Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:33 AM UTC

PDB ID	:	6YLA / pdb_00006yla
Title	:	Crystal structure of the SARS-CoV-2 receptor binding domain in complex with CR3022 Fab
Authors	:	Huo, J.; Zhao, Y.; Ren, J.; Zhou, D.; Ginn, H.M.; Fry, E.E.; Owens, R.; Stuart, D.I.
Deposited on	:	2020-04-06
Resolution	:	2.42 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:

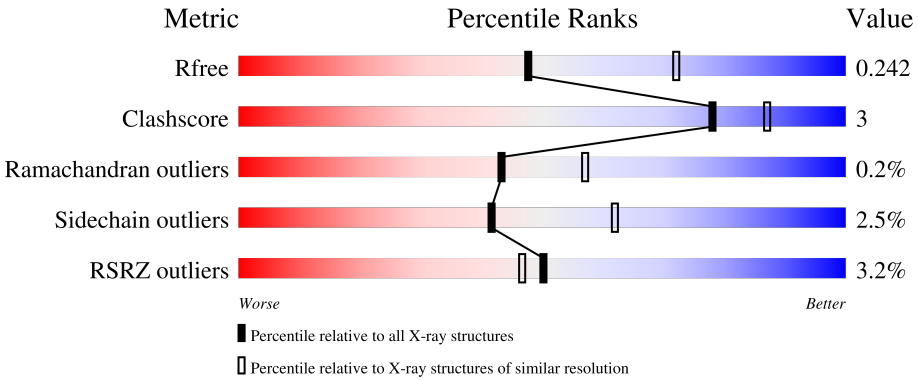
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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 <=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	213	6% 80% 12% • 7%
1	E	213	4% 83% 12% 5%
2	B	229	4% 86% 9% 5%
2	H	229	2% 88% 7% 6%
3	C	220	2% 93% 6%

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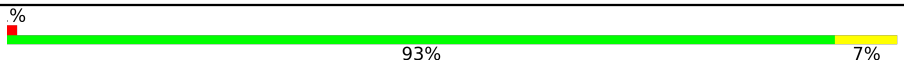
Mol	Chain	Length	Quality of chain
3	L	220	

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	DMS	C	303	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10090 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	203	Total	C	N	O	S	0	0	0
			1604	1027	268	301	8			
1	A	199	Total	C	N	O	S	0	0	0
			1582	1014	264	296	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	327	GLU	-	expression tag	UNP P0DTC2
E	328	THR	-	expression tag	UNP P0DTC2
E	329	GLY	-	expression tag	UNP P0DTC2
E	533	LYS	-	expression tag	UNP P0DTC2
E	534	HIS	-	expression tag	UNP P0DTC2
E	535	HIS	-	expression tag	UNP P0DTC2
E	536	HIS	-	expression tag	UNP P0DTC2
E	537	HIS	-	expression tag	UNP P0DTC2
E	538	HIS	-	expression tag	UNP P0DTC2
E	539	HIS	-	expression tag	UNP P0DTC2
A	327	GLU	-	expression tag	UNP P0DTC2
A	328	THR	-	expression tag	UNP P0DTC2
A	329	GLY	-	expression tag	UNP P0DTC2
A	533	LYS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2
A	538	HIS	-	expression tag	UNP P0DTC2
A	539	HIS	-	expression tag	UNP P0DTC2

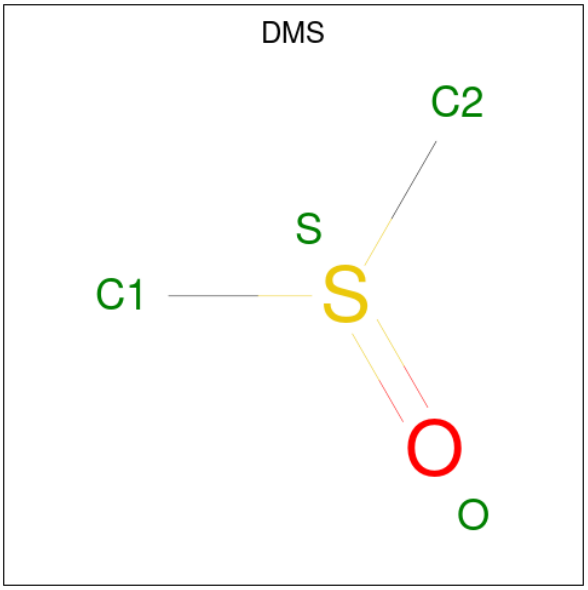
- Molecule 2 is a protein called Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	1	0
			1609	1023	261	317	8			
2	B	217	Total	C	N	O	S	0	1	0
			1615	1026	262	318	9			

