



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:05 AM UTC

PDB ID : 3K8K / pdb_00003k8k
Title : Crystal structure of SusG
Authors : Koropatkin, N.M.; Smith, T.J.
Deposited on : 2009-10-14
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

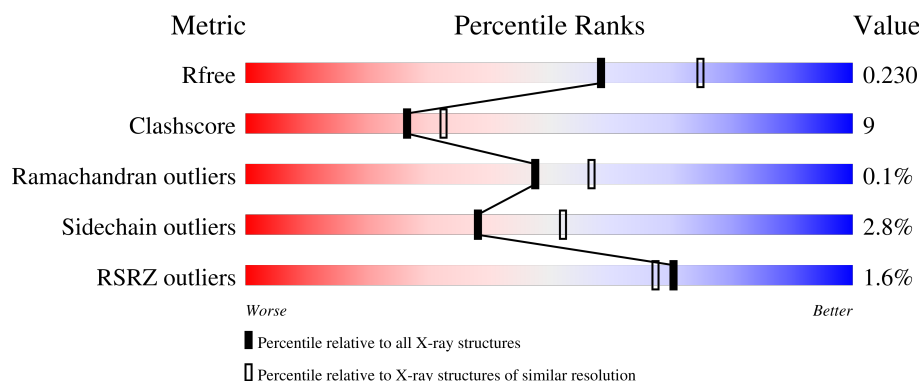
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	669	
1	B	669	

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
5	PEG	A	951	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10894 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 Alpha-amylase, susG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	Se	0	0	0
			5178	3293	837	1032	5	11			
1	B	649	Total	C	N	O	S	Se	0	0	0
			5169	3288	835	1030	5	11			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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

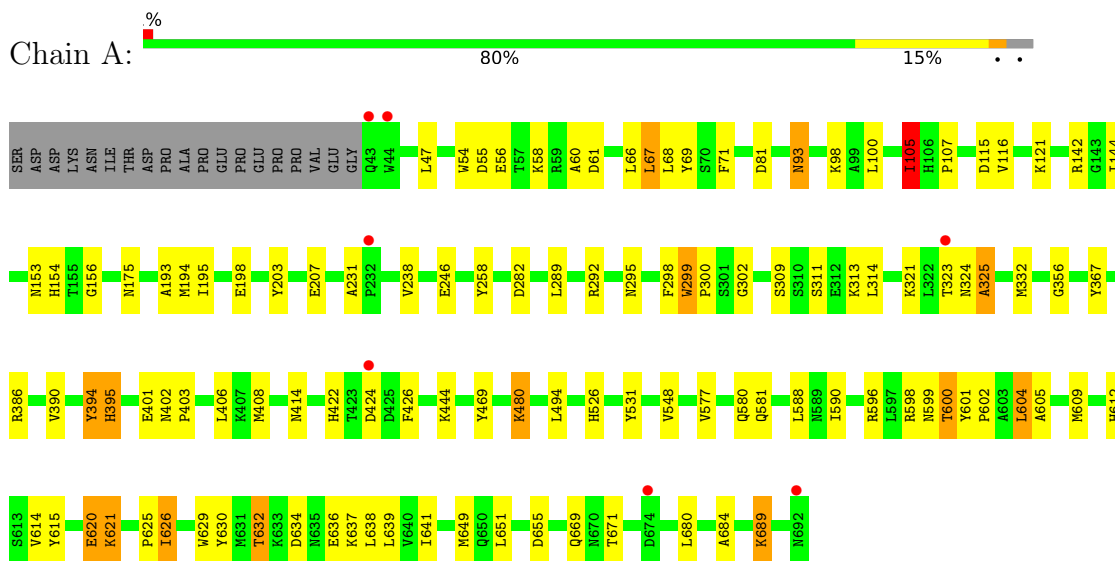
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	335	Total	O	0	0
			335	335		
7	B	129	Total	O	0	0
			129	129		

