



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 02:21 AM UTC

PDB ID : 2Y5Y / pdb_00002y5y
Title : Crystal structure of LacY in complex with an affinity inactivator
Authors : Chaptal, V.; Kwon, S.; Sawaya, M.R.; Guan, L.; Kaback, H.R.; Abramson, J.
Deposited on : 2011-01-19
Resolution : 3.38 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

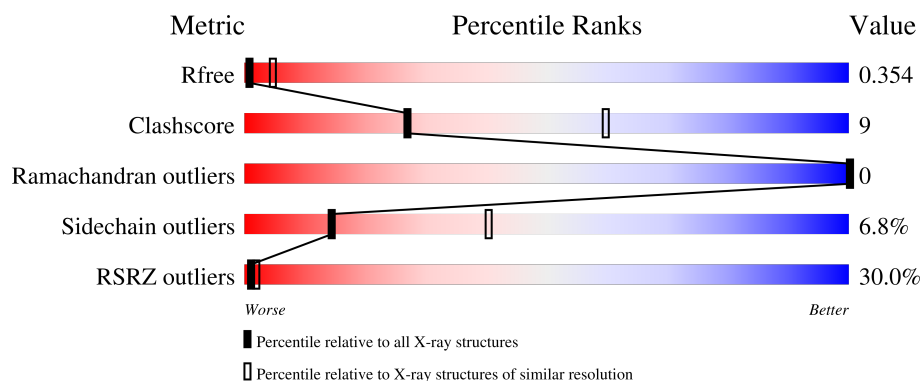
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	423	25% 67% 22% 9%
1	B	423	30% 69% 21% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6209 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 LACTOSE PERMEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3065	2086	466	498	15			
1	B	394	Total	C	N	O	S	0	0	0
			3112	2114	475	508	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	SER	CYS	engineered mutation	UNP P02920
A	122	CYS	ALA	engineered mutation	UNP P02920
A	148	ALA	CYS	engineered mutation	UNP P02920
A	154	VAL	CYS	engineered mutation	UNP P02920
A	176	MET	CYS	engineered mutation	UNP P02920
A	234	SER	CYS	engineered mutation	UNP P02920
A	333	SER	CYS	engineered mutation	UNP P02920
A	353	ALA	CYS	engineered mutation	UNP P02920
A	355	ALA	CYS	engineered mutation	UNP P02920
A	418	HIS	-	expression tag	UNP P02920
A	419	HIS	-	expression tag	UNP P02920
A	420	HIS	-	expression tag	UNP P02920
A	421	HIS	-	expression tag	UNP P02920
A	422	HIS	-	expression tag	UNP P02920
A	423	HIS	-	expression tag	UNP P02920
B	117	SER	CYS	engineered mutation	UNP P02920
B	122	CYS	ALA	engineered mutation	UNP P02920
B	148	ALA	CYS	engineered mutation	UNP P02920
B	154	VAL	CYS	engineered mutation	UNP P02920
B	176	MET	CYS	engineered mutation	UNP P02920
B	234	SER	CYS	engineered mutation	UNP P02920
B	333	SER	CYS	engineered mutation	UNP P02920
B	353	ALA	CYS	engineered mutation	UNP P02920
B	355	ALA	CYS	engineered mutation	UNP P02920
B	418	HIS	-	expression tag	UNP P02920

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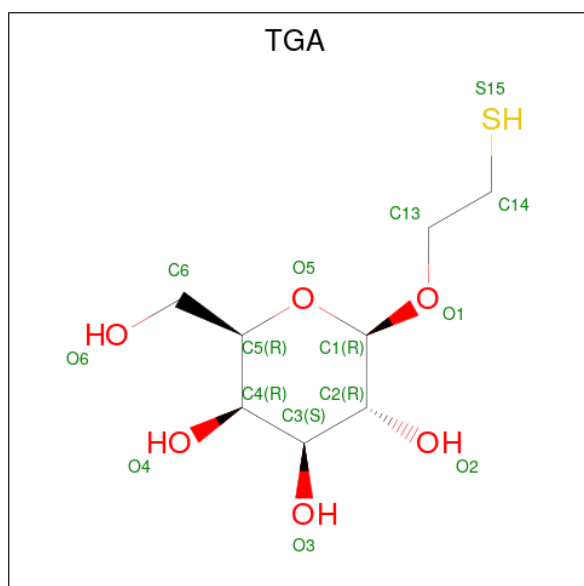
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Chain	Residue	Modelled	Actual	Comment	Reference
B	419	HIS	-	expression tag	UNP P02920
B	420	HIS	-	expression tag	UNP P02920
B	421	HIS	-	expression tag	UNP P02920
B	422	HIS	-	expression tag	UNP P02920
B	423	HIS	-	expression tag	UNP P02920

- Molecule 2 is BARIUM ION (CCD ID: BA) (formula: Ba).

