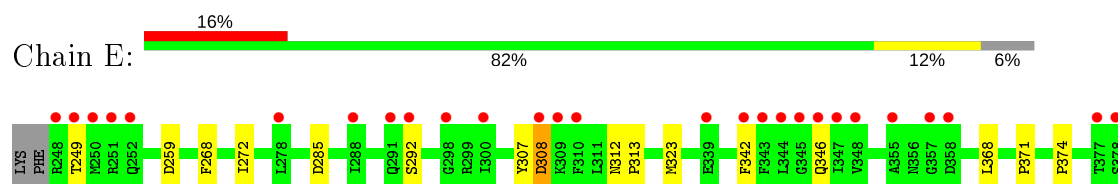
- Molecule 1: DNA polymerase alpha subunit B

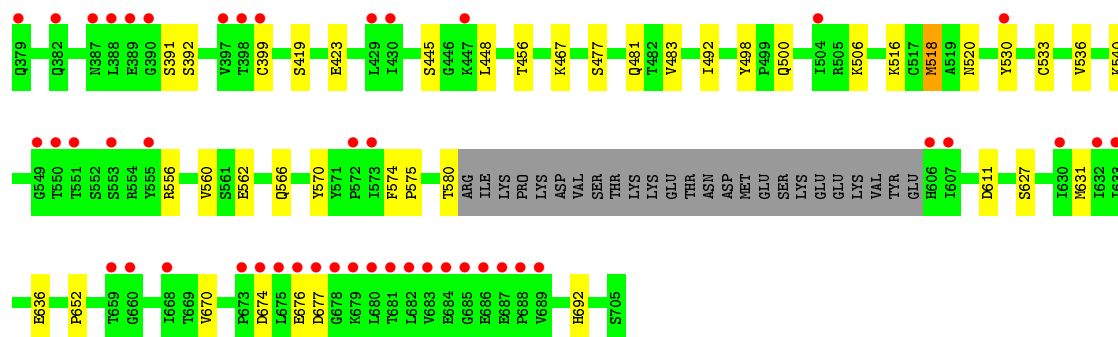


- Molecule 1: DNA polymerase alpha subunit B

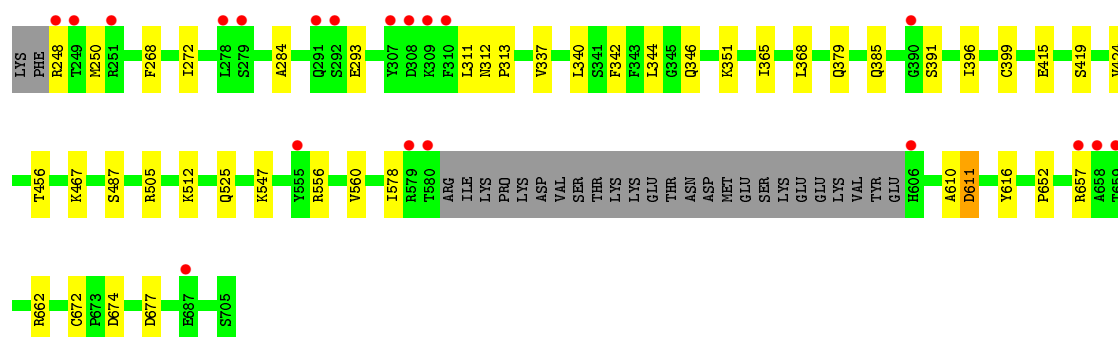
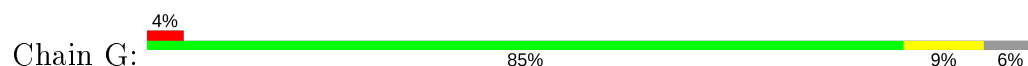


- Molecule 1: DNA polymerase alpha subunit B





• Molecule 1: DNA polymerase alpha subunit B



• Molecule 2: DNA polymerase alpha catalytic subunit A



There are no outlier residues recorded for this chain.

• Molecule 2: DNA polymerase alpha catalytic subunit A



There are no outlier residues recorded for this chain.

• Molecule 2: DNA polymerase alpha catalytic subunit A



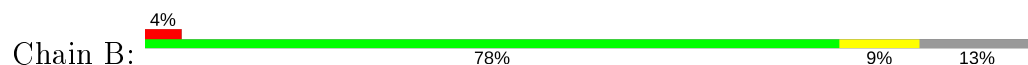
There are no outlier residues recorded for this chain.

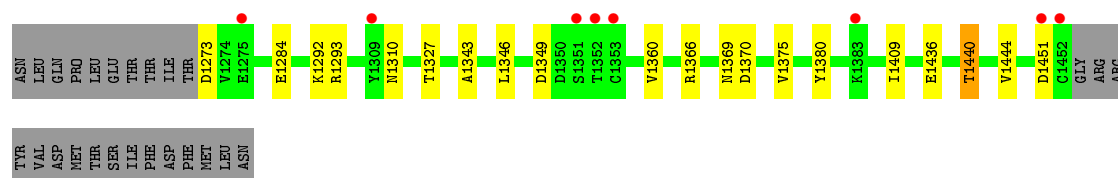
• Molecule 2: DNA polymerase alpha catalytic subunit A



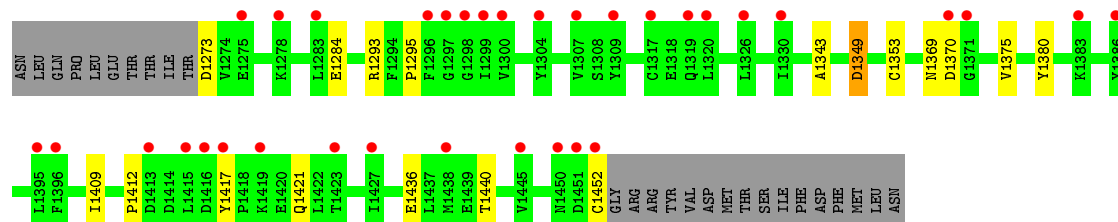
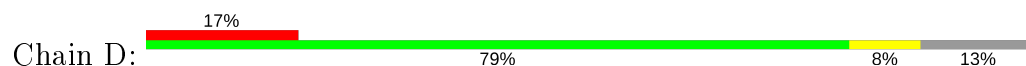
There are no outlier residues recorded for this chain.