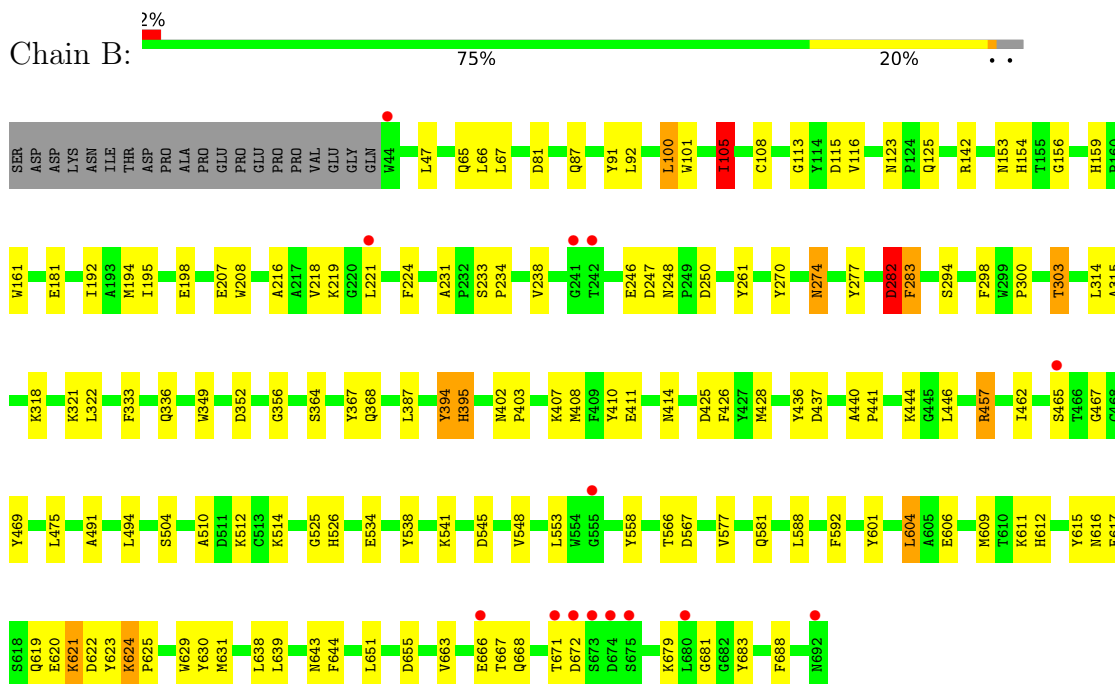
3 Residue-property plots [i](#)

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: Alpha-amylase, susG



- Molecule 1: Alpha-amylase, susG



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	128.04Å 128.04Å 129.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.2 (50.00-2.20) 89.2 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.230 0.197 , 0.230	Depositor DCC
R_{free} test set	9556 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.006 for -h,l,k 0.006 for l,-k,h 0.018 for -l,-k,-h 0.030 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10894	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: PEG, EDO, MG, ACT, CA

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	0.44	0/5306	0.89	19/7193 (0.3%)
1	B	0.39	0/5297	0.85	14/7181 (0.2%)
All	All	0.41	0/10603	0.87	33/14374 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	LEU	N-CA-C	-8.09	102.14	108.78
1	A	626	ILE	N-CA-C	6.82	117.89	108.89
1	B	116	VAL	N-CA-C	6.20	117.58	109.58
1	A	105	ILE	N-CA-C	6.19	118.05	112.17
1	B	394	TYR	N-CA-C	-6.06	100.63	110.20
1	A	116	VAL	N-CA-C	6.00	118.26	109.63
1	B	395	HIS	N-CA-C	5.93	118.23	111.11
1	B	525	GLY	N-CA-C	5.89	119.23	111.52
1	A	156	GLY	N-CA-C	-5.85	105.05	112.54
1	A	282	ASP	N-CA-C	-5.82	98.43	108.56
1	A	246	GLU	N-CA-C	-5.79	102.74	110.55
1	A	395	HIS	N-CA-C	5.56	118.06	111.33
1	B	349	TRP	N-CA-C	-5.56	106.50	113.28
1	A	386	ARG	N-CA-C	-5.51	99.75	108.73
1	A	107	PRO	N-CA-C	-5.50	102.57	111.14
1	A	548	VAL	N-CA-C	-5.48	106.96	112.17
1	B	156	GLY	N-CA-C	-5.46	105.09	112.14
1	A	494	LEU	N-CA-C	-5.45	99.19	110.80
1	B	105	ILE	N-CA-C	5.36	117.26	112.17
1	A	325	ALA	N-CA-C	5.29	117.91	110.23
1	A	401	GLU	N-CA-C	5.28	117.47	111.02
1	A	299	TRP	CA-C-N	5.28	125.04	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	TRP	C-N-CA	5.28	125.04	119.76
1	A	394	TYR	N-CA-C	-5.20	101.49	109.76
1	A	689	LYS	N-CA-C	-5.18	100.85	109.46
1	B	123	ASN	CA-C-N	5.16	124.96	119.28
1	B	123	ASN	C-N-CA	5.16	124.96	119.28
1	B	548	VAL	N-CA-C	-5.12	107.76	112.83
1	B	601	TYR	N-CA-C	5.12	116.81	109.04
1	A	634	ASP	CB-CA-C	-5.10	110.29	117.23
1	B	282	ASP	N-CA-C	-5.05	102.04	109.62
1	B	283	PHE	N-CA-C	5.03	117.64	110.24
1	A	121	LYS	N-CA-C	5.02	117.50	109.81