- Molecule 3 is a protein called Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			
3	C	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	O	S	0	0
			4	2	1	1		
4	E	1	Total	C	O	S	0	0
			4	2	1	1		
4	E	1	Total	C	O	S	0	0
			4	2	1	1		
4	E	1	Total	C	O	S	0	0
			4	2	1	1		
4	H	1	Total	C	O	S	0	0
			4	2	1	1		
4	H	1	Total	C	O	S	0	0
			4	2	1	1		

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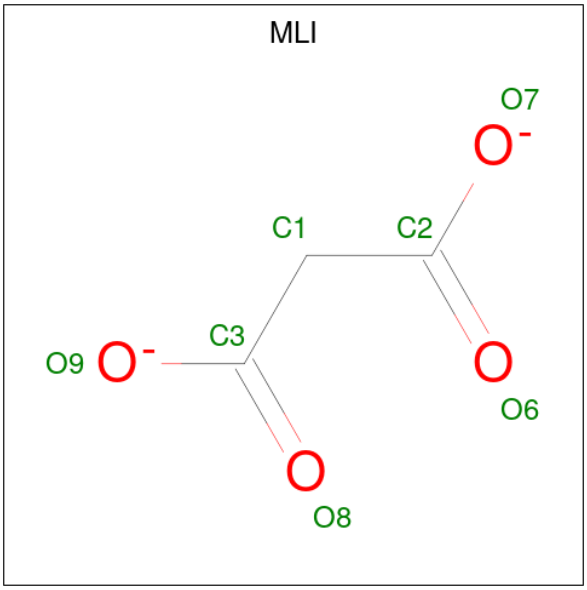
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O S 4 2 1 1	0	0
4	L	1	Total C O S 4 2 1 1	0	0
4	A	1	Total C O S 4 2 1 1	0	0
4	A	1	Total C O S 4 2 1 1	0	0
4	A	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 7 3 4	0	0
5	E	1	Total C O 7 3 4	0	0
5	H	1	Total C O 7 3 4	0	0

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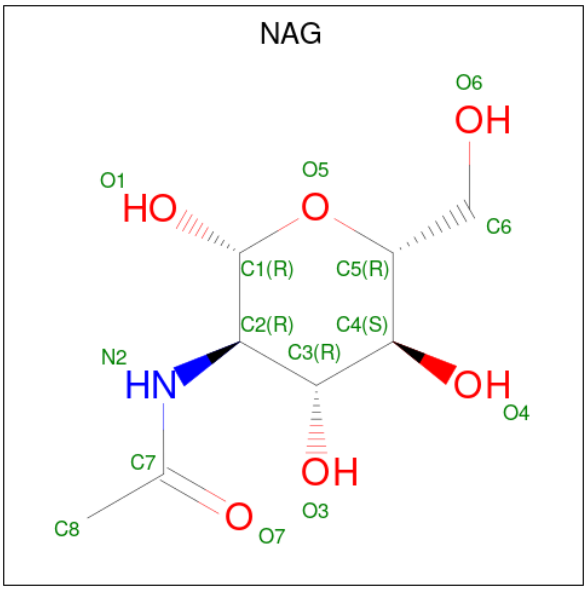
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 7 3 4	0	0
5	H	1	Total C O 7 3 4	0	0
5	B	1	Total C O 7 3 4	0	0
5	B	1	Total C O 7 3 4	0	0
5	B	1	Total C O 7 3 4	0	0
5	B	1	Total C O 7 3 4	0	0
5	C	1	Total C O 7 3 4	0	0
5	C	1	Total C O 7 3 4	0	0
5	C	1	Total C O 7 3 4	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0