• Molecule 3: DNA polymerase alpha catalytic subunit A

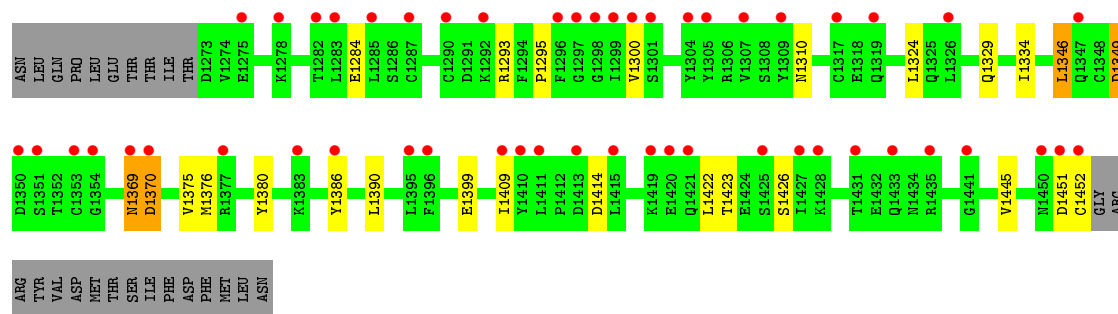
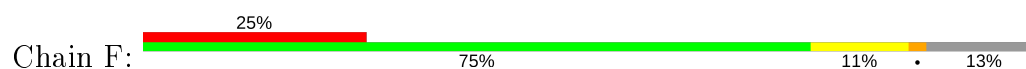




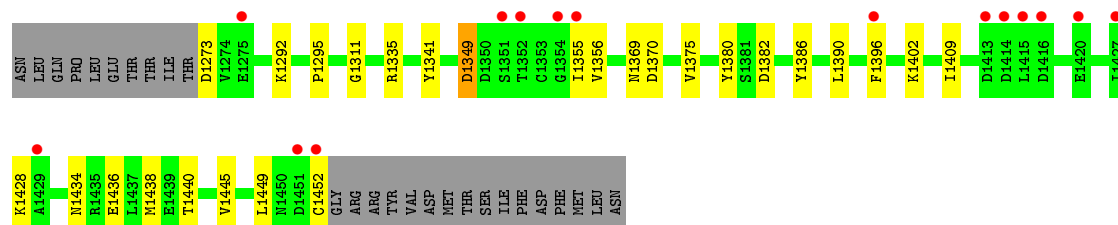
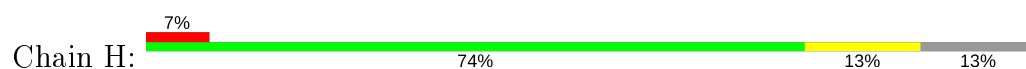
• Molecule 3: DNA polymerase alpha catalytic subunit A



• Molecule 3: DNA polymerase alpha catalytic subunit A



• Molecule 3: DNA polymerase alpha catalytic subunit A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.41Å 142.63Å 175.25Å 90.00° 102.33° 90.00°	Depositor
Resolution (Å)	31.90 – 2.50 31.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.90-2.50) 99.8 (31.90-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.218 0.214 , 0.236	Depositor DCC
R_{free} test set	7082 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20656	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

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	0.83	0/3537	0.81	3/4801 (0.1%)
1	C	0.77	0/3537	0.79	3/4801 (0.1%)
1	E	0.70	3/3537 (0.1%)	0.76	3/4801 (0.1%)
1	G	0.83	1/3537 (0.0%)	0.82	2/4801 (0.0%)
3	B	0.88	0/1500	0.81	0/2024
3	D	0.67	0/1492	0.75	1/2013 (0.0%)
3	F	0.63	0/1492	0.71	0/2013
3	H	0.69	0/1492	0.77	2/2013 (0.1%)
All	All	0.77	4/20124 (0.0%)	0.79	14/27267 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	415	GLU	CG-CD	6.25	1.61	1.51
1	E	533	CYS	CB-SG	-5.52	1.72	1.81
1	E	676	GLU	CD-OE2	5.49	1.31	1.25
1	E	676	GLU	CD-OE1	5.28	1.31	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	518	MET	CG-SD-CE	6.32	110.31	100.20
1	C	662	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	E	611	ASP	CB-CG-OD2	-5.74	113.14	118.30
3	D	1349	ASP	CB-CA-C	-5.71	98.99	110.40
1	C	259	ASP	CB-CG-OD1	5.68	123.41	118.30
1	G	611	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	G	578	ILE	CB-CA-C	-5.49	100.62	111.60
1	A	568	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	366	LEU	CA-CB-CG	5.21	127.28	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	611	ASP	CB-CG-OD2	-5.18	113.64	118.30
3	H	1349	ASP	CB-CA-C	-5.12	100.17	110.40
3	H	1335	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	E	285	ASP	CB-CG-OD2	-5.07	113.73	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3444	21	0
1	C	3458	0	3444	31	0
1	E	3458	0	3444	40	0
1	G	3458	0	3444	26	0
2	I	15	0	5	0	0
2	J	15	0	5	0	0
2	K	15	0	5	0	0
2	L	15	0	5	0	0
3	B	1471	0	1422	9	0
3	D	1463	0	1419	9	0
3	F	1463	0	1419	13	0
3	H	1463	0	1419	14	0
4	A	65	0	0	1	0
4	B	30	0	0	0	0
4	C	55	0	0	1	0
4	D	20	0	0	0	0
4	E	60	0	0	1	0
4	F	20	0	0	0	0
4	G	55	0	0	0	0
4	H	20	0	0	0	0
5	B	2	0	0	0	0
5	D	2	0	0	0	0
5	F	2	0	0	0	0
5	H	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	135	0	0	1	0
6	B	79	0	0	0	0
6	C	106	0	0	1	0
6	D	13	0	0	0	0
6	E	65	0	0	0	0
6	F	8	0	0	0	0
6	G	138	0	0	1	0
6	H	27	0	0	0	0
All	All	20656	0	19475	153	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 4.