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	5178	0	4878	85	0
1	B	5169	0	4870	103	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	36	0	45	5	0
4	B	16	0	20	1	0
5	A	7	0	10	2	0
6	A	16	0	12	0	0
6	B	4	0	3	0	0
7	A	335	0	0	6	0
7	B	129	0	0	3	0
All	All	10894	0	9838	189	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 9.

All (189) 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:394:TYR:H	1:A:402:ASN:HD21	1.06	0.96
1:B:394:TYR:H	1:B:402:ASN:HD21	1.11	0.96
1:B:159:HIS:HD2	1:B:161:TRP:H	1.14	0.95
1:B:609:MSE:HB2	1:B:631:MSE:HE1	1.49	0.95
1:B:153:ASN:HD22	1:B:154:HIS:HD2	1.15	0.92
1:A:313:LYS:HE2	1:A:332:MSE:HE3	1.54	0.86
1:A:612:HIS:HD2	1:A:615:TYR:H	1.24	0.85
1:B:663:VAL:HG23	1:B:667:THR:HG21	1.60	0.83
1:A:422:HIS:NE2	4:A:910:EDO:H21	1.93	0.83
1:A:153:ASN:HD22	1:A:154:HIS:HD2	1.24	0.81
1:A:238:VAL:HG21	1:A:314:LEU:HD21	1.63	0.81
1:A:194:MSE:HE1	1:A:356:GLY:O	1.85	0.76
1:B:612:HIS:HD2	1:B:615:TYR:H	1.30	0.76
1:B:238:VAL:HG21	1:B:314:LEU:HD21	1.67	0.75
1:B:153:ASN:HD22	1:B:154:HIS:CD2	2.03	0.74
1:A:626:ILE:HD11	1:A:649:MSE:HE3	1.70	0.73
1:A:302:GLY:HA2	1:A:324:ASN:HD21	1.54	0.73
1:B:194:MSE:HE1	1:B:356:GLY:O	1.89	0.72
1:B:414:ASN:ND2	1:B:426:PHE:H	1.88	0.71
1:B:604:LEU:HD13	1:B:638:LEU:HD12	1.72	0.70
1:B:629:TRP:CD1	1:B:631:MSE:HE3	2.27	0.70
1:A:632:THR:HG23	7:A:722:HOH:O	1.92	0.68
1:A:596:ARG:O	1:A:600:THR:HG23	1.94	0.68
1:B:465:SER:HA	1:B:644:PHE:O	1.93	0.68
1:A:198:GLU:OE1	1:A:395:HIS:HD2	1.77	0.67
1:B:195:ILE:HG12	1:B:395:HIS:HB2	1.75	0.67
1:B:609:MSE:CB	1:B:631:MSE:HE1	2.23	0.67
1:B:621:LYS:HA	1:B:621:LYS:HE2	1.77	0.66
1:B:238:VAL:CG2	1:B:314:LEU:HD21	2.25	0.65
1:A:480:LYS:HE3	7:A:725:HOH:O	1.97	0.63
1:A:639:LEU:HD11	1:A:641:ILE:HD11	1.80	0.63
1:A:632:THR:HG21	1:A:637:LYS:NZ	2.13	0.63
1:A:671:THR:HG22	1:A:671:THR:O	1.99	0.63
1:B:444:LYS:HE3	7:B:813:HOH:O	1.98	0.63
1:B:300:PRO:O	1:B:303:THR:HB	1.98	0.63
1:B:234:PRO:HG2	1:B:322:LEU:HB2	1.82	0.62
1:A:203:TYR:OH	4:A:904:EDO:H21	2.01	0.61
1:A:604:LEU:HD13	1:A:638:LEU:HD12	1.83	0.60
1:B:666:GLU:HB3	1:B:681:GLY:HA3	1.84	0.60
1:B:462:ILE:HG22	1:B:512:LYS:HE3	1.83	0.60
1:B:629:TRP:NE1	1:B:631:MSE:HE3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:HIS:CD2	1:B:161:TRP:H	2.06	0.59
