



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2016 – 01:28 AM EDT

PDB ID : 5DJC
Title : Fc Heterodimer Design 8.1 L368V/Y407A + T366V/K409F
Authors : Atwell, S.; Leaver-Fay, A.; Froning, K.J.; Aldaz, H.; Pustilnik, A.; Lu, F.;
Huang, F.; Yuan, R.; Dhanani, S.H.; Chamberlain, A.K.; Fitchett, J.R.;
Gutierrez, B.; Hendle, J.; Secrist, E.; Demarest, S.J.; Kuhlman, B.
Deposited on : 2015-09-01
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027257
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027257

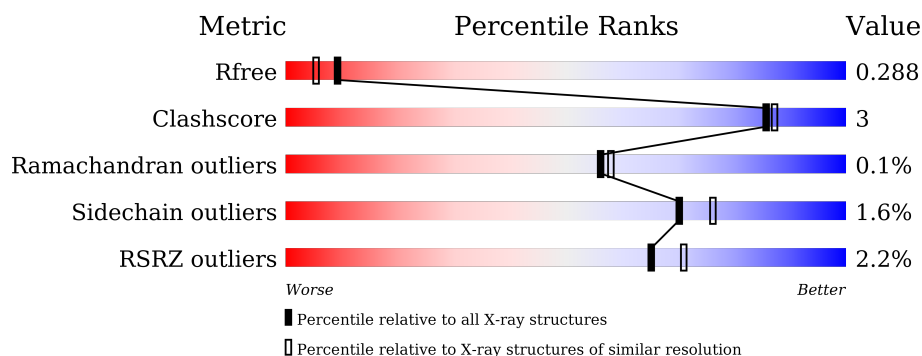
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	227	<div> <div>81%</div> <div>10%</div> <div>9%</div> </div>
1	D	227	<div> <div>82%</div> <div>8%</div> <div>9%</div> </div>
2	B	240	<div> <div>3%</div> <div>81%</div> <div>5%</div> <div>14%</div> </div>
2	E	240	<div> <div>4%</div> <div>76%</div> <div>10%</div> <div>14%</div> </div>
3	C	13	<div> <div>8%</div> <div>92%</div> <div>8%</div> </div>
3	F	13	<div> <div>92%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GAL	A	506	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7227 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1637	1041	273	316	7			
1	D	207	Total	C	N	O	S	1	0	0
			1635	1042	270	316	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	GLU	ASP	variant	UNP P01857
A	358	MET	LEU	variant	UNP P01857
A	368	VAL	LEU	engineered mutation	UNP P01857
A	407	ALA	TYR	engineered mutation	UNP P01857
D	356	GLU	ASP	variant	UNP P01857
D	358	MET	LEU	variant	UNP P01857
D	368	VAL	LEU	engineered mutation	UNP P01857
D	407	ALA	TYR	engineered mutation	UNP P01857

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	0	0
			1587	1020	261	300	6			
2	E	207	Total	C	N	O	S	0	0	0
			1580	1014	260	300	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	208	HIS	-	expression tag	UNP P01857
B	209	HIS	-	expression tag	UNP P01857
B	210	HIS	-	expression tag	UNP P01857
B	211	HIS	-	expression tag	UNP P01857

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	212	HIS	-	expression tag	UNP P01857
B	213	HIS	-	expression tag	UNP P01857
B	214	HIS	-	expression tag	UNP P01857
B	215	HIS	-	expression tag	UNP P01857
B	216	SER	-	expression tag	UNP P01857
B	217	GLY	-	expression tag	UNP P01857
B	218	SER	-	expression tag	UNP P01857
B	219	GLY	-	expression tag	UNP P01857
B	220	SER	-	expression tag	UNP P01857
B	252	GLU	MET	engineered mutation	UNP P01857
B	253	ALA	ILE	engineered mutation	UNP P01857
B	356	GLU	ASP	variant	UNP P01857
B	358	MET	LEU	variant	UNP P01857
B	366	VAL	THR	engineered mutation	UNP P01857
B	409	PHE	LYS	engineered mutation	UNP P01857
B	435	ALA	HIS	engineered mutation	UNP P01857
E	208	HIS	-	expression tag	UNP P01857
E	209	HIS	-	expression tag	UNP P01857
E	210	HIS	-	expression tag	UNP P01857
E	211	HIS	-	expression tag	UNP P01857
E	212	HIS	-	expression tag	UNP P01857
E	213	HIS	-	expression tag	UNP P01857
E	214	HIS	-	expression tag	UNP P01857
E	215	HIS	-	expression tag	UNP P01857
E	216	SER	-	expression tag	UNP P01857
E	217	GLY	-	expression tag	UNP P01857
E	218	SER	-	expression tag	UNP P01857
E	219	GLY	-	expression tag	UNP P01857
E	220	SER	-	expression tag	UNP P01857
E	252	GLU	MET	engineered mutation	UNP P01857
E	253	ALA	ILE	engineered mutation	UNP P01857
E	356	GLU	ASP	variant	UNP P01857
E	358	MET	LEU	variant	UNP P01857
E	366	VAL	THR	engineered mutation	UNP P01857
E	409	PHE	LYS	engineered mutation	UNP P01857
E	435	ALA	HIS	engineered mutation	UNP P01857

- Molecule 3 is a protein called Fc-III peptide.