All (153) 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:E:374:PRO:HB2	1:E:530:TYR:CE2	1.48	1.49
1:E:374:PRO:CB	1:E:530:TYR:CE2	2.01	1.42
1:C:474:LYS:NZ	6:C:807:HOH:O	1.67	1.28
1:A:399[B]:CYS:SG	1:A:652:PRO:HG2	1.87	1.13
1:E:374:PRO:CG	1:E:530:TYR:CD2	2.37	1.08
1:E:374:PRO:HG3	1:E:530:TYR:CD2	1.89	1.07
1:G:399[B]:CYS:SG	1:G:652:PRO:HG2	2.00	0.99
1:E:374:PRO:HB3	1:E:530:TYR:CE2	1.96	0.97
1:E:374:PRO:HB2	1:E:530:TYR:HE2	0.81	0.93
1:E:374:PRO:CB	1:E:530:TYR:CD2	2.55	0.90
1:E:399[B]:CYS:SG	1:E:652:PRO:HG2	2.13	0.88
1:E:272:ILE:HD11	1:E:368:LEU:HD23	1.60	0.83
1:C:399[B]:CYS:SG	1:C:652:PRO:HG2	2.20	0.81
3:B:1436:GLU:O	3:B:1440:THR:HG23	1.82	0.78
1:A:399[B]:CYS:SG	1:A:652:PRO:CG	2.70	0.76
1:G:293:GLU:OE1	1:G:351:LYS:NZ	2.19	0.75
1:E:374:PRO:CG	1:E:530:TYR:HD2	2.00	0.73
3:B:1284:GLU:HG2	3:B:1293:ARG:NH2	2.04	0.72
1:E:307:TYR:HD1	1:E:308:ASP:O	1.74	0.69
3:H:1436:GLU:O	3:H:1440:THR:HG23	1.92	0.69
1:G:396:ILE:HD11	1:G:424:VAL:HG11	1.76	0.68
1:G:399[B]:CYS:SG	1:G:652:PRO:CG	2.79	0.68
1:E:399[B]:CYS:SG	1:E:652:PRO:CG	2.83	0.66
1:C:456:THR:O	1:C:467:LYS:HE3	1.99	0.63
1:E:307:TYR:CD1	1:E:308:ASP:O	2.52	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:ILE:HD11	1:E:368:LEU:CD2	2.29	0.62
3:H:1295:PRO:HB2	3:H:1409:ILE:HD13	1.84	0.59
1:A:661:ASN:ND2	4:A:50:SO4:O1	2.34	0.59
1:C:292:SER:OG	4:C:69:SO4:S	2.62	0.57
1:G:248:ARG:HD2	1:G:616:TYR:CZ	2.41	0.56
1:E:456:THR:O	1:E:467:LYS:HE3	2.05	0.56
3:B:1369:ASN:O	3:B:1370:ASP:C	2.44	0.56
1:C:371:PRO:HG2	1:C:627:SER:HB3	1.88	0.56
1:G:337:VAL:HG11	1:G:365:ILE:HD11	1.87	0.55
1:G:674:ASP:HB3	1:G:677:ASP:HB2	1.87	0.55
1:C:570:TYR:HE1	1:C:631:MET:HE2	1.72	0.54
1:E:448:LEU:HD13	3:F:1324:LEU:HG	1.88	0.54
1:E:371:PRO:HG2	1:E:627:SER:HB3	1.88	0.54
1:C:249:THR:HG23	1:C:251:ARG:HG3	1.90	0.53
1:G:284:ALA:HB1	6:G:1105:HOH:O	2.09	0.53
3:D:1436:GLU:O	3:D:1440:THR:HG23	2.10	0.52
3:D:1284:GLU:HG2	3:D:1293:ARG:NH2	2.24	0.52
3:H:1355:ILE:HD13	3:H:1369:ASN:OD1	2.09	0.52
3:F:1295:PRO:HB2	3:F:1409:ILE:HD13	1.92	0.51
3:H:1341:TYR:OH	3:H:1382:ASP:HB3	2.09	0.51
3:D:1369:ASN:O	3:D:1370:ASP:C	2.48	0.51
3:H:1369:ASN:O	3:H:1370:ASP:C	2.47	0.51
1:E:500:GLN:HB3	1:E:520:ASN:HB3	1.91	0.51
1:A:272:ILE:HD11	1:A:368:LEU:HD23	1.91	0.51
1:G:311:LEU:CD1	1:G:344:LEU:HD11	2.40	0.51
1:C:465:PHE:CE2	1:C:508:LEU:HD22	2.47	0.50
1:C:443:ILE:HD13	1:C:448:LEU:HD21	1.95	0.49
1:G:250:MET:CE	3:H:1452:CYS:HB2	2.43	0.48
1:G:657:ARG:HD2	1:G:662:ARG:O	2.13	0.48
3:D:1284:GLU:HG2	3:D:1293:ARG:CZ	2.43	0.48
1:G:456:THR:O	1:G:467:LYS:HE3	2.12	0.48
1:A:312:ASN:HB2	1:A:313:PRO:CD	2.44	0.48
1:G:342:PHE:HA	1:G:346:GLN:OE1	2.12	0.48
1:E:498:TYR:CD2	1:E:536:VAL:CG2	2.97	0.48
1:E:483:VAL:HG13	1:E:518:MET:HG2	1.95	0.48
1:C:365:ILE:O	1:C:367:PRO:HD3	2.14	0.47
1:A:488:THR:HG23	6:A:753:HOH:O	2.13	0.47
1:C:248:ARG:HD2	1:C:616:TYR:CE2	2.49	0.47
1:C:682:LEU:HD12	1:C:683:VAL:N	2.30	0.47
3:D:1412:PRO:HA	3:D:1417:TYR:CG	2.50	0.47
1:C:376:SER:OG	1:C:692:HIS:NE2	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1310:ASN:N	3:F:1310:ASN:OD1	2.48	0.46
1:A:285:ASP:OD2	1:A:328:ARG:NH2	2.48	0.46
1:E:374:PRO:HB3	1:E:530:TYR:CZ	2.46	0.46
1:G:505:ARG:CZ	1:G:512:LYS:HB2	2.44	0.46
1:C:249:THR:CG2	1:C:251:ARG:HG3	2.46	0.46
1:G:610:ALA:O	1:G:611:ASP:C	2.53	0.46
3:H:1396:PHE:HD2	3:H:1438:MET:HE2	1.81	0.46
1:C:578:ILE:HD11	3:D:1343:ALA:HB1	1.98	0.46
1:C:498:TYR:CD2	1:C:536:VAL:CG2	2.98	0.46
3:H:1445:VAL:HG12	3:H:1449:LEU:HD12	1.98	0.46
3:H:1402:LYS:HD2	3:H:1428:LYS:HD2	1.97	0.46
1:C:561:SER:HB2	1:C:644:VAL:HG11	1.97	0.46
3:F:1346:LEU:HD23	3:F:1376:MET:HB3	1.97	0.46
1:G:312:ASN:HB2	1:G:313:PRO:CD	2.46	0.46
1:A:456:THR:O	1:A:467:LYS:HE3	2.16	0.46
1:G:268:PHE:CE1	1:G:368:LEU:HD13	2.51	0.45