1:A:612:HIS:CD2	1:A:615:TYR:H	2.15	0.58
1:A:100:LEU:HD13	1:A:144:ILE:HG21	1.84	0.58
1:A:596:ARG:HE	5:A:951:PEG:H21	1.67	0.58
1:B:142:ARG:HH11	1:B:142:ARG:HG3	1.69	0.58
1:A:620:GLU:OE2	1:A:621:LYS:HE2	2.04	0.58
1:A:58:LYS:O	1:A:98:LYS:HE3	2.03	0.58
1:A:469:TYR:OH	1:A:620:GLU:HG3	2.04	0.57
1:A:207:GLU:OE1	1:A:395:HIS:HE1	1.87	0.57
1:A:632:THR:HG21	1:A:637:LYS:HZ1	1.69	0.57
1:A:238:VAL:CG2	1:A:314:LEU:HD21	2.34	0.57
1:A:367:TYR:CZ	1:A:408:MSE:HE3	2.39	0.57
1:B:91:TYR:OH	1:B:534:GLU:OE1	2.22	0.57
1:B:504:SER:OG	1:B:538:TYR:HB2	2.04	0.57
1:A:60:ALA:H	1:A:599:ASN:HD22	1.51	0.56
1:A:444:LYS:HG2	7:A:822:HOH:O	2.04	0.56
1:A:47:LEU:HD22	1:A:669:GLN:HE21	1.70	0.56
1:B:541:LYS:HE3	1:B:545:ASP:OD1	2.06	0.56
1:A:67:LEU:HD22	1:A:531:TYR:HE2	1.71	0.55
1:A:612:HIS:CD2	1:A:614:VAL:H	2.23	0.55
1:A:100:LEU:HD13	1:A:144:ILE:CG2	2.37	0.55
1:A:302:GLY:CA	1:A:324:ASN:HD21	2.19	0.54
1:A:321:LYS:HD2	1:A:321:LYS:H	1.72	0.54
1:A:680:LEU:HD22	1:A:684:ALA:HB3	1.89	0.54
1:B:125:GLN:NE2	4:B:905:EDO:O2	2.41	0.54
4:A:911:EDO:O2	1:B:321:LYS:HE2	2.09	0.53
1:A:323:THR:HG22	1:A:325:ALA:H	1.73	0.53
1:B:92:LEU:HD13	1:B:100:LEU:HD11	1.89	0.53
1:B:663:VAL:HG21	1:B:667:THR:OG1	2.09	0.52
1:B:510:ALA:O	1:B:514:LYS:HG3	2.10	0.52
1:A:66:LEU:HD12	1:A:66:LEU:C	2.34	0.52
1:A:414:ASN:ND2	1:A:426:PHE:H	2.08	0.52
1:A:422:HIS:CE1	4:A:910:EDO:H21	2.45	0.52
1:B:66:LEU:C	1:B:66:LEU:HD12	2.34	0.52
1:A:47:LEU:HD22	1:A:669:GLN:NE2	2.25	0.52
1:B:153:ASN:ND2	1:B:154:HIS:HD2	1.96	0.51
1:A:402:ASN:HB2	1:A:403:PRO:HD3	1.93	0.51
1:B:577:VAL:O	1:B:581:GLN:HG3	2.11	0.51
1:A:612:HIS:HE1	1:A:655:ASP:OD2	1.94	0.51
1:B:440:ALA:HB3	1:B:441:PRO:HD3	1.93	0.50
1:A:67:LEU:HD22	1:A:531:TYR:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:TYR:H	1:B:402:ASN:ND2	1.94	0.50
1:B:364:SER:O	1:B:368:GLN:HG3	2.12	0.50
1:A:298:PHE:O	1:A:300:PRO:HD3	2.11	0.50
1:A:596:ARG:O	1:A:600:THR:CG2	2.60	0.50
1:B:616:ASN:HB2	1:B:617:GLU:OE1	2.12	0.50
1:A:612:HIS:HD2	1:A:615:TYR:N	2.03	0.49
1:B:387:LEU:HD11	1:B:428:MSE:HE3	1.94	0.49
1:A:636:GLU:HG3	1:A:689:LYS:NZ	2.27	0.49
1:B:410:TYR:HB2	1:B:428:MSE:HE2	1.94	0.49
1:A:67:LEU:HG	1:A:69:TYR:OH	2.13	0.49
1:B:315:ALA:HB3	1:B:318:LYS:HD2	1.93	0.49