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

- Molecule 3 is 2-sulfanylethyl beta-D-galactopyranoside (CCD ID: TGA) (formula: C₈H₁₆O₆S).

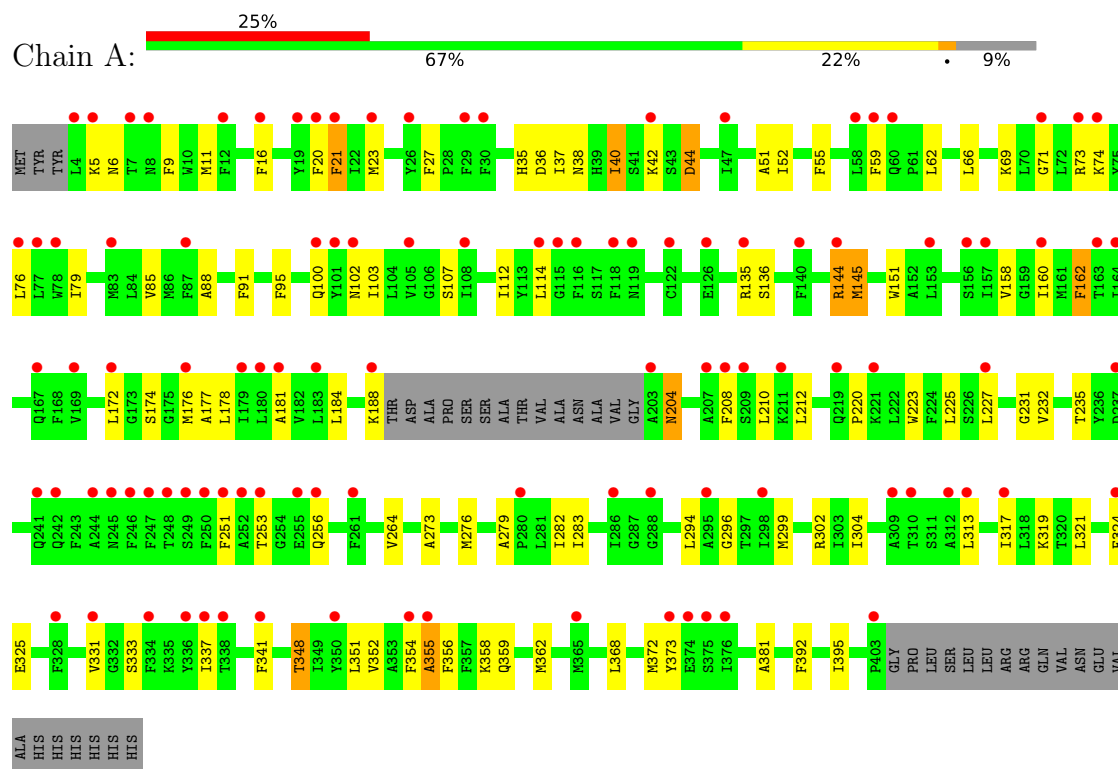


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 15 8 6 1	0	0
3	B	1	Total C O S 15 8 6 1	0	0

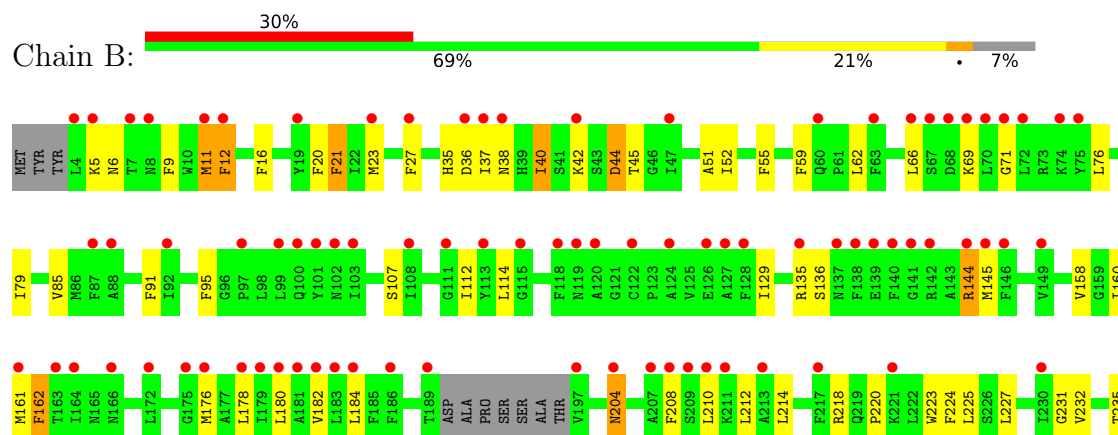
3 Residue-property plots [i](#)