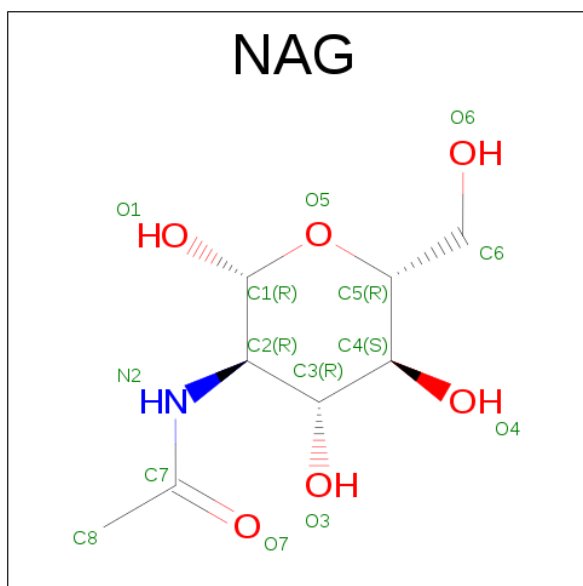
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	S	0	0	0
			107	69	17	19	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	13	Total	C	N	O	S	0	0	0
			107	69	17	19	2			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



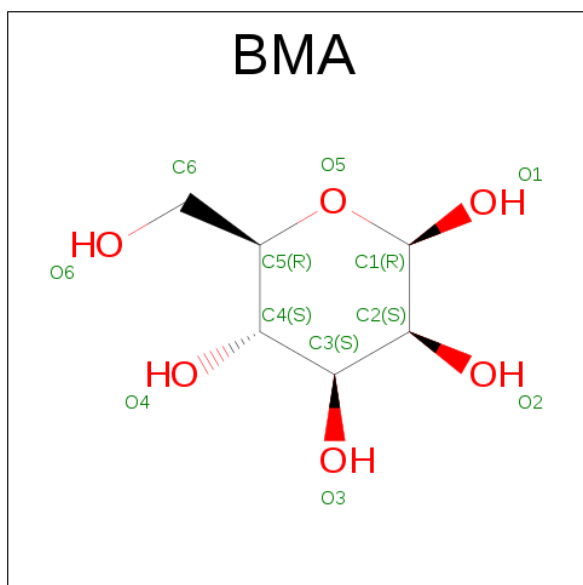
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O		0	0
			14	8	1	5			
4	A	1	Total	C	N	O		0	0
			14	8	1	5			
4	A	1	Total	C	N	O		0	0
			14	8	1	5			
4	B	1	Total	C	N	O		0	0
			14	8	1	5			
4	B	1	Total	C	N	O		0	0
			14	8	1	5			
4	B	1	Total	C	N	O		0	0
			14	8	1	5			
4	D	1	Total	C	N	O		0	0
			14	8	1	5			
4	D	1	Total	C	N	O		0	0
			14	8	1	5			
4	D	1	Total	C	N	O		0	0
			14	8	1	5			
4	E	1	Total	C	N	O		0	0
			14	8	1	5			

Continued on next page...

Continued from previous page...

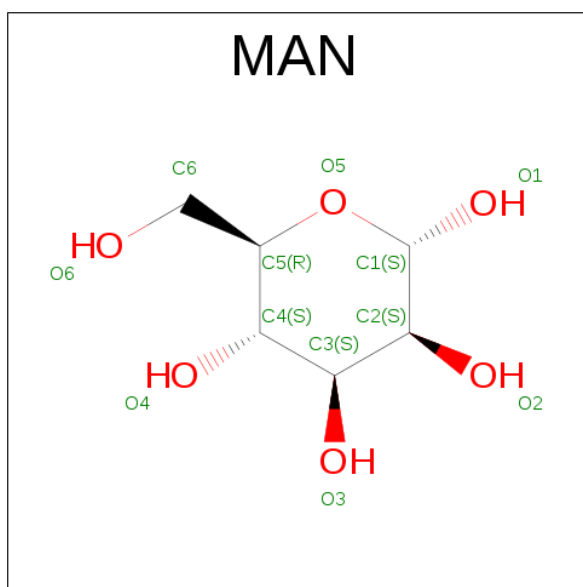
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