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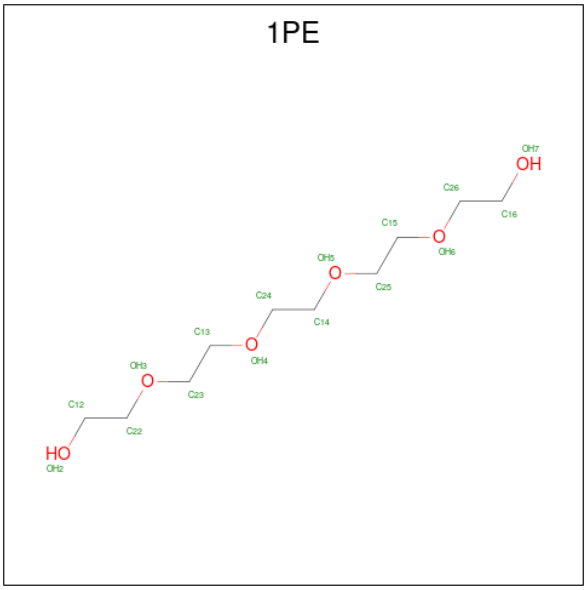
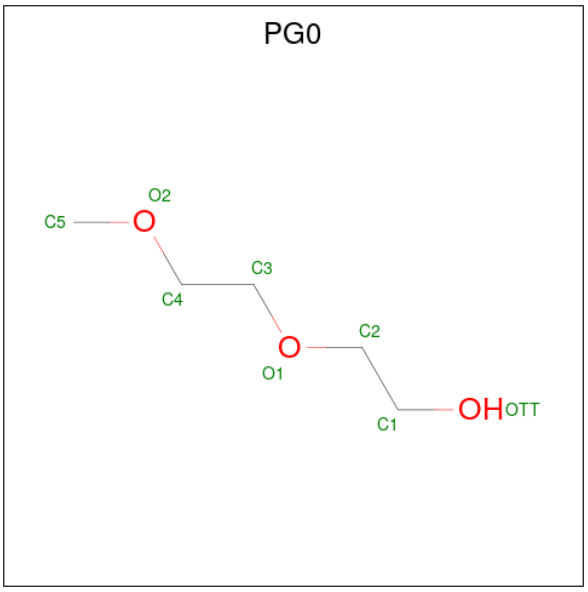
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 16 10 6	0	0
7	C	1	Total C O 16 10 6	0	0

- Molecule 8 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 8 5 3	0	0

- Molecule 9 is water.

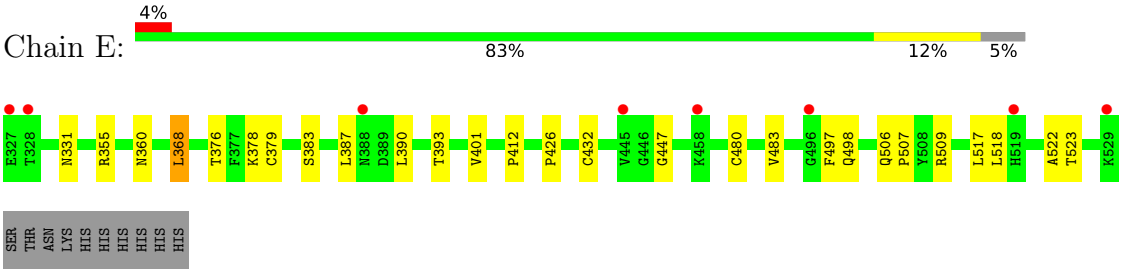
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	6	Total O 6 6	0	0
9	H	9	Total O 9 9	0	0
9	L	9	Total O 9 9	0	0
9	A	4	Total O 4 4	0	0
9	B	10	Total O 10 10	0	0
9	C	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

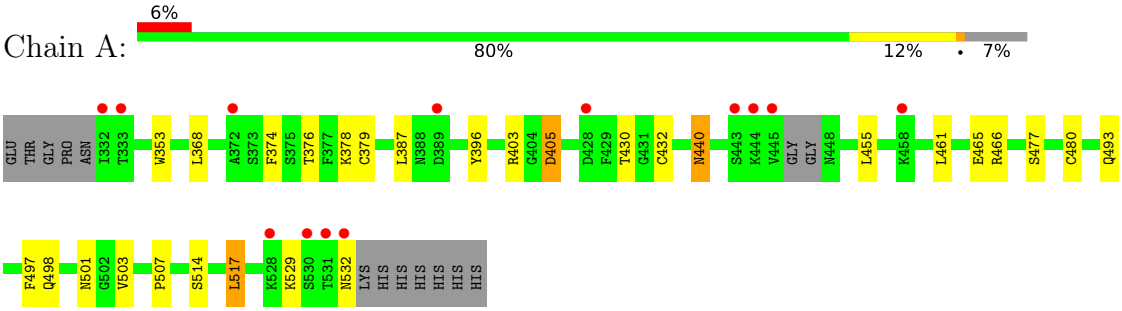
• Molecule 1: Spike glycoprotein

Chain E:



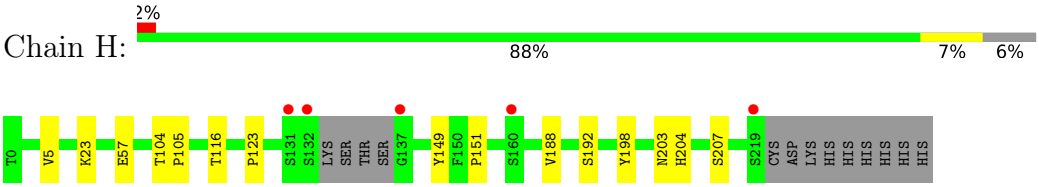
• Molecule 1: Spike glycoprotein

Chain A:



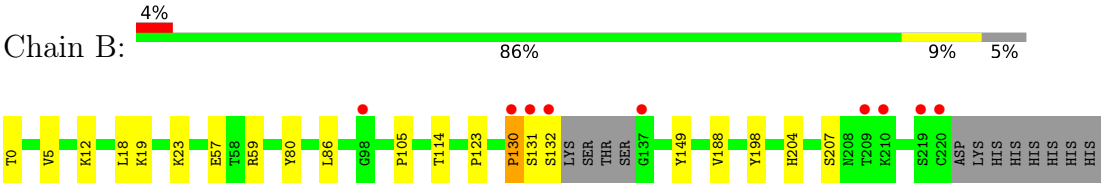
• Molecule 2: Heavy Chain

Chain H:



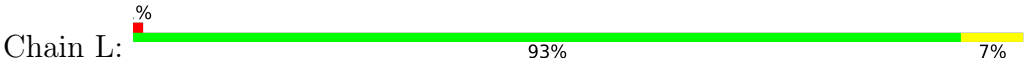
• Molecule 2: Heavy Chain

Chain B:



• Molecule 3: Light chain

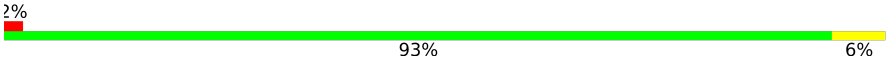
Chain L:

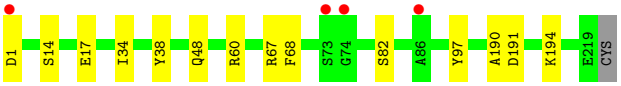




• Molecule 3: Light chain

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.12Å 163.12Å 189.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.31 – 2.42 55.31 – 2.42	Depositor EDS
% Data completeness (in resolution range)	96.8 (55.31-2.42) 92.9 (55.31-2.42)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.68 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.213 , 0.237 0.216 , 0.242	Depositor DCC
R_{free} test set	4986 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	73.6	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10090	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MLI, 1PE, PG0, DMS, NAG

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	0.12	0/1625	0.31	0/2210
1	E	0.09	0/1649	0.29	0/2244
2	B	0.10	0/1660	0.31	0/2261
2	H	0.08	0/1654	0.28	0/2253
3	C	0.09	0/1741	0.30	0/2367
3	L	0.09	0/1741	0.30	0/2367
All	All	0.10	0/10070	0.30	0/13702

There are no bond length outliers.

There are no bond angle outliers.

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	1582	0	1507	13	0
1	E	1604	0	1524	13	0
2	B	1615	0	1590	12	0
2	H	1609	0	1585	8	0
3	C	1703	0	1649	9	0
3	L	1703	0	1649	12	0
4	A	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	6	0	0
4	C	8	0	12	0	0
4	E	16	0	24	1	0
4	H	8	0	12	0	0
4	L	8	0	12	0	0
5	B	28	0	8	1	0
5	C	21	0	6	0	0
5	E	14	0	4	0	0
5	H	21	0	6	0	0
6	A	14	0	13	0	0
6	E	28	0	26	0	0
7	C	16	0	22	0	0
7	L	16	0	22	4	0
8	A	8	0	12	0	0
9	A	4	0	0	0	0
9	B	10	0	0	0	0
9	C	14	0	0	0	0
9	E	6	0	0	0	0
9	H	9	0	0	0	0
9	L	9	0	0	0	0
All	All	10090	0	9707	56	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 3.