3:B:1366:ARG:HH11	1:E:323:MET:HE1	1.80	0.45
1:C:302:PRO:HD3	1:C:344:LEU:HD22	1.98	0.45
1:A:682:LEU:HD13	1:A:690:TYR:CZ	2.51	0.45
1:E:574:PHE:HA	1:E:575:PRO:C	2.37	0.45
1:C:470:THR:O	1:C:474:LYS:HG3	2.17	0.45
1:C:468:LEU:O	1:C:472:ILE:HD12	2.17	0.45
3:H:1311:GLY:HA2	3:H:1434:ASN:ND2	2.32	0.45
1:G:556:ARG:O	1:G:560:VAL:HG23	2.18	0.44
3:D:1349:ASP:HB2	3:D:1375:VAL:H	1.82	0.44
3:H:1311:GLY:HA2	3:H:1434:ASN:HD21	1.82	0.44
3:F:1386:TYR:CE2	3:F:1390:LEU:HD11	2.52	0.44
1:E:312:ASN:HB2	1:E:313:PRO:CD	2.48	0.44
1:C:342:PHE:HA	1:C:346:GLN:OE1	2.18	0.44
1:E:674:ASP:HB2	1:E:677:ASP:HB2	1.99	0.44
1:C:307:TYR:HD1	1:C:308:ASP:O	2.01	0.44
1:C:248:ARG:NH2	1:C:495[A]:HIS:HE1	2.16	0.44
3:F:1284:GLU:HG2	3:F:1293:ARG:NH2	2.32	0.44
1:C:248:ARG:HD2	1:C:616:TYR:CZ	2.53	0.44
1:E:540:LYS:HD2	1:E:636:GLU:CD	2.38	0.44
1:C:674:ASP:HB3	1:C:677:ASP:OD2	2.18	0.44
1:A:307:TYR:HD1	1:A:308:ASP:O	2.01	0.43
1:E:268:PHE:CE1	1:E:368:LEU:HD13	2.54	0.43
1:G:250:MET:HE2	3:H:1452:CYS:HB2	1.99	0.43
1:E:342:PHE:HA	1:E:346:GLN:OE1	2.18	0.43
1:A:500:GLN:HB3	1:A:520:ASN:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ILE:HD13	1:C:578:ILE:HG21	1.76	0.43
3:F:1300:VAL:HA	3:F:1422:LEU:HD12	2.00	0.43
3:F:1423:THR:OG1	3:F:1426:SER:OG	2.25	0.43
3:F:1334:ILE:HD11	3:F:1445:VAL:HG22	2.00	0.43
1:C:279:SER:N	1:C:282:ASP:OD2	2.51	0.43
1:E:392:SER:HB2	1:E:670:VAL:O	2.19	0.42
1:A:259:ASP:OD2	1:E:259:ASP:OD2	2.37	0.42
1:A:333:ASP:HB3	1:A:361:THR:HA	2.00	0.42
1:C:312:ASN:HB2	1:C:313:PRO:CD	2.49	0.42
1:E:481:GLN:HE21	1:E:516:LYS:HG3	1.85	0.42
1:A:578:ILE:HD11	3:B:1343:ALA:HB1	2.01	0.42
1:A:311:LEU:HD11	1:A:344:LEU:HD11	2.01	0.42
3:D:1295:PRO:HB2	3:D:1409:ILE:HD13	2.02	0.42
1:E:374:PRO:HG2	1:E:530:TYR:HD2	1.81	0.42
3:F:1369:ASN:O	3:F:1370:ASP:C	2.57	0.42
1:C:574:PHE:HA	1:C:575:PRO:C	2.40	0.42
3:H:1349:ASP:HB2	3:H:1375:VAL:H	1.85	0.42
1:G:340:LEU:HG	1:G:547:LYS:HB2	2.01	0.41
3:H:1386:TYR:CZ	3:H:1390:LEU:HD11	2.55	0.41
1:A:307:TYR:CD1	1:A:308:ASP:O	2.73	0.41
1:A:440:HIS:HB3	1:A:443:ILE:HD12	2.02	0.41
1:C:268:PHE:CE1	1:C:368:LEU:HD13	2.54	0.41
1:A:248:ARG:HD2	1:A:616:TYR:CE2	2.55	0.41
1:E:570:TYR:HE1	1:E:631:MET:HE2	1.84	0.41
1:G:311:LEU:HD13	1:G:344:LEU:HD11	2.03	0.41
1:E:249:THR:HA	3:F:1451:ASP:O	2.20	0.41
1:G:312:ASN:HB2	1:G:313:PRO:HD2	2.01	0.41
1:G:385:GLN:HG3	1:G:672:CYS:SG	2.61	0.41
1:G:311:LEU:CD1	1:G:344:LEU:CD1	2.98	0.41
1:A:677:ASP:OD1	1:A:677:ASP:C	2.59	0.41
1:E:506:LYS:HE2	4:E:26:SO4:O2	2.20	0.41
3:D:1417:TYR:CZ	3:D:1421:GLN:NE2	2.89	0.41
1:A:248:ARG:HD2	1:A:616:TYR:CZ	2.56	0.41
3:B:1327:THR:HB	3:B:1444:VAL:HG21	2.02	0.41
1:E:562:GLU:O	1:E:566:GLN:HG3	2.21	0.41
3:B:1346:LEU:HD11	3:B:1360:VAL:HG22	2.03	0.41
1:E:419:SER:O	1:E:423:GLU:HB2	2.21	0.41
3:B:1366:ARG:HH11	1:E:323:MET:CE	2.34	0.40
1:G:272:ILE:HD11	1:G:368:LEU:HD22	2.03	0.40
3:B:1349:ASP:HB2	3:B:1375:VAL:H	1.85	0.40
1:E:445:SER:O	3:F:1329:GLN:NE2	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1349:ASP:HB2	3:F:1375:VAL:H	1.86	0.40
1:G:248:ARG:HD2	1:G:616:TYR:CE2	2.56	0.40
1:A:622:PHE:CZ	1:A:631:MET:HE1	2.56	0.40
1:C:303:ASP:OD2	1:C:331:ARG:NH1	2.53	0.40
1:E:556:ARG:O	1:E:560:VAL:HG23	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	432/460 (94%)	421 (98%)	10 (2%)	1 (0%)	47	68
1	C	432/460 (94%)	419 (97%)	12 (3%)	1 (0%)	47	68
1	E	432/460 (94%)	421 (98%)	10 (2%)	1 (0%)	47	68
1	G	432/460 (94%)	421 (98%)	10 (2%)	1 (0%)	47	68
3	B	179/206 (87%)	173 (97%)	6 (3%)	0	100	100
3	D	178/206 (86%)	171 (96%)	7 (4%)	0	100	100
3	F	178/206 (86%)	173 (97%)	5 (3%)	0	100	100
3	H	178/206 (86%)	172 (97%)	6 (3%)	0	100	100
All	All	2441/2664 (92%)	2371 (97%)	66 (3%)	4 (0%)	47	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	391	SER
1	A	391	SER
1	C	391	SER
1	E	391	SER