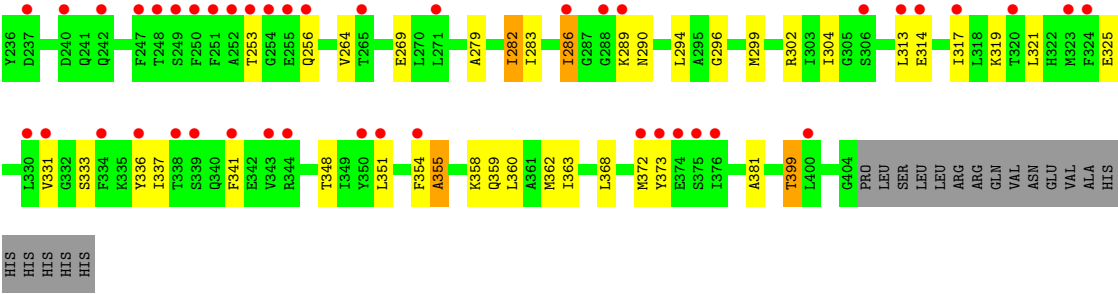
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LACTOSE PERMEASE



• Molecule 1: LACTOSE PERMEASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.56Å 127.84Å 189.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.28 – 3.38 28.28 – 3.38	Depositor EDS
% Data completeness (in resolution range)	(Not available) (28.28-3.38) 98.2 (28.28-3.38)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.286 , 0.303 0.349 , 0.354	Depositor DCC
R_{free} test set	1760 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	105.2	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 110.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6209	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: BA, TGA

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	0.74	0/3157	1.57	26/4273 (0.6%)
1	B	0.74	0/3204	1.56	22/4338 (0.5%)
All	All	0.74	0/6361	1.57	48/8611 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ILE	N-CA-C	12.86	122.44	110.74
1	B	232	VAL	N-CA-C	10.39	120.20	110.74
1	A	232	VAL	N-CA-C	10.25	120.07	110.74
1	B	135	ARG	CB-CA-C	10.08	127.99	110.85
1	A	36	ASP	CB-CA-C	9.63	125.79	110.96
1	A	135	ARG	CB-CA-C	9.36	126.76	110.85
1	B	36	ASP	CB-CA-C	8.16	123.69	110.88
1	B	107	SER	N-CA-C	7.62	119.58	111.28
1	B	355	ALA	N-CA-C	7.48	122.54	113.41
1	B	136	SER	N-CA-C	7.30	121.49	109.96
1	A	325	GLU	N-CA-C	7.13	118.84	111.14
1	B	11	MET	CB-CA-C	7.11	122.05	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	SER	N-CA-C	7.00	118.92	111.28
1	A	145	MET	CB-CA-C	6.97	123.53	110.63
1	A	103	ILE	N-CA-CB	6.77	120.41	112.35
1	A	136	SER	N-CA-C	6.76	120.64	109.96
1	B	136	SER	N-CA-CB	-6.64	98.72	110.14
1	A	324	PHE	CB-CA-C	6.50	122.60	110.70
1	B	354	PHE	CB-CA-C	6.39	121.04	110.81
1	B	162	PHE	N-CA-C	6.31	118.68	111.11
1	A	356	PHE	N-CA-C	6.28	119.07	111.40
1	B	12	PHE	N-CA-C	6.27	121.01	113.23
1	A	162	PHE	N-CA-C	6.25	118.62	111.11
1	B	399	THR	N-CA-C	6.21	120.69	113.18
1	A	136	SER	N-CA-CB	-6.17	99.53	110.14
1	B	325	GLU	N-CA-C	6.15	117.78	111.14
1	A	355	ALA	N-CA-C	6.14	120.80	113.12
1	A	69	LYS	N-CA-C	5.94	123.45	110.80
1	A	264	VAL	N-CA-C	5.67	115.86	110.53
1	A	355	ALA	CB-CA-C	5.64	118.87	109.56
1	B	264	VAL	N-CA-C	5.62	115.81	110.53
1	A	204	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	352	VAL	N-CA-C	5.53	115.99	110.23
1	B	37	ILE	N-CA-C	5.51	120.80	109.34
1	B	204	ASN	CA-CB-CG	5.45	118.05	112.60
1	B	69	LYS	N-CA-C	5.43	122.37	110.80
1	A	354	PHE	CB-CA-C	5.39	119.33	110.88
1	A	103	ILE	N-CA-C	-5.30	97.17	106.61
1	B	59	PHE	N-CA-C	5.13	118.00	111.69
1	B	161	MET	N-CA-C	5.12	119.37	113.18
1	A	59	PHE	N-CA-C	5.11	117.97	111.69
1	A	21	PHE	N-CA-C	-5.09	105.64	111.14
1	B	21	PHE	N-CA-C	-5.08	105.65	111.14
1	A	27	PHE	N-CA-C	5.08	121.04	109.81
1	B	27	PHE	N-CA-C	5.08	121.03	109.81
1	A	251	PHE	CA-C-N	5.03	128.37	120.82
1	A	251	PHE	C-N-CA	5.03	128.37	120.82
1	B	399	THR	CB-CA-C	5.02	119.95	109.95