1:B:609:MSE:HE2	1:B:629:TRP:CD2	2.48	0.49
1:A:142:ARG:HH11	1:A:142:ARG:HG3	1.78	0.49
1:A:195:ILE:HG12	1:A:395:HIS:HB2	1.95	0.48
1:B:553:LEU:O	1:B:577:VAL:HG23	2.13	0.48
1:B:87:GLN:NE2	1:B:558:TYR:OH	2.46	0.48
1:B:298:PHE:O	1:B:300:PRO:HD3	2.13	0.48
1:A:55:ASP:O	1:A:56:GLU:HB2	2.14	0.48
1:B:231:ALA:HA	1:B:233:SER:N	2.27	0.48
1:B:108:CYS:SG	1:B:113:GLY:HA2	2.53	0.48
4:A:910:EDO:H22	7:A:702:HOH:O	2.14	0.48
1:B:105:ILE:HG23	7:B:769:HOH:O	2.14	0.48
1:A:626:ILE:CD1	1:A:649:MSE:HE3	2.40	0.48
1:B:216:ALA:O	1:B:336:GLN:HG2	2.14	0.48
1:B:620:GLU:N	1:B:620:GLU:OE1	2.46	0.48
1:B:671:THR:HG22	1:B:671:THR:O	2.14	0.48
1:B:207:GLU:OE1	1:B:395:HIS:HE1	1.96	0.47
1:B:643:ASN:O	1:B:683:TYR:HA	2.14	0.47
1:B:101:TRP:C	1:B:101:TRP:CD1	2.93	0.47
1:A:625:PRO:HD2	1:A:649:MSE:HE1	1.95	0.47
1:B:294:SER:HB3	1:B:303:THR:HG21	1.97	0.47
1:B:231:ALA:HA	1:B:234:PRO:HD3	1.97	0.47
1:B:428:MSE:HE2	1:B:446:LEU:CD2	2.45	0.47
1:A:394:TYR:H	1:A:402:ASN:ND2	1.91	0.46
1:B:231:ALA:HA	1:B:233:SER:H	1.81	0.46
1:B:668:GLN:OE1	1:B:679:LYS:HD3	2.15	0.46
1:B:663:VAL:HG23	1:B:667:THR:CG2	2.40	0.46
1:B:142:ARG:HG3	1:B:142:ARG:NH1	2.30	0.46
1:B:624:LYS:HB2	1:B:624:LYS:NZ	2.30	0.46
1:A:193:ALA:C	1:A:194:MSE:HE2	2.41	0.46
1:A:54:TRP:CZ2	1:A:56:GLU:HA	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:TYR:CZ	1:B:408:MSE:HE3	2.51	0.45
1:B:491:ALA:HA	1:B:526:HIS:O	2.15	0.45
1:B:467:GLY:C	1:B:469:TYR:H	2.24	0.45
1:B:248:ASN:HA	1:B:270:TYR:OH	2.17	0.45
1:A:580:GLN:HG2	7:A:896:HOH:O	2.16	0.45
1:A:71:PHE:HB3	7:A:733:HOH:O	2.16	0.45
1:A:577:VAL:O	1:A:581:GLN:HG3	2.17	0.45
1:A:153:ASN:HD22	1:A:154:HIS:CD2	2.16	0.44
1:B:219:LYS:HA	1:B:283:PHE:O	2.17	0.44
1:A:596:ARG:NE	5:A:951:PEG:H11	2.32	0.44
1:B:261:TYR:C	1:B:261:TYR:CD1	2.95	0.44
1:B:402:ASN:HB2	1:B:403:PRO:HD3	1.99	0.44
1:B:619:GLN:HB3	1:B:623:TYR:HB2	1.99	0.44
1:A:323:THR:HG22	1:A:324:ASN:N	2.33	0.44
1:A:609:MSE:HA	1:A:630:TYR:O	2.18	0.44
1:B:198:GLU:OE1	1:B:395:HIS:HD2	1.99	0.44
1:A:198:GLU:OE1	1:A:395:HIS:CD2	2.64	0.43
1:B:609:MSE:HA	1:B:631:MSE:HE2	2.00	0.43
1:B:566:THR:HG22	1:B:567:ASP:N	2.33	0.43
1:B:457:ARG:HA	1:B:457:ARG:HD3	1.83	0.43
1:A:598:ARG:O	1:A:605:ALA:HB2	2.18	0.43