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	392/416 (94%)	388 (99%)	4 (1%)	76	90
1	C	392/416 (94%)	389 (99%)	3 (1%)	81	93
1	E	392/416 (94%)	386 (98%)	6 (2%)	65	85
1	G	392/416 (94%)	388 (99%)	4 (1%)	76	90
3	B	169/193 (88%)	162 (96%)	7 (4%)	30	55
3	D	168/193 (87%)	164 (98%)	4 (2%)	49	74
3	F	168/193 (87%)	160 (95%)	8 (5%)	25	48
3	H	168/193 (87%)	164 (98%)	4 (2%)	49	74
All	All	2241/2436 (92%)	2201 (98%)	40 (2%)	59	81

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	SER
1	A	293	GLU
1	A	358	ASP
1	A	677	ASP
3	B	1273	ASP
3	B	1292	LYS
3	B	1310	ASN
3	B	1380	TYR
3	B	1409	ILE
3	B	1440	THR
3	B	1451	ASP
1	C	358	ASP
1	C	487	SER
1	C	682	LEU
3	D	1273	ASP
3	D	1353	CYS
3	D	1380	TYR
3	D	1452	CYS
1	E	292	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	308	ASP
1	E	477	SER
1	E	492	ILE
1	E	580	THR
1	E	692	HIS
3	F	1346	LEU
3	F	1349	ASP
3	F	1369	ASN
3	F	1370	ASP
3	F	1380	TYR
3	F	1399	GLU
3	F	1414	ASP
3	F	1452	CYS
1	G	379	GLN
1	G	419	SER
1	G	487	SER
1	G	525	GLN
3	H	1273	ASP
3	H	1292	LYS
3	H	1356	VAL
3	H	1380	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	C	639	HIS
3	D	1421	GLN
1	E	363	ASN
1	G	372	ASN
1	G	525	GLN
3	H	1434	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 73 ligands modelled in this entry, 8 are monoatomic - leaving 65 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	$\# Z > 2$
4	SO4	A	49	-	4,4,4	0.13	0	6,6,6	0.51	0
4	SO4	A	12	-	4,4,4	0.17	0	6,6,6	0.26	0
4	SO4	D	39	-	4,4,4	0.13	0	6,6,6	0.26	0
4	SO4	D	63	-	4,4,4	0.21	0	6,6,6	0.25	0
4	SO4	F	64	-	4,4,4	0.22	0	6,6,6	0.14	0
4	SO4	C	53	-	4,4,4	0.17	0	6,6,6	0.34	0
4	SO4	G	1	-	4,4,4	0.14	0	6,6,6	0.28	0
4	SO4	A	50	-	4,4,4	0.10	0	6,6,6	0.24	0
4	SO4	A	3	-	4,4,4	0.19	0	6,6,6	0.57	0
4	SO4	A	32	-	4,4,4	0.18	0	6,6,6	0.12	0
4	SO4	A	35	-	4,4,4	0.15	0	6,6,6	0.24	0
4	SO4	A	47	-	4,4,4	0.22	0	6,6,6	0.25	0
4	SO4	E	4	-	4,4,4	0.11	0	6,6,6	0.19	0
4	SO4	C	15	-	4,4,4	0.22	0	6,6,6	0.59	0
4	SO4	E	23	-	4,4,4	0.20	0	6,6,6	0.26	0
4	SO4	A	13	-	4,4,4	0.13	0	6,6,6	0.53	0
4	SO4	A	34	-	4,4,4	0.14	0	6,6,6	0.17	0
4	SO4	A	5	-	4,4,4	0.21	0	6,6,6	0.18	0
4	SO4	A	30	-	4,4,4	0.06	0	6,6,6	0.65	0
4	SO4	F	41	-	4,4,4	0.15	0	6,6,6	0.14	0
4	SO4	G	2	-	4,4,4	0.15	0	6,6,6	0.29	0
4	SO4	E	58	-	4,4,4	0.17	0	6,6,6	0.15	0
4	SO4	E	26	-	4,4,4	0.23	0	6,6,6	0.45	0
4	SO4	B	38	-	4,4,4	0.13	0	6,6,6	0.20	0
4	SO4	C	11	-	4,4,4	0.15	0	6,6,6	0.58	0
4	SO4	C	43	-	4,4,4	0.14	0	6,6,6	0.16	0
4	SO4	H	65	-	4,4,4	0.20	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	E	44	-	4,4,4	0.16	0	6,6,6	0.16	0
4	SO4	G	7	-	4,4,4	0.18	0	6,6,6	0.33	0
4	SO4	G	42	-	4,4,4	0.18	0	6,6,6	0.22	0
4	SO4	G	16	-	4,4,4	0.13	0	6,6,6	0.30	0
4	SO4	G	55	-	4,4,4	0.26	0	6,6,6	0.43	0
4	SO4	B	68	-	4,4,4	0.28	0	6,6,6	0.35	0
4	SO4	G	56	-	4,4,4	0.16	0	6,6,6	0.22	0
4	SO4	E	22	-	4,4,4	0.16	0	6,6,6	0.29	0
4	SO4	E	45	-	4,4,4	0.20	0	6,6,6	0.17	0
4	SO4	C	8	-	4,4,4	0.28	0	6,6,6	0.22	0
4	SO4	C	6	-	4,4,4	0.11	0	6,6,6	0.21	0
4	SO4	A	31	-	4,4,4	0.23	0	6,6,6	0.40	0
4	SO4	B	37	-	4,4,4	0.15	0	6,6,6	0.24	0
4	SO4	H	60	-	4,4,4	0.17	0	6,6,6	0.36	0
4	SO4	A	48	-	4,4,4	0.08	0	6,6,6	0.56	0
4	SO4	C	10	-	4,4,4	0.12	0	6,6,6	0.25	0
4	SO4	E	25	-	4,4,4	0.10	0	6,6,6	0.23	0
4	SO4	G	18	-	4,4,4	0.14	0	6,6,6	0.54	0