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	144	ARG	Sidechain

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	3065	0	3112	55	0
1	B	3112	0	3159	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	15	1	0
3	B	15	0	15	3	0
All	All	6209	0	6301	115	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 (115) 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:B:55:PHE:HB2	1:B:112:ILE:HG21	1.41	1.02
1:A:55:PHE:HB2	1:A:112:ILE:HG21	1.41	0.99
1:A:55:PHE:CD2	1:A:112:ILE:HG22	2.10	0.87
1:B:55:PHE:CD2	1:B:112:ILE:HG22	2.12	0.85
1:B:253:THR:OG1	1:B:256:GLN:HG2	1.77	0.84
1:A:253:THR:OG1	1:A:256:GLN:HG2	1.77	0.84
1:A:55:PHE:CB	1:A:112:ILE:HG21	2.16	0.74
1:B:55:PHE:CB	1:B:112:ILE:HG21	2.16	0.74
1:B:11:MET:O	1:B:184:LEU:HD22	1.89	0.73
1:B:66:LEU:HD23	1:B:71:GLY:HA3	1.70	0.72
1:B:231:GLY:O	1:B:235:THR:OG1	2.06	0.72
1:A:66:LEU:HD23	1:A:71:GLY:HA3	1.71	0.72
1:B:55:PHE:HB2	1:B:112:ILE:CG2	2.19	0.70
1:A:55:PHE:HB2	1:A:112:ILE:CG2	2.19	0.69
1:A:55:PHE:CB	1:A:112:ILE:CG2	2.70	0.69
1:A:231:GLY:O	1:A:235:THR:OG1	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PHE:CG	1:A:112:ILE:HG22	2.27	0.68
1:B:55:PHE:CB	1:B:112:ILE:CG2	2.71	0.68
1:A:51:ALA:CB	1:A:112:ILE:HD13	2.24	0.68
1:B:51:ALA:CB	1:B:112:ILE:HD13	2.23	0.68
1:A:355:ALA:O	1:A:359:GLN:HG2	1.95	0.67
1:B:55:PHE:CG	1:B:112:ILE:HG22	2.29	0.66
1:B:51:ALA:HB1	1:B:112:ILE:HD13	1.79	0.64
1:A:172:LEU:O	1:A:176:MET:HG2	1.99	0.63
1:B:224:PHE:HB3	1:B:399:THR:HB	1.80	0.63
1:B:224:PHE:CG	1:B:399:THR:O	2.52	0.63
1:A:55:PHE:CG	1:A:112:ILE:CG2	2.82	0.62
1:B:224:PHE:CD2	1:B:399:THR:O	2.52	0.62
1:A:51:ALA:HB1	1:A:112:ILE:HD13	1.80	0.62
1:B:178:LEU:O	1:B:182:VAL:HG22	2.00	0.62
1:B:55:PHE:CG	1:B:112:ILE:CG2	2.83	0.61
1:B:282:ILE:HG22	1:B:286:ILE:HD11	1.82	0.61
1:A:358:LYS:HG2	1:A:362:MET:HE2	1.83	0.61
1:B:52:ILE:HA	1:B:112:ILE:HG12	1.82	0.60
1:A:52:ILE:HA	1:A:112:ILE:HG12	1.83	0.60
1:A:74:LYS:HE3	1:A:188:LYS:HD3	1.84	0.60
1:A:208:PHE:HB2	1:A:348:THR:HG23	1.83	0.59
1:B:358:LYS:HG2	1:B:362:MET:HE2	1.83	0.59
1:B:355:ALA:O	1:B:359:GLN:HG2	2.04	0.58
1:B:208:PHE:HB2	1:B:348:THR:HG23	1.85	0.57
1:B:20:PHE:HA	1:B:23:MET:HB3	1.86	0.57
1:A:151:TRP:CG	3:A:701:TGA:H61C	2.40	0.57
1:A:20:PHE:HA	1:A:23:MET:HB3	1.86	0.57
1:A:114:LEU:HD23	1:A:114:LEU:O	2.05	0.56
1:A:35:HIS:HD2	1:A:42:LYS:HE3	1.71	0.56
1:B:35:HIS:HD2	1:B:42:LYS:HE3	1.71	0.56
1:B:302:ARG:HH21	1:B:319:LYS:HA	1.69	0.56
1:A:11:MET:O	1:A:184:LEU:HD22	2.07	0.55
1:A:21:PHE:CE1	1:A:176:MET:HG3	2.45	0.52
1:A:296:GLY:HA2	1:A:299:MET:HE3	1.91	0.52
1:A:392:PHE:HA	1:A:395:ILE:HG22	1.93	0.51
1:A:181:ALA:HA	1:A:184:LEU:HD12	1.93	0.51
1:A:279:ALA:O	1:A:283:ILE:HG12	2.11	0.51
1:B:40:ILE:HG23	1:B:44:ASP:HB2	1.93	0.50
1:B:279:ALA:O	1:B:283:ILE:HG12	2.11	0.50
1:A:40:ILE:HG23	1:A:44:ASP:HB2	1.94	0.50