All (56) 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:A:455:LEU:HD11	1:A:493:GLN:HG3	1.64	0.79
3:L:47:GLY:H	7:L:1603:1PE:H221	1.52	0.74
1:E:378:LYS:NZ	2:H:57:GLU:OE2	2.24	0.70
1:A:378:LYS:NZ	2:B:57:GLU:OE2	2.27	0.67
2:B:123:PRO:HB3	2:B:149:TYR:HB3	1.82	0.61
1:A:403:ARG:NH1	1:A:405:ASP:OD2	2.33	0.61
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.82	0.61
3:L:46:PRO:HA	7:L:1603:1PE:H232	1.85	0.58
2:B:204:HIS:ND1	2:B:207:SER:OG	2.38	0.55
1:E:383:SER:OG	2:H:104:THR:OG1	2.21	0.53
1:A:430:THR:HG21	3:C:34:ILE:HG12	1.91	0.52
3:L:48:GLN:HE21	2:B:23:LYS:HE2	1.74	0.52
3:L:190:ALA:O	3:L:194:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:ARG:HB3	4:E:904:DMS:H13	1.92	0.51
2:H:23:LYS:HE2	3:C:48:GLN:HE21	1.77	0.50
1:A:440:ASN:OD1	1:A:440:ASN:N	2.42	0.49
3:C:34:ILE:HD11	3:C:38:TYR:OH	2.13	0.48
1:E:517:LEU:HB2	3:L:34:ILE:HG22	1.96	0.47
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.49	0.47
2:B:105:PRO:HG3	3:C:97:TYR:CZ	2.50	0.47
3:L:67:ARG:HB2	3:L:82:SER:O	2.15	0.47
3:L:91:VAL:HG21	7:L:1603:1PE:H241	1.97	0.47
2:H:116:THR:HG21	2:H:151:PRO:HG3	1.96	0.47
1:A:379:CYS:HA	1:A:432:CYS:HA	1.97	0.46
3:L:34:ILE:O	3:L:36:LYS:N	2.48	0.46
3:C:190:ALA:O	3:C:194:LYS:HG3	2.15	0.46
3:L:56:TRP:CD1	3:L:97:TYR:HH	2.33	0.46
2:B:114:THR:OG1	5:B:304:MLI:O7	2.22	0.45
1:A:498:GLN:H	1:A:501:ASN:ND2	2.14	0.44
1:E:379:CYS:HA	1:E:432:CYS:HA	2.00	0.44
1:A:396:TYR:HB2	1:A:514:SER:OG	2.18	0.43
2:H:105:PRO:HG3	3:L:97:TYR:CZ	2.54	0.43
3:L:47:GLY:N	7:L:1603:1PE:H221	2.28	0.43
2:H:204:HIS:ND1	2:H:207:SER:OG	2.44	0.43
1:A:461:LEU:HD22	1:A:465:GLU:HB3	2.00	0.43
1:E:497:PHE:CE2	1:E:507:PRO:HB3	2.54	0.43
1:A:374:PHE:CE1	4:A:901:DMS:H23	2.54	0.43
3:C:14:SER:HB2	3:C:17:GLU:HG3	2.00	0.42
1:E:393:THR:HA	1:E:522:ALA:HA	2.02	0.42
2:B:19:LYS:HE3	2:B:80:TYR:CD1	2.54	0.42
2:B:130:PRO:O	2:B:131[A]:SER:OG	2.30	0.42
3:C:60:ARG:NH1	3:C:68:PHE:O	2.52	0.42
1:E:447:GLY:HA2	1:E:498:GLN:HG2	2.00	0.42
1:A:353:TRP:O	1:A:466:ARG:NH2	2.53	0.42
1:A:517:LEU:N	3:C:34:ILE:HG22	2.34	0.41
2:B:18:LEU:HB2	2:B:86:LEU:HD11	2.03	0.41
1:E:393:THR:HG21	1:E:518:LEU:H	1.85	0.41
3:L:51:LYS:NZ	2:B:0:THR:O	2.50	0.41
2:B:131[A]:SER:HB2	2:B:132:SER:H	1.69	0.41
2:B:188:VAL:HG11	2:B:198:TYR:CE1	2.55	0.41
1:E:360:ASN:H	1:E:523:THR:HB	1.86	0.40
1:E:401:VAL:HG22	1:E:509:ARG:HG2	2.03	0.40
1:E:368:LEU:HD12	1:E:368:LEU:HA	1.89	0.40
1:E:412:PRO:HB3	1:E:426:PRO:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:188:VAL:HG11	2:H:198:TYR:CE1	2.56	0.40
3:C:67:ARG:HB2	3:C:82:SER:O	2.22	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	195/213 (92%)	179 (92%)	16 (8%)	0	100	100
1	E	201/213 (94%)	190 (94%)	11 (6%)	0	100	100
2	B	214/229 (93%)	204 (95%)	9 (4%)	1 (0%)	24	35
2	H	213/229 (93%)	208 (98%)	5 (2%)	0	100	100
3	C	217/220 (99%)	207 (95%)	10 (5%)	0	100	100
3	L	217/220 (99%)	208 (96%)	8 (4%)	1 (0%)	24	35
All	All	1257/1324 (95%)	1196 (95%)	59 (5%)	2 (0%)	43	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	130	PRO
3	L	35	ASN