4	SO4	D	40	-	4,4,4	0.15	0	6,6,6	0.18	0
4	SO4	B	62	-	4,4,4	0.25	0	6,6,6	0.56	0
4	SO4	E	20	-	4,4,4	0.12	0	6,6,6	0.22	0
4	SO4	G	27	-	4,4,4	0.16	0	6,6,6	0.42	0
4	SO4	C	46	-	4,4,4	0.19	0	6,6,6	0.20	0
4	SO4	E	33	-	4,4,4	0.12	0	6,6,6	0.38	0
4	SO4	B	57	-	4,4,4	0.20	0	6,6,6	0.22	0
4	SO4	C	52	-	4,4,4	0.17	0	6,6,6	0.30	0
4	SO4	E	24	-	4,4,4	0.13	0	6,6,6	0.33	0
4	SO4	H	19	-	4,4,4	0.07	0	6,6,6	0.23	0
4	SO4	C	69	-	4,4,4	0.66	0	6,6,6	0.35	0
4	SO4	G	17	-	4,4,4	0.17	0	6,6,6	0.32	0
4	SO4	C	9	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	F	28	-	4,4,4	0.18	0	6,6,6	0.16	0
4	SO4	E	54	-	4,4,4	0.15	0	6,6,6	0.21	0
4	SO4	B	59	-	4,4,4	0.19	0	6,6,6	0.42	0
4	SO4	F	66	-	4,4,4	0.19	0	6,6,6	0.32	0
4	SO4	G	51	-	4,4,4	0.16	0	6,6,6	0.28	0
4	SO4	H	61	-	4,4,4	0.13	0	6,6,6	0.26	0
4	SO4	D	67	-	4,4,4	0.19	0	6,6,6	0.41	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	50	SO4	1	0
4	E	26	SO4	1	0
4	C	69	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	433/460 (94%)	0.01	26 (6%) 21 22	10, 37, 95, 141	0
1	C	433/460 (94%)	0.39	34 (7%) 12 12	20, 49, 109, 165	0
1	E	433/460 (94%)	0.90	73 (16%) 1 1	28, 67, 153, 211	0
1	G	433/460 (94%)	0.03	20 (4%) 32 34	14, 38, 94, 143	0
2	I	0/3	-	-	-	-
2	J	0/3	-	-	-	-
2	K	0/3	-	-	-	-
2	L	0/3	-	-	-	-
3	B	180/206 (87%)	0.17	8 (4%) 34 37	19, 46, 77, 87	0
3	D	180/206 (87%)	1.03	34 (18%) 1 1	35, 82, 176, 213	0
3	F	180/206 (87%)	1.45	51 (28%) 0 0	50, 103, 210, 256	0
3	H	180/206 (87%)	0.57	15 (8%) 11 11	30, 68, 151, 189	0
All	All	2452/2676 (91%)	0.47	261 (10%) 6 5	10, 52, 139, 256	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	309	LYS	8.7
3	D	1452	CYS	7.4
1	C	309	LYS	7.3
1	E	688	PRO	7.2
3	F	1451	ASP	6.8
1	C	249	THR	6.7
1	C	251	ARG	6.5
3	B	1451	ASP	6.4
1	E	555	TYR	6.3
3	F	1452	CYS	6.2
1	G	310	PHE	6.1
1	A	309	LYS	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	684	GLU	5.9
1	E	683	VAL	5.8
1	E	687	GLU	5.8
1	E	685	GLY	5.7
1	A	251	ARG	5.6
1	A	686	GLU	5.5
3	B	1452	CYS	5.5
1	E	389	GLU	5.4
1	C	248	ARG	5.4
1	A	687	GLU	5.4
1	E	308	ASP	5.4
1	G	580	THR	5.3
1	E	251	ARG	5.2
1	G	249	THR	5.1
1	C	555	TYR	5.1
1	E	689	VAL	4.9
1	G	579	ARG	4.9
1	E	249	THR	4.9
3	D	1309	TYR	4.9
3	F	1317	CYS	4.8
3	H	1415	LEU	4.7
1	E	310	PHE	4.7
3	D	1413	ASP	4.7
1	E	248	ARG	4.6
1	C	308	ASP	4.6
3	F	1296	PHE	4.6
1	A	390	GLY	4.6
3	D	1451	ASP	4.6
1	A	685	GLY	4.5
1	E	676	GLU	4.5
1	E	684	GLU	4.4
1	E	677	ASP	4.4
1	G	390	GLY	4.3
1	A	310	PHE	4.3
3	D	1415	LEU	4.2
3	D	1299	ILE	4.2
3	H	1452	CYS	4.2
1	E	675	LEU	4.2
3	F	1415	LEU	4.1
3	F	1413	ASP	4.1
1	C	310	PHE	4.1
3	D	1396	PHE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	1297	GLY	4.0
3	D	1296	PHE	4.0
1	E	357	GLY	4.0
3	F	1278	LYS	3.9
3	F	1395	LEU	3.9
1	E	530	TYR	3.9
3	F	1299	ILE	3.9
3	H	1413	ASP	3.9
3	F	1304	TYR	3.9
3	F	1419	LYS	3.8
1	G	308	ASP	3.8
1	A	308	ASP	3.8
1	E	686	GLU	3.7
1	E	679	LYS	3.7
3	F	1369	ASN	3.7
3	D	1297	GLY	3.6
3	F	1283	LEU	3.6
1	G	251	ARG	3.5
1	G	309	LYS	3.5
3	D	1283	LEU	3.5
1	G	307	TYR	3.4
3	D	1304	TYR	3.4
1	E	278	LEU	3.4
1	C	687	GLU	3.3
3	F	1370	ASP	3.3
3	F	1275	GLU	3.3
3	B	1352	THR	3.3
1	A	659	THR	3.3
3	F	1420	GLU	3.3
1	G	291	GLN	3.3
1	E	673	PRO	3.3
3	F	1396	PHE	3.3
1	E	553	SER	3.3
1	G	292	SER	3.3
3	D	1419	LYS	3.3
3	F	1351	SER	3.3
1	E	377	THR	3.2