1:B:6:ASN:HB2	1:B:9:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ILE:HG13	1:B:331:VAL:HG13	1.94	0.49
1:B:114:LEU:HD23	1:B:114:LEU:O	2.12	0.49
1:A:88:ALA:H	1:A:174:SER:HB3	1.78	0.48
1:B:85:VAL:HG13	1:B:178:LEU:HD12	1.96	0.48
1:B:66:LEU:HD22	1:B:76:LEU:HD22	1.94	0.48
1:A:66:LEU:HD22	1:A:76:LEU:HD22	1.95	0.48
1:B:372:MET:HB3	1:B:381:ALA:HB2	1.96	0.48
1:A:112:ILE:CG2	1:A:112:ILE:O	2.62	0.48
1:A:283:ILE:HG13	1:A:331:VAL:HG13	1.95	0.48
1:A:372:MET:HB3	1:A:381:ALA:HB2	1.96	0.47
1:A:85:VAL:HG13	1:A:178:LEU:HD12	1.96	0.47
1:A:55:PHE:CB	1:A:112:ILE:HG22	2.43	0.47
1:B:51:ALA:HB3	1:B:112:ILE:CD1	2.44	0.47
1:B:55:PHE:CB	1:B:112:ILE:HG22	2.44	0.47
1:B:296:GLY:HA2	1:B:299:MET:HE3	1.97	0.47
1:A:51:ALA:HB3	1:A:112:ILE:CD1	2.45	0.46
1:A:273:ALA:HA	1:A:276:MET:HG2	1.97	0.46
1:B:112:ILE:CG2	1:B:112:ILE:O	2.62	0.46
1:A:220:PRO:HA	1:A:223:TRP:HD1	1.81	0.46
1:B:158:VAL:O	1:B:162:PHE:HB2	2.16	0.46
1:B:220:PRO:HA	1:B:223:TRP:HD1	1.80	0.45
1:A:66:LEU:HD22	1:A:76:LEU:HD13	1.99	0.45
1:A:158:VAL:O	1:A:162:PHE:HB2	2.17	0.45
1:B:51:ALA:CB	1:B:112:ILE:CD1	2.93	0.44
1:B:21:PHE:CE1	1:B:176:MET:HG3	2.52	0.44
1:A:51:ALA:CB	1:A:112:ILE:CD1	2.94	0.44
1:A:337:ILE:HA	1:A:341:PHE:HD2	1.83	0.44
1:B:337:ILE:HA	1:B:341:PHE:HD2	1.83	0.44
1:B:286:ILE:HG22	1:B:290:ASN:HB2	2.00	0.44
1:B:42:LYS:HB3	1:B:373:TYR:HB2	1.99	0.44
1:A:333:SER:O	1:A:337:ILE:HG12	2.18	0.43
1:A:302:ARG:HH21	1:A:319:LYS:HA	1.84	0.43
1:B:253:THR:H	1:B:256:GLN:HB2	1.83	0.43
1:B:333:SER:O	1:B:337:ILE:HG12	2.19	0.43
1:A:253:THR:H	1:A:256:GLN:HB2	1.83	0.43
1:A:6:ASN:HB2	1:A:9:PHE:HB3	2.00	0.43
1:B:66:LEU:HD22	1:B:76:LEU:HD13	2.01	0.43
1:A:42:LYS:HB3	1:A:373:TYR:HB2	2.00	0.43
1:B:20:PHE:HZ	3:B:801:TGA:H142	1.84	0.43
1:B:269:GLU:OE1	3:B:801:TGA:H4	2.19	0.42
1:A:73:ARG:O	1:A:74:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:HD3	1:B:145:MET:HE2	2.02	0.42
1:A:144:ARG:HD3	1:A:145:MET:HE2	2.01	0.42
1:B:176:MET:SD	1:B:180:LEU:CD1	3.07	0.42
1:B:214:LEU:HD23	1:B:218:ARG:HH21	1.84	0.42
1:A:91:PHE:HA	1:A:95:PHE:HB3	2.02	0.42
1:B:91:PHE:HA	1:B:95:PHE:HB3	2.02	0.42
1:A:76:LEU:HA	1:A:79:ILE:HD12	2.02	0.41
1:A:66:LEU:CD2	1:A:71:GLY:HA3	2.47	0.41
1:A:100:GLN:C	1:A:102:ASN:H	2.29	0.41
1:B:20:PHE:CZ	3:B:801:TGA:H142	2.55	0.41
1:B:282:ILE:O	1:B:286:ILE:HG13	2.21	0.41
1:B:76:LEU:HA	1:B:79:ILE:HD12	2.02	0.41
1:B:289:LYS:HG2	1:B:336:TYR:HE1	1.85	0.41
1:A:177:ALA:O	1:A:181:ALA:HB3	2.21	0.40
1:B:12:PHE:CD1	1:B:129:ILE:HG12	2.55	0.40
1:B:66:LEU:CD2	1:B:71:GLY:HA3	2.46	0.40
1:B:360:LEU:HA	1:B:363:ILE:HD12	2.02	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	382/423 (90%)	359 (94%)	23 (6%)	0	100	100
1	B	390/423 (92%)	365 (94%)	25 (6%)	0	100	100
All	All	772/846 (91%)	724 (94%)	48 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/350 (91%)	299 (93%)	21 (7%)	15	41
1	B	324/350 (93%)	301 (93%)	23 (7%)	13	39
All	All	644/700 (92%)	600 (93%)	44 (7%)	14	40