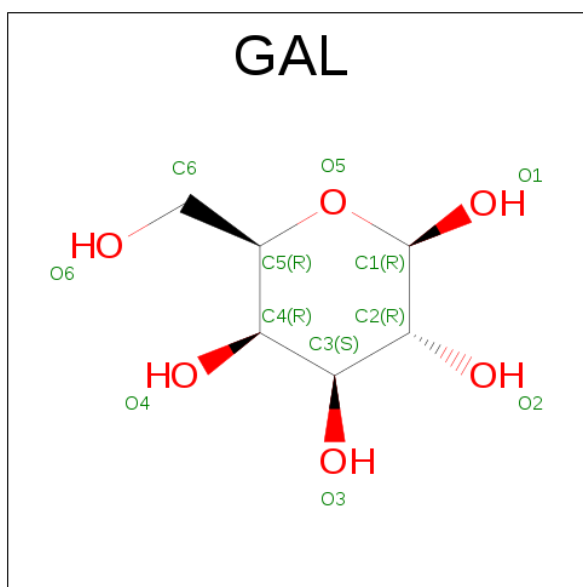
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



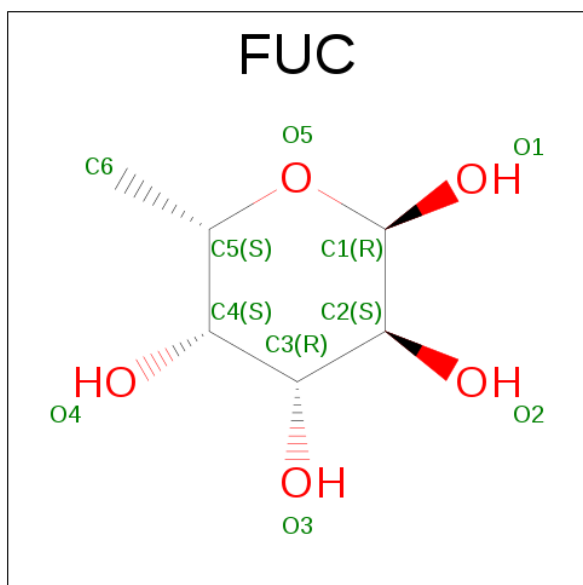
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	B	1	Total	C	O	0	0
			10	6	4		
8	D	1	Total	C	O	0	0
			10	6	4		
8	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	I	0	0
			1	1		

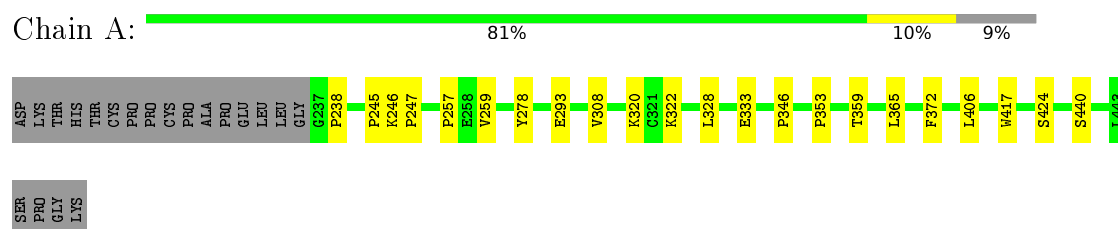
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	64	Total	O	0	0
			64	64		
10	B	25	Total	O	0	0
			25	25		
10	C	1	Total	O	0	0
			1	1		
10	D	67	Total	O	0	0
			67	67		
10	E	32	Total	O	0	0
			32	32		

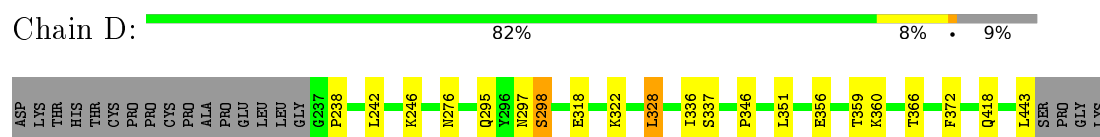
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