3	F	1305	TYR	3.2
1	A	248	ARG	3.2
3	F	1300	VAL	3.2
3	H	1451	ASP	3.2
1	E	347	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	1395	LEU	3.2
1	E	549	GLY	3.2
1	E	430	ILE	3.2
1	C	291	GLN	3.2
1	C	659	THR	3.1
1	E	388	LEU	3.2
1	E	300	ILE	3.1
1	A	307	TYR	3.1
3	D	1298	GLY	3.1
1	E	346	GLN	3.1
1	E	674	ASP	3.1
1	G	659	THR	3.1
3	F	1386	TYR	3.1
3	F	1450	ASN	3.1
1	C	430	ILE	3.0
1	E	378	SER	3.0
3	F	1326	LEU	3.0
1	C	307	TYR	3.0
1	E	680	LEU	3.0
1	C	632	ILE	3.0
1	E	632	ILE	3.0
1	C	580	THR	3.0
3	F	1433	GLN	2.9
1	E	550	THR	2.9
3	D	1371	GLY	2.9
3	D	1427	ILE	2.9
3	D	1317	CYS	2.9
1	G	606	HIS	2.9
1	G	248	ARG	2.9
3	B	1275	GLU	2.9
3	B	1351	SER	2.9
3	F	1428	LYS	2.9
1	E	399[A]	CYS	2.9
1	E	633	ILE	2.9
3	F	1347	GLN	2.9
1	C	279	SER	2.8
1	E	345	GLY	2.8
3	D	1370	ASP	2.8
1	C	423	GLU	2.8
1	E	447	LYS	2.8
1	E	288	ILE	2.8
1	C	379	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	678	GLY	2.7
1	A	386	ALA	2.7
3	D	1417	TYR	2.7
1	E	397	VAL	2.7
1	A	249	THR	2.7
1	E	291	GLN	2.7
3	D	1423	THR	2.7
1	E	343	PHE	2.7
1	A	356	ASN	2.7
1	C	357	GLY	2.7
1	E	678	GLY	2.7
1	A	292	SER	2.7
1	A	391	SER	2.6
1	E	390	GLY	2.6
3	F	1441	GLY	2.6
3	H	1414	ASP	2.6
1	A	657	ARG	2.6
3	D	1275	GLU	2.6
3	D	1450	ASN	2.6
1	E	250	MET	2.6
1	A	579	ARG	2.6
1	G	658	ALA	2.6
3	F	1427	ILE	2.6
3	H	1354	GLY	2.6
3	H	1352	THR	2.5
3	D	1319	GLN	2.5
1	C	530	TYR	2.5
3	H	1429	ALA	2.5
3	F	1431	THR	2.5
1	E	379	GLN	2.5
3	H	1416	ASP	2.5
3	B	1309	TYR	2.5
1	C	657	ARG	2.5
3	F	1377	ARG	2.5
3	H	1275	GLU	2.5
1	E	429	LEU	2.5
3	D	1445	VAL	2.5
1	C	661	ASN	2.4
1	C	399[A]	CYS	2.4
3	H	1351	SER	2.4
1	C	432	PHE	2.4
3	F	1435	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	551	THR	2.4
1	G	555	TYR	2.4
3	F	1421	GLN	2.4
1	A	555	TYR	2.4
1	E	252	GLN	2.4
3	F	1350	ASP	2.4
3	F	1411	LEU	2.4
3	F	1298	GLY	2.4
1	E	607	ILE	2.4
1	E	342	PHE	2.4
1	E	572	PRO	2.4
1	E	659	THR	2.4
1	A	291	GLN	2.4
1	C	473	LEU	2.4
1	A	689	VAL	2.3
3	F	1307	VAL	2.3
3	H	1355	ILE	2.3
1	C	553	SER	2.3
1	G	279	SER	2.3
3	D	1307	VAL	2.3
1	E	355	ALA	2.3
1	E	681	THR	2.3
1	A	389	GLU	2.3
3	D	1300	VAL	2.3
1	E	358	ASP	2.3
1	E	382	GLN	2.3
3	F	1383	LYS	2.3
1	E	292	SER	2.3
1	E	660	GLY	2.3
1	C	431	MET	2.3
1	C	250	MET	2.2
1	G	687	GLU	2.2
1	A	355	ALA	2.2
1	E	573	ILE	2.2
3	H	1427	ILE	2.2
1	E	682	LEU	2.2
3	F	1290	CYS	2.2
3	D	1386	TYR	2.2
3	F	1301	SER	2.2
1	E	504	ILE	2.2
1	E	630	ILE	2.2
3	D	1278	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	1425	SER	2.2
1	E	348	VAL	2.2
3	D	1438	MET	2.2
3	D	1383	LYS	2.2
1	C	630	ILE	2.2
3	D	1416	ASP	2.2
1	E	339	GLU	2.2
3	F	1287	CYS	2.2
3	F	1353	CYS	2.2
1	C	606	HIS	2.1
1	G	657	ARG	2.1
3	F	1409	ILE	2.1
3	B	1383	LYS	2.1
1	E	606	HIS	2.1
3	B	1353	CYS	2.1
3	F	1309	TYR	2.1
1	E	398	THR	2.1
1	C	281	ASN	2.1
1	A	530	TYR	2.1
3	D	1320	LEU	2.1
3	F	1319	GLN	2.1
1	C	292	SER	2.1
1	E	298	GLY	2.1
3	F	1354	GLY	2.1
3	F	1282	THR	2.1
1	E	668	ILE	2.1
1	C	705	SER	2.1
1	E	344	LEU	2.1
1	C	355	ALA	2.0
1	E	387	ASN	2.0
3	D	1330	ILE	2.0
3	F	1292	LYS	2.0
1	C	429	LEU	2.0
3	D	1326	LEU	2.0
3	H	1420	GLU	2.0
1	G	278	LEU	2.0
3	F	1285	LEU	2.0
3	F	1410	TYR	2.0
3	H	1396	PHE	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 carbohydrates 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(\AA^2)	Q<0.9
4	SO4	F	28	5/5	0.43	0.35	136,136,137,137	0