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	16	PHE
1	A	38	ASN
1	A	40	ILE
1	A	44	ASP
1	A	62	LEU
1	A	160	ILE
1	A	204	ASN
1	A	210	LEU
1	A	212	LEU
1	A	225	LEU
1	A	227	LEU
1	A	282	ILE
1	A	294	LEU
1	A	304	ILE
1	A	313	LEU
1	A	317	ILE
1	A	321	LEU
1	A	348	THR
1	A	351	LEU
1	A	368	LEU
1	B	5	LYS
1	B	16	PHE
1	B	38	ASN
1	B	40	ILE
1	B	44	ASP
1	B	45	THR

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Mol	Chain	Res	Type
1	B	62	LEU
1	B	160	ILE
1	B	204	ASN
1	B	210	LEU
1	B	212	LEU
1	B	225	LEU
1	B	227	LEU
1	B	282	ILE
1	B	286	ILE
1	B	294	LEU
1	B	304	ILE
1	B	313	LEU
1	B	314	GLU
1	B	317	ILE
1	B	321	LEU
1	B	351	LEU
1	B	368	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	35	HIS
1	A	39	HIS
1	A	102	ASN
1	A	167	GLN
1	A	241	GLN
1	A	242	GLN
1	A	284	ASN
1	A	290	ASN
1	A	359	GLN
1	A	371	ASN
1	B	8	ASN
1	B	35	HIS
1	B	102	ASN
1	B	137	ASN
1	B	167	GLN
1	B	241	GLN
1	B	242	GLN
1	B	284	ASN
1	B	359	GLN
1	B	371	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TGA	A	701	1	15,15,15	0.94	1 (6%)	19,20,20	1.10	2 (10%)
3	TGA	B	801	1	15,15,15	0.78	0	19,20,20	1.20	3 (15%)