5.3.2 Protein sidechains (i)

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	174/185 (94%)	163 (94%)	11 (6%)	16	27
1	E	175/185 (95%)	167 (95%)	8 (5%)	24	39
2	B	183/194 (94%)	180 (98%)	3 (2%)	55	74
2	H	182/194 (94%)	179 (98%)	3 (2%)	55	74
3	C	194/195 (100%)	192 (99%)	2 (1%)	68	82
3	L	194/195 (100%)	193 (100%)	1 (0%)	81	90
All	All	1102/1148 (96%)	1074 (98%)	28 (2%)	42	62

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	331	ASN
1	E	368	LEU
1	E	376	THR
1	E	387	LEU
1	E	390	LEU
1	E	480	CYS
1	E	483	VAL
1	E	506	GLN
2	H	5	VAL
2	H	192	SER
2	H	203	ASN
3	L	1	ASP
1	A	368	LEU
1	A	376	THR
1	A	387	LEU
1	A	405	ASP
1	A	440	ASN
1	A	477	SER
1	A	480	CYS
1	A	503	VAL
1	A	517	LEU
1	A	529	LYS
1	A	532	ASN
2	B	5	VAL
2	B	12	LYS
2	B	59	ARG
3	C	1	ASP
3	C	191	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	E	487	ASN
3	L	35	ASN
3	L	37	ASN
3	L	195	HIS
1	A	388	ASN
1	A	450	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)

32 ligands 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	$\#\|Z\| > 2$
6	NAG	E	906	1	14,14,15	0.31	0	17,19,21	0.62	0
5	MLI	H	305	-	6,6,6	1.33	0	7,7,7	1.27	0
4	DMS	C	303	-	3,3,3	0.67	0	3,3,3	0.65	0
5	MLI	B	304	-	6,6,6	1.41	0	7,7,7	1.33	0
4	DMS	E	905	-	3,3,3	0.67	0	3,3,3	0.48	0
5	MLI	C	305	-	6,6,6	1.42	0	7,7,7	1.32	0
4	DMS	E	904	-	3,3,3	0.66	0	3,3,3	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DMS	C	302	-	3,3,3	0.66	0	3,3,3	0.54	0
4	DMS	H	303	-	3,3,3	0.67	0	3,3,3	0.54	0
5	MLI	H	304	-	6,6,6	1.34	0	7,7,7	1.25	0
5	MLI	B	302	-	6,6,6	1.40	0	7,7,7	1.21	0
5	MLI	H	301	-	6,6,6	1.33	0	7,7,7	1.29	0
4	DMS	A	901	-	3,3,3	0.66	0	3,3,3	0.50	0
4	DMS	E	902	-	3,3,3	0.67	0	3,3,3	0.54	0
5	MLI	B	303	-	6,6,6	1.35	0	7,7,7	1.26	0
6	NAG	E	907	1	14,14,15	0.36	0	17,19,21	0.40	0
8	PG0	A	902	-	7,7,7	0.50	0	6,6,6	0.24	0
5	MLI	B	301	-	6,6,6	1.39	0	7,7,7	1.33	1 (14%)
6	NAG	A	904	1	14,14,15	0.79	1 (7%)	17,19,21	0.63	0
5	MLI	C	304	-	6,6,6	1.38	0	7,7,7	1.20	0
5	MLI	C	306	-	6,6,6	1.35	0	7,7,7	1.23	0
4	DMS	E	901	-	3,3,3	0.66	0	3,3,3	0.51	0
4	DMS	B	305	-	3,3,3	0.67	0	3,3,3	0.54	0
7	1PE	C	301	-	15,15,15	0.55	0	14,14,14	0.27	0
5	MLI	E	903	-	6,6,6	1.43	0	7,7,7	1.39	1 (14%)
4	DMS	L	1601	-	3,3,3	0.66	0	3,3,3	0.84	0
4	DMS	A	905	-	3,3,3	0.67	0	3,3,3	1.15	0
4	DMS	L	1602	-	3,3,3	0.65	0	3,3,3	0.49	0
7	1PE	L	1603	-	15,15,15	0.55	0	14,14,14	0.24	0
4	DMS	H	302	-	3,3,3	0.66	0	3,3,3	0.51	0
4	DMS	A	903	-	3,3,3	0.67	0	3,3,3	0.53	0
5	MLI	E	908	-	6,6,6	1.39	0	7,7,7	1.43	1 (14%)