1:B:277:TYR:N	1:B:277:TYR:CD2	2.85	0.43
1:B:630:TYR:O	1:B:631:MSE:HE2	2.19	0.43
1:B:274:ASN:HD22	1:B:274:ASN:HA	1.54	0.43
1:B:414:ASN:HD21	1:B:425:ASP:HA	1.84	0.43
1:B:436:TYR:CG	1:B:437:ASP:N	2.87	0.43
1:A:54:TRP:CD1	1:A:600:THR:HG22	2.54	0.43
1:A:258:TYR:CE1	1:A:295:ASN:HB3	2.53	0.43
1:B:629:TRP:CD1	1:B:631:MSE:CE	2.99	0.43
1:A:54:TRP:CE2	1:A:56:GLU:HA	2.53	0.43
1:A:60:ALA:H	1:A:599:ASN:ND2	2.16	0.42
1:B:623:TYR:CE1	1:B:651:LEU:HD23	2.54	0.42
1:B:609:MSE:CB	1:B:631:MSE:CE	2.95	0.42
1:A:93:ASN:HD22	1:A:93:ASN:HA	1.64	0.42
1:B:588:LEU:HG	1:B:592:PHE:CE2	2.55	0.42
1:B:624:LYS:HB3	1:B:625:PRO:HD3	2.01	0.42
1:A:626:ILE:HD12	1:A:651:LEU:HD11	2.02	0.42
1:A:61:ASP:OD2	1:A:526:HIS:HD2	2.02	0.42
1:B:224:PHE:CD2	1:B:238:VAL:HG22	2.55	0.42
1:B:407:LYS:O	1:B:411:GLU:HG3	2.20	0.42
1:A:258:TYR:CZ	1:A:295:ASN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:VAL:HB	1:A:406:LEU:HD11	2.01	0.42
1:B:221:LEU:HD23	1:B:282:ASP:HA	2.01	0.42
1:A:302:GLY:HA2	1:A:324:ASN:ND2	2.28	0.42
1:B:192:ILE:HD13	1:B:208:TRP:CH2	2.55	0.42
1:A:292:ARG:HD2	1:A:299:TRP:CH2	2.55	0.42
1:A:601:TYR:HA	1:A:602:PRO:HD3	1.94	0.42
1:A:609:MSE:HE2	1:A:629:TRP:CD2	2.54	0.41
1:B:303:THR:CG2	7:B:796:HOH:O	2.67	0.41
1:A:289:LEU:C	1:A:289:LEU:HD12	2.44	0.41
1:B:639:LEU:HB3	1:B:688:PHE:HB2	2.01	0.41
1:B:671:THR:O	1:B:672:ASP:C	2.62	0.41
1:B:612:HIS:HE1	1:B:655:ASP:OD2	2.04	0.41
1:A:636:GLU:HG3	1:A:689:LYS:HZ1	1.84	0.41
1:B:192:ILE:HD13	1:B:208:TRP:HH2	1.85	0.41
1:B:250:ASP:OD1	1:B:250:ASP:C	2.63	0.41
1:A:68:LEU:HD11	1:A:105:ILE:HG22	2.03	0.41
1:A:580:GLN:NE2	1:A:588:LEU:H	2.19	0.41
1:B:475:LEU:CD1	1:B:611:LYS:HG3	2.51	0.41
1:B:609:MSE:HE2	1:B:629:TRP:CE2	2.56	0.41
1:B:47:LEU:HD12	1:B:667:THR:HB	2.02	0.41
1:B:65:GLN:HG3	1:B:101:TRP:CE3	2.56	0.41
1:B:247:ASP:O	1:B:248:ASN:C	2.63	0.41
1:B:218:VAL:HG21	1:B:333:PHE:CD2	2.56	0.40
1:A:309:SER:C	1:A:311:SER:H	2.30	0.40
1:B:428:MSE:CE	1:B:446:LEU:CD2	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	648/669 (97%)	625 (96%)	22 (3%)	1 (0%)	43	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	647/669 (97%)	605 (94%)	42 (6%)	0	100	100
All	All	1295/1338 (97%)	1230 (95%)	64 (5%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ALA