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
3	TGA	A	701	1	-	1/6/26/26	0/1/1/1
3	TGA	B	801	1	-	3/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	TGA	O1-C1	2.77	1.44	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	TGA	O5-C5-C6	3.30	114.61	106.44
3	B	801	TGA	C13-O1-C1	-2.78	108.93	113.68
3	A	701	TGA	O5-C1-C2	2.53	115.57	110.37
3	A	701	TGA	O5-C5-C6	2.48	112.58	106.44
3	B	801	TGA	C1-O5-C5	-2.04	109.73	113.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	TGA	O1-C13-C14-S15
3	B	801	TGA	C4-C5-C6-O6
3	B	801	TGA	O5-C5-C6-O6
3	A	701	TGA	O1-C13-C14-S15

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	TGA	1	0
3	B	801	TGA	3	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	386/423 (91%)	1.41	107 (27%) ⓘ ⓘ	113, 158, 207, 251	0
1	B	394/423 (93%)	1.60	127 (32%) ⓘ ⓘ	104, 160, 214, 264	0
All	All	780/846 (92%)	1.51	234 (30%) ⓘ ⓘ	104, 159, 212, 264	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	375	SER	7.6
1	B	7	THR	7.3
1	B	252	ALA	7.2
1	B	119	ASN	7.1
1	B	341	PHE	6.9
1	B	179	ILE	6.8
1	A	252	ALA	6.6
1	B	139	GLU	5.9
1	A	341	PHE	5.8
1	B	181	ALA	5.8
1	B	317	ILE	5.8
1	B	376	ILE	5.7
1	A	334	PHE	5.6
1	B	374	GLU	5.5
1	A	375	SER	5.5
1	A	376	ILE	5.5
1	A	163	THR	5.4
1	A	118	PHE	5.4
1	A	19	TYR	5.4
1	B	334	PHE	5.4
1	A	207	ALA	5.2
1	B	182	VAL	5.1
1	B	164	ILE	5.1
1	A	30	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	23	MET	5.0
1	B	400	LEU	4.9
1	A	8	ASN	4.8
1	B	207	ALA	4.8
1	A	219	GLN	4.8
1	A	115	GLY	4.7
1	B	138	PHE	4.6
1	A	4	LEU	4.6
1	A	324	PHE	4.6
1	B	115	GLY	4.5
1	A	221	LYS	4.5
1	B	71	GLY	4.4
1	A	12	PHE	4.4
1	A	354	PHE	4.4
1	B	141	GLY	4.4
1	B	354	PHE	4.3
1	B	68	ASP	4.3
1	B	74	LYS	4.2
1	A	29	PHE	4.1
1	B	183	LEU	4.0
1	B	101	TYR	4.0
1	A	119	ASN	4.0
1	B	118	PHE	4.0
1	A	317	ILE	4.0
1	B	60	GLN	3.9
1	A	176	MET	3.9
1	A	78	TRP	3.9
1	B	209	SER	3.9
1	B	211	LYS	3.8
1	A	286	ILE	3.8
1	B	100	GLN	3.8
1	B	249	SER	3.8
1	B	210	LEU	3.8
1	B	178	LEU	3.8
1	A	312	ALA	3.7
1	A	211	LYS	3.7
1	A	295	ALA	3.7
1	A	83	MET	3.7
1	A	114	LEU	3.7
1	B	5	LYS	3.7
1	A	179	ILE	3.6
1	B	186	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLU	3.6
1	A	253	THR	3.6
1	A	251	PHE	3.6
1	B	331	VAL	3.6
1	A	164	ILE	3.6
1	B	265	THR	3.6
1	A	74	LYS	3.5
1	A	188	LYS	3.5
1	B	66	LEU	3.5
1	A	245	ASN	3.5
1	A	7	THR	3.5
1	B	338	THR	3.5
1	A	100	GLN	3.5
1	B	37	ILE	3.5
1	B	237	ASP	3.5
1	A	102	ASN	3.4
1	A	71	GLY	3.4
1	B	180	LEU	3.4
1	A	58	LEU	3.4
1	A	208	PHE	3.3
1	B	92	ILE	3.3
1	B	172	LEU	3.3
1	A	250	PHE	3.2
1	A	338	THR	3.2
1	B	70	LEU	3.2
1	B	135	ARG	3.2
1	B	12	PHE	3.2
1	B	339	SER	3.2
1	B	103	ILE	3.2
1	A	20	PHE	3.1
1	B	149	VAL	3.1
1	B	250	PHE	3.1