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
8	PG0	A	902	-	-	3/5/5/5	-
5	MLI	B	301	-	-	2/4/4/4	-
6	NAG	E	906	1	-	3/6/23/26	0/1/1/1
6	NAG	A	904	1	-	2/6/23/26	0/1/1/1
5	MLI	C	305	-	-	4/4/4/4	-
5	MLI	H	305	-	-	0/4/4/4	-
5	MLI	H	304	-	-	0/4/4/4	-
5	MLI	B	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLI	C	304	-	-	2/4/4/4	-
5	MLI	C	306	-	-	2/4/4/4	-
5	MLI	B	304	-	-	2/4/4/4	-
7	1PE	C	301	-	-	5/13/13/13	-
5	MLI	E	903	-	-	0/4/4/4	-
7	1PE	L	1603	-	-	7/13/13/13	-
5	MLI	H	301	-	-	2/4/4/4	-
5	MLI	E	908	-	-	2/4/4/4	-
5	MLI	B	303	-	-	2/4/4/4	-
6	NAG	E	907	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	904	NAG	C1-C2	2.73	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	903	MLI	O7-C2-C1	2.25	121.48	114.51
5	E	908	MLI	O9-C3-C1	2.08	120.95	114.51
5	B	301	MLI	O9-C3-C1	2.01	120.74	114.51

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	906	NAG	C8-C7-N2-C2
6	E	906	NAG	O7-C7-N2-C2
6	E	907	NAG	C8-C7-N2-C2
6	E	907	NAG	O7-C7-N2-C2
6	A	904	NAG	C8-C7-N2-C2
6	A	904	NAG	O7-C7-N2-C2
7	C	301	1PE	OH6-C15-C25-OH5
7	L	1603	1PE	OH5-C14-C24-OH4
7	C	301	1PE	OH5-C14-C24-OH4
7	C	301	1PE	OH4-C13-C23-OH3
7	C	301	1PE	OH7-C16-C26-OH6
6	E	906	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	301	MLI	C3-C1-C2-O7
5	B	302	MLI	C2-C1-C3-O9
5	B	301	MLI	C3-C1-C2-O6
7	L	1603	1PE	OH2-C12-C22-OH3
5	E	908	MLI	C3-C1-C2-O6
5	B	302	MLI	C2-C1-C3-O8
7	L	1603	1PE	C14-C24-OH4-C13
7	L	1603	1PE	C25-C15-OH6-C26
7	L	1603	1PE	OH4-C13-C23-OH3
7	C	301	1PE	C16-C26-OH6-C15
5	E	908	MLI	C3-C1-C2-O7
5	H	301	MLI	C2-C1-C3-O8
5	H	301	MLI	C2-C1-C3-O9
5	B	303	MLI	C3-C1-C2-O6
5	C	306	MLI	C2-C1-C3-O8
5	C	306	MLI	C2-C1-C3-O9
5	B	303	MLI	C3-C1-C2-O7
5	B	304	MLI	C2-C1-C3-O8
5	B	304	MLI	C2-C1-C3-O9
5	C	305	MLI	C2-C1-C3-O8
7	L	1603	1PE	C23-C13-OH4-C24
5	C	304	MLI	C2-C1-C3-O8
5	C	305	MLI	C2-C1-C3-O9
8	A	902	PG0	OTT-C1-C2-O1
5	C	305	MLI	C3-C1-C2-O6
8	A	902	PG0	C1-C2-O1-C3
8	A	902	PG0	O1-C3-C4-O2
7	L	1603	1PE	C24-C14-OH5-C25
5	C	304	MLI	C2-C1-C3-O9
5	C	305	MLI	C3-C1-C2-O7