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	551/557 (99%)	537 (98%)	14 (2%)	42	56
1	B	550/557 (99%)	533 (97%)	17 (3%)	35	48
All	All	1101/1114 (99%)	1070 (97%)	31 (3%)	38	52

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	81	ASP
1	A	93	ASN
1	A	105	ILE
1	A	115	ASP
1	A	175	ASN
1	A	424	ASP
1	A	480	LYS
1	A	590	ILE
1	A	600	THR
1	A	604	LEU
1	A	620	GLU
1	A	621	LYS
1	A	632	THR
1	B	67	LEU

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Mol	Chain	Res	Type
1	B	81	ASP
1	B	100	LEU
1	B	105	ILE
1	B	115	ASP
1	B	181	GLU
1	B	246	GLU
1	B	274	ASN
1	B	282	ASP
1	B	303	THR
1	B	352	ASP
1	B	457	ARG
1	B	604	LEU
1	B	606	GLU
1	B	621	LYS
1	B	622	ASP
1	B	624	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	93	ASN
1	A	94	GLN
1	A	154	HIS
1	A	197	GLN
1	A	274	ASN
1	A	317	ASN
1	A	324	ASN
1	A	330	ASN
1	A	337	GLN
1	A	342	HIS
1	A	395	HIS
1	A	402	ASN
1	A	414	ASN
1	A	464	ASN
1	A	526	HIS
1	A	543	ASN
1	A	561	ASN
1	A	573	ASN
1	A	580	GLN
1	A	581	GLN
1	A	589	ASN