1	B	251	PHE	3.1
1	B	350	TYR	3.1
1	A	135	ARG	3.1
1	A	180	LEU	3.1
1	B	72	LEU	3.1
1	A	331	VAL	3.1
1	A	122	CYS	3.1
1	A	256	GLN	3.1
1	A	249	SER	3.1
1	A	403	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	108	ILE	3.1
1	A	242	GLN	3.0
1	B	87	PHE	3.0
1	A	47	ILE	3.0
1	B	176	MET	3.0
1	B	163	THR	3.0
1	A	157	ILE	3.0
1	B	42	LYS	3.0
1	B	253	THR	3.0
1	A	280	PRO	3.0
1	B	4	LEU	3.0
1	A	73	ARG	3.0
1	A	5	LYS	2.9
1	A	126	GLU	2.9
1	B	67	SER	2.9
1	B	142	ARG	2.9
1	B	144	ARG	2.9
1	B	254	GLY	2.9
1	A	60	GLN	2.8
1	B	145	MET	2.8
1	B	256	GLN	2.8
1	A	237	ASP	2.8
1	B	248	THR	2.8
1	B	111	GLY	2.8
1	A	313	LEU	2.8
1	B	323	MET	2.8
1	A	172	LEU	2.8
1	B	247	PHE	2.7
1	B	314	GLU	2.7
1	A	42	LYS	2.7
1	A	209	SER	2.7
1	B	113	TYR	2.7
1	A	355	ALA	2.7
1	B	343	VAL	2.7
1	B	330	LEU	2.7
1	A	160	ILE	2.6
1	B	146	PHE	2.6
1	A	328	PHE	2.6
1	B	175	GLY	2.6
1	A	116	PHE	2.6
1	B	324	PHE	2.6
1	A	241	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	88	ALA	2.6
1	B	213	ALA	2.6
1	A	108	ILE	2.5
1	B	23	MET	2.5
1	B	242	GLN	2.5
1	B	11	MET	2.5
1	A	246	PHE	2.5
1	B	19	TYR	2.5
1	A	298	ILE	2.5
1	A	144	ARG	2.5
1	A	156	SER	2.5
1	B	127	ALA	2.5
1	A	337	ILE	2.5
1	B	286	ILE	2.5
1	A	26	TYR	2.5
1	B	97	PRO	2.5
1	B	336	TYR	2.5
1	B	344	ARG	2.5
1	B	99	LEU	2.5
1	B	271	LEU	2.4
1	B	313	LEU	2.4
1	B	351	LEU	2.4
1	B	288	GLY	2.4
1	A	309	ALA	2.4
1	B	372	MET	2.4
1	B	208	PHE	2.4
1	B	197	VAL	2.4
1	A	101	TYR	2.4
1	B	140	PHE	2.4
1	B	217	PHE	2.4
1	A	181	ALA	2.3
1	B	230	ILE	2.3
1	B	240	ASP	2.3
1	B	161	MET	2.3
1	A	153	LEU	2.3
1	A	255	GLU	2.3
1	A	169	VAL	2.3
1	A	87	PHE	2.3
1	A	247	PHE	2.3
1	B	36	ASP	2.3
1	B	255	GLU	2.3
1	A	365	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	288	GLY	2.3
1	A	76	LEU	2.3
1	A	140	PHE	2.3
1	B	166	ASN	2.3
1	B	204	ASN	2.3
1	B	289	LYS	2.3
1	A	374	GLU	2.2
1	B	124	ALA	2.2
1	B	102	ASN	2.2
1	B	137	ASN	2.2
1	A	77	LEU	2.2
1	B	69	LYS	2.2
1	A	59	PHE	2.2
1	B	189	THR	2.2
1	B	373	TYR	2.2
1	B	306	SER	2.2
1	A	373	TYR	2.2
1	A	310	THR	2.1
1	B	47	ILE	2.1
1	A	167	GLN	2.1
1	B	128	PHE	2.1
1	B	75	TYR	2.1
1	B	184	LEU	2.1
1	B	221	LYS	2.1
1	A	183	LEU	2.1
1	B	122	CYS	2.1
1	A	350	TYR	2.1
1	A	203	ALA	2.1
1	A	244	ALA	2.1
1	B	63	PHE	2.1
1	B	8	ASN	2.1
1	B	38	ASN	2.1
1	A	248	THR	2.1
1	B	320	THR	2.1
1	B	120	ALA	2.0
1	A	336	TYR	2.0
1	A	16	PHE	2.0
1	A	21	PHE	2.0
1	A	261	PHE	2.0
1	B	27	PHE	2.0
1	A	105	VAL	2.0
1	A	227	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BA	A	501	1/1	0.85	0.15	232,232,232,232	0
3	TGA	B	801	15/15	0.87	0.13	37,157,237,244	0
3	TGA	A	701	15/15	0.92	0.13	121,167,242,253	0
2	BA	B	501	1/1	0.98	0.13	205,205,205,205	0

6.5 Other polymers [i](#)

There are no such residues in this entry.