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	MLI	1	0
4	E	904	DMS	1	0
4	A	901	DMS	1	0
7	L	1603	1PE	4	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	199/213 (93%)	0.57	13 (6%)	25	21	70, 90, 129, 153	0
1	E	203/213 (95%)	0.34	8 (3%)	43	39	60, 81, 120, 168	0
2	B	217/229 (94%)	0.38	9 (4%)	41	37	55, 89, 140, 179	1 (0%)
2	H	216/229 (94%)	0.18	5 (2%)	61	57	56, 84, 135, 170	1 (0%)
3	C	219/220 (99%)	0.20	4 (1%)	67	64	57, 86, 125, 144	0
3	L	219/220 (99%)	0.12	2 (0%)	81	79	58, 83, 109, 124	0
All	All	1273/1324 (96%)	0.29	41 (3%)	50	47	55, 86, 128, 179	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	137	GLY	6.1
3	C	73	SER	4.6
2	B	220	CYS	4.2
1	E	445	VAL	4.2
2	B	131[A]	SER	3.6
1	E	529	LYS	3.5
2	B	132	SER	3.4
1	A	445	VAL	3.4
2	H	131[A]	SER	3.4
2	H	132	SER	3.3
1	A	332	ILE	3.2
1	E	458	LYS	3.0
1	A	532	ASN	2.9
1	A	333	THR	2.9
2	H	219	SER	2.8
2	H	137	GLY	2.7
3	C	86	ALA	2.6
1	A	458	LYS	2.6
1	A	530	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	327	GLU	2.5
1	A	531	THR	2.5
1	A	389	ASP	2.5
1	E	388	ASN	2.4
1	A	444	LYS	2.3
1	A	528	LYS	2.3
1	E	328	THR	2.3
1	A	372	ALA	2.2
1	A	428	ASP	2.2
3	L	148	ARG	2.1
3	C	1	ASP	2.1
1	E	496	GLY	2.1
1	E	519	HIS	2.1
1	A	443	SER	2.1
2	B	209	THR	2.1
3	L	32	SER	2.1
2	B	130	PRO	2.1
3	C	74	GLY	2.0
2	B	210	LYS	2.0
2	H	160	SER	2.0
2	B	98	GLY	2.0
2	B	219	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	C	303	4/4	0.55	0.52	149,149,150,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	H	302	4/4	0.62	0.36	144,147,149,154	0
5	MLI	B	303	7/7	0.68	0.20	135,136,137,140	0
5	MLI	B	304	7/7	0.70	0.23	116,123,137,137	0
5	MLI	H	304	7/7	0.72	0.16	126,130,132,133	0
4	DMS	E	905	4/4	0.74	0.29	129,130,131,132	0
5	MLI	B	302	7/7	0.75	0.20	120,123,134,134	0
8	PG0	A	902	8/8	0.75	0.27	93,96,104,105	0
4	DMS	H	303	4/4	0.78	0.31	123,124,124,125	0
6	NAG	E	906	14/15	0.78	0.19	82,90,102,107	0
4	DMS	L	1602	4/4	0.78	0.38	160,163,164,175	0
6	NAG	E	907	14/15	0.79	0.17	80,99,120,127	0
5	MLI	H	305	7/7	0.79	0.19	134,136,139,139	0
5	MLI	E	903	7/7	0.81	0.18	132,133,134,135	0
6	NAG	A	904	14/15	0.81	0.15	72,97,109,117	0
5	MLI	E	908	7/7	0.81	0.15	97,101,109,109	0
4	DMS	A	903	4/4	0.82	0.34	142,146,146,147	0
4	DMS	L	1601	4/4	0.83	0.30	137,138,139,147	0
4	DMS	B	305	4/4	0.83	0.39	136,137,139,139	0
4	DMS	C	302	4/4	0.85	0.30	136,136,138,138	0
5	MLI	C	306	7/7	0.85	0.18	115,118,138,139	0
5	MLI	H	301	7/7	0.85	0.14	125,126,127,127	0
4	DMS	E	904	4/4	0.88	0.27	141,142,143,144	0
5	MLI	C	305	7/7	0.89	0.14	131,135,136,137	0
4	DMS	A	901	4/4	0.89	0.24	101,102,107,113	0
4	DMS	E	902	4/4	0.90	0.26	125,129,129,130	0
4	DMS	A	905	4/4	0.90	0.30	148,149,151,160	0
7	1PE	L	1603	16/16	0.90	0.20	81,91,108,109	0
5	MLI	B	301	7/7	0.90	0.10	107,109,113,113	0
7	1PE	C	301	16/16	0.91	0.15	84,90,95,96	0
5	MLI	C	304	7/7	0.91	0.17	123,124,128,129	0
4	DMS	E	901	4/4	0.94	0.16	95,95,98,98	0

6.5 Other polymers (i)

There are no such residues in this entry.