4	SO4	A	34	5/5	0.48	0.55	144,144,145,145	0
4	SO4	H	60	5/5	0.51	0.38	129,129,130,130	0
4	SO4	F	41	5/5	0.53	0.38	144,144,144,144	0
4	SO4	B	38	5/5	0.65	0.60	139,139,139,139	0
4	SO4	G	55	5/5	0.66	0.32	101,103,104,105	0
4	SO4	E	54	5/5	0.68	0.41	129,129,129,130	0
4	SO4	D	67	5/5	0.68	0.44	117,118,120,120	0
4	SO4	G	42	5/5	0.69	0.47	105,106,107,107	0
4	SO4	A	47	5/5	0.69	0.42	136,137,137,138	0
4	SO4	B	68	5/5	0.69	0.40	111,112,112,113	0
4	SO4	E	22	5/5	0.69	0.41	121,122,122,123	0
4	SO4	E	45	5/5	0.70	0.64	140,140,140,141	0
4	SO4	B	59	5/5	0.72	0.40	120,120,121,122	0
4	SO4	C	46	5/5	0.72	0.38	127,127,128,128	0
4	SO4	G	17	5/5	0.74	0.45	122,122,123,123	0
4	SO4	C	52	5/5	0.75	0.35	125,125,126,126	0
4	SO4	C	53	5/5	0.75	0.44	119,119,120,120	0
4	SO4	A	31	5/5	0.76	0.36	102,102,103,104	0
4	SO4	A	35	5/5	0.76	0.41	137,137,137,138	0
4	SO4	G	56	5/5	0.76	0.60	135,135,135,136	0
4	SO4	D	39	5/5	0.77	0.47	133,133,134,134	0
4	SO4	G	16	5/5	0.77	0.31	114,114,115,115	0
4	SO4	B	57	5/5	0.77	0.24	123,123,123,124	0
4	SO4	H	65	5/5	0.78	0.43	105,106,106,107	0
4	SO4	A	32	5/5	0.79	0.44	138,139,139,140	0
4	SO4	A	30	5/5	0.79	0.30	96,97,97,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	50	5/5	0.80	0.65	136,136,136,137	0
4	SO4	C	43	5/5	0.80	0.33	120,120,120,121	0
4	SO4	H	19	5/5	0.81	0.28	123,124,124,124	0
4	SO4	C	10	5/5	0.81	0.19	128,128,128,129	0
4	SO4	G	51	5/5	0.81	0.38	125,126,127,127	0
4	SO4	E	44	5/5	0.81	0.39	148,148,148,148	0
4	SO4	E	26	5/5	0.82	0.42	112,112,113,114	0
4	SO4	D	40	5/5	0.82	0.30	119,120,120,121	0
4	SO4	E	33	5/5	0.82	0.35	116,117,117,117	0
4	SO4	D	63	5/5	0.83	0.33	121,122,122,123	0
4	SO4	E	25	5/5	0.84	0.32	110,111,111,111	0
4	SO4	A	48	5/5	0.84	0.28	98,100,101,102	0
4	SO4	B	37	5/5	0.84	0.29	118,119,120,120	0
4	SO4	F	66	5/5	0.85	0.32	121,121,122,122	0
4	SO4	C	11	5/5	0.85	0.39	97,97,98,99	0
4	SO4	A	49	5/5	0.85	0.49	112,112,112,113	0
4	SO4	E	4	5/5	0.86	0.20	123,123,124,124	0
4	SO4	A	3	5/5	0.86	0.18	93,94,95,95	0
4	SO4	A	12	5/5	0.86	0.35	117,117,118,118	0
4	SO4	E	20	5/5	0.86	0.54	117,117,118,118	0
4	SO4	C	69	5/5	0.87	0.42	81,82,82,83	0
4	SO4	G	2	5/5	0.87	0.52	106,106,107,107	0
4	SO4	E	24	5/5	0.87	0.43	105,106,107,107	0
4	SO4	C	8	5/5	0.87	0.38	93,93,94,94	0
4	SO4	H	61	5/5	0.88	0.33	111,111,112,112	0
4	SO4	G	18	5/5	0.88	0.42	101,102,102,103	0
4	SO4	A	13	5/5	0.89	0.51	99,100,101,101	0
5	ZN	D	1	1/1	0.89	0.09	70,70,70,70	0
4	SO4	B	62	5/5	0.89	0.27	97,97,98,99	0
4	SO4	C	9	5/5	0.89	0.39	114,114,115,115	0
4	SO4	C	15	5/5	0.90	0.26	89,89,90,91	0
4	SO4	A	5	5/5	0.91	0.21	96,97,97,98	0
5	ZN	F	1	1/1	0.91	0.22	72,72,72,72	0
4	SO4	C	6	5/5	0.91	0.19	120,121,121,121	0
5	ZN	H	1	1/1	0.91	0.07	67,67,67,67	0
4	SO4	G	7	5/5	0.92	0.30	87,87,88,88	0
4	SO4	G	27	5/5	0.92	0.40	91,91,92,93	0
5	ZN	D	2	1/1	0.92	0.05	66,66,66,66	0
4	SO4	E	23	5/5	0.92	0.32	91,92,92,93	0
4	SO4	E	58	5/5	0.92	0.55	123,123,124,124	0
5	ZN	B	2	1/1	0.93	0.06	63,63,63,63	0
5	ZN	F	2	1/1	0.94	0.08	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	F	64	5/5	0.94	0.29	115,115,115,116	0
4	SO4	G	1	5/5	0.94	0.14	89,90,91,92	0
5	ZN	B	1	1/1	0.96	0.05	59,59,59,59	0
5	ZN	H	2	1/1	0.97	0.05	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.