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Mol	Chain	Res	Type
1	A	599	ASN
1	A	612	HIS
1	A	668	GLN
1	A	669	GLN
1	B	65	GLN
1	B	87	GLN
1	B	94	GLN
1	B	125	GLN
1	B	154	HIS
1	B	159	HIS
1	B	197	GLN
1	B	274	ASN
1	B	395	HIS
1	B	402	ASN
1	B	414	ASN
1	B	422	HIS
1	B	561	ASN
1	B	589	ASN
1	B	612	HIS
1	B	650	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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	$\# Z > 2$
6	ACT	A	962	-	3,3,3	1.09	0	3,3,3	0.85	0
4	EDO	A	902	-	3,3,3	2.22	1 (33%)	2,2,2	0.32	0
4	EDO	B	907	-	3,3,3	2.27	1 (33%)	2,2,2	0.36	0
4	EDO	A	903	-	3,3,3	2.27	1 (33%)	2,2,2	0.34	0
4	EDO	B	912	-	3,3,3	2.26	1 (33%)	2,2,2	0.30	0
4	EDO	A	909	-	3,3,3	2.22	1 (33%)	2,2,2	0.32	0
4	EDO	A	910	-	3,3,3	2.25	1 (33%)	2,2,2	0.33	0
6	ACT	A	972	-	3,3,3	0.99	0	3,3,3	0.91	0
4	EDO	B	906	-	3,3,3	2.28	1 (33%)	2,2,2	0.37	0
4	EDO	A	904	-	3,3,3	2.27	1 (33%)	2,2,2	0.32	0
5	PEG	A	951	-	6,6,6	0.94	0	5,5,5	2.37	3 (60%)
4	EDO	A	901	-	3,3,3	2.30	1 (33%)	2,2,2	0.37	0
6	ACT	A	973	-	3,3,3	1.02	0	3,3,3	0.86	0
4	EDO	A	911	-	3,3,3	2.25	1 (33%)	2,2,2	0.39	0
4	EDO	B	905	-	3,3,3	2.26	1 (33%)	2,2,2	0.37	0
6	ACT	A	961	-	3,3,3	0.99	0	3,3,3	0.84	0
4	EDO	A	900	-	3,3,3	2.33	1 (33%)	2,2,2	0.37	0
4	EDO	A	908	-	3,3,3	2.25	1 (33%)	2,2,2	0.37	0
6	ACT	B	971	-	3,3,3	1.02	0	3,3,3	0.87	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	EDO	A	904	-	-	1/1/1/1	-
4	EDO	A	908	-	-	0/1/1/1	-
4	EDO	A	902	-	-	0/1/1/1	-
4	EDO	B	912	-	-	0/1/1/1	-
4	EDO	A	900	-	-	1/1/1/1	-
4	EDO	A	909	-	-	1/1/1/1	-
4	EDO	B	907	-	-	1/1/1/1	-
4	EDO	A	901	-	-	0/1/1/1	-
4	EDO	A	910	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	951	-	-	4/4/4/4	-
4	EDO	A	911	-	-	1/1/1/1	-
4	EDO	B	905	-	-	0/1/1/1	-
4	EDO	B	906	-	-	1/1/1/1	-
4	EDO	A	903	-	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	EDO	O1-C1	-3.88	1.22	1.42
4	A	901	EDO	O1-C1	-3.84	1.22	1.42
4	B	906	EDO	O1-C1	-3.79	1.22	1.42
4	A	911	EDO	O1-C1	-3.76	1.22	1.42
4	A	908	EDO	O1-C1	-3.76	1.22	1.42
4	A	904	EDO	O1-C1	-3.76	1.22	1.42
4	A	903	EDO	O1-C1	-3.75	1.23	1.42
4	B	905	EDO	O1-C1	-3.75	1.23	1.42
4	B	907	EDO	O1-C1	-3.75	1.23	1.42
4	B	912	EDO	O1-C1	-3.73	1.23	1.42
4	A	910	EDO	O1-C1	-3.71	1.23	1.42
4	A	902	EDO	O1-C1	-3.66	1.23	1.42
4	A	909	EDO	O1-C1	-3.66	1.23	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	951	PEG	C3-O2-C2	3.12	126.92	113.26
5	A	951	PEG	O2-C2-C1	2.86	122.73	110.11
5	A	951	PEG	O2-C3-C4	2.77	122.30	110.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	951	PEG	O2-C3-C4-O4
4	A	903	EDO	O1-C1-C2-O2
4	A	904	EDO	O1-C1-C2-O2
4	A	911	EDO	O1-C1-C2-O2
5	A	951	PEG	O1-C1-C2-O2
5	A	951	PEG	C1-C2-O2-C3
4	A	900	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	909	EDO	O1-C1-C2-O2
4	B	907	EDO	O1-C1-C2-O2
5	A	951	PEG	C4-C3-O2-C2
4	B	906	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	910	EDO	3	0
4	A	904	EDO	1	0
5	A	951	PEG	2	0
4	A	911	EDO	1	0
4	B	905	EDO	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	639/669 (95%)	-0.25	7 (1%) 78 76	22, 37, 52, 65	0
1	B	638/669 (95%)	0.40	14 (2%) 62 59	31, 48, 59, 66	0
All	All	1277/1338 (95%)	0.08	21 (1%) 70 67	22, 42, 57, 66	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	GLY	3.4
1	A	232	PRO	3.0
1	B	242	THR	3.0
1	B	675	SER	2.8
1	A	323	THR	2.8
1	B	680	LEU	2.8
1	B	666	GLU	2.7
1	B	674	ASP	2.6
1	B	44	TRP	2.5
1	B	555	GLY	2.4
1	A	692	ASN	2.3
1	A	674	ASP	2.3
1	B	672	ASP	2.2
1	A	43	GLN	2.2
1	A	44	TRP	2.2
1	B	221	LEU	2.1
1	B	465	SER	2.1
1	B	692	ASN	2.1
1	A	424	ASP	2.1
1	B	673	SER	2.0
1	B	671	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	A	972	4/4	0.65	0.21	55,55,57,58	0
4	EDO	A	902	4/4	0.73	0.15	54,55,56,57	0
4	EDO	A	910	4/4	0.75	0.23	61,61,61,62	0
4	EDO	A	909	4/4	0.83	0.15	55,58,58,58	0
4	EDO	B	905	4/4	0.84	0.18	58,58,58,60	0
4	EDO	B	907	4/4	0.86	0.14	60,60,61,61	0
5	PEG	A	951	7/7	0.87	0.14	49,50,54,58	0
4	EDO	A	904	4/4	0.87	0.16	48,51,52,52	0
4	EDO	B	912	4/4	0.88	0.14	57,57,59,59	0
6	ACT	A	962	4/4	0.89	0.16	50,52,53,55	0
4	EDO	A	911	4/4	0.89	0.13	59,60,60,64	0
4	EDO	A	908	4/4	0.90	0.16	47,52,53,56	0
6	ACT	A	961	4/4	0.91	0.16	53,54,55,57	0
6	ACT	A	973	4/4	0.92	0.11	59,62,63,64	0
6	ACT	B	971	4/4	0.93	0.13	53,55,55,56	0
4	EDO	B	906	4/4	0.94	0.11	50,50,52,52	0
4	EDO	A	900	4/4	0.94	0.10	43,46,48,50	0
4	EDO	A	903	4/4	0.94	0.08	46,48,49,49	0
4	EDO	A	901	4/4	0.98	0.07	42,43,44,45	0
2	MG	B	800	1/1	0.98	0.04	53,53,53,53	0
3	CA	A	710	1/1	0.99	0.02	31,31,31,31	0
3	CA	B	810	1/1	0.99	0.02	38,38,38,38	0
2	MG	A	700	1/1	0.99	0.03	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.