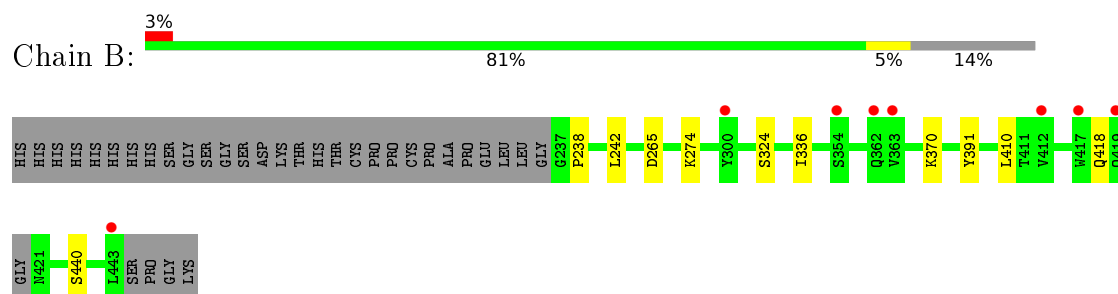
- Molecule 1: Ig gamma-1 chain C region



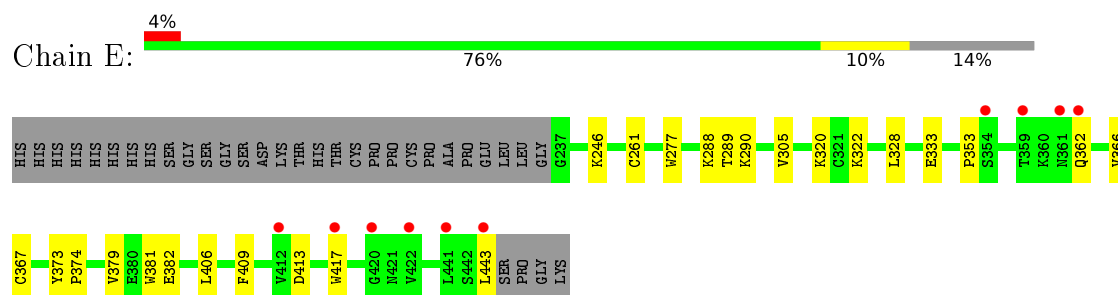
- Molecule 1: Ig gamma-1 chain C region



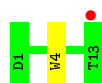
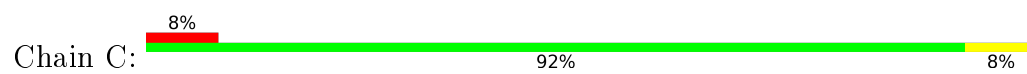
- Molecule 2: Ig gamma-1 chain C region



- Molecule 2: Ig gamma-1 chain C region



- Molecule 3: Fc-III peptide



- Molecule 3: Fc-III peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.24Å 66.86Å 72.77Å 85.17° 80.71° 89.69°	Depositor
Resolution (Å)	30.00 – 2.10 59.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-2.10) 93.6 (59.45-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0017	Depositor
R, R_{free}	0.229 , 0.285 0.232 , 0.288	Depositor DCC
R_{free} test set	3179 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7227	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, GAL, FUC, IOD, MAN

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	0.53	1/1682 (0.1%)	0.58	0/2295
1	D	0.56	1/1680 (0.1%)	0.65	1/2293 (0.0%)
2	B	0.50	0/1631	0.54	0/2230
2	E	0.50	1/1624 (0.1%)	0.54	0/2224
3	C	1.02	1/111 (0.9%)	0.69	0/151
3	F	1.03	1/111 (0.9%)	0.62	0/151
All	All	0.55	5/6839 (0.1%)	0.58	1/9344 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	360	LYS	CG-CD	-7.29	1.27	1.52
1	A	417	TRP	CD2-CE2	5.60	1.48	1.41
3	F	4	TRP	CD2-CE2	5.19	1.47	1.41
2	E	417	TRP	CD2-CE2	5.07	1.47	1.41
3	C	4	TRP	CD2-CE2	5.03	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	360	LYS	CB-CG-CD	12.72	144.66	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1637	0	1583	10	0
1	D	1635	0	1570	13	0
2	B	1587	0	1501	4	0
2	E	1580	0	1497	11	0
3	C	107	0	93	0	0
3	F	107	0	93	0	0
4	A	42	0	35	0	0
4	B	42	0	35	0	0
4	D	42	0	35	1	0
4	E	42	0	35	0	0
5	A	11	0	8	0	0
5	B	11	0	8	0	0
5	D	11	0	8	0	0
5	E	11	0	8	0	0
6	A	22	0	19	0	0
6	B	22	0	19	0	0
6	D	22	0	19	0	0
6	E	22	0	19	0	0
7	A	11	0	10	0	0
7	B	11	0	10	0	0
7	D	11	0	10	1	0
7	E	11	0	10	1	0
8	A	10	0	10	0	0
8	B	10	0	10	0	0
8	D	10	0	10	0	0
8	E	10	0	10	0	0
9	D	1	0	0	0	0
10	A	64	0	0	0	0
10	B	25	0	0	0	0
10	C	1	0	0	0	0
10	D	67	0	0	1	0
10	E	32	0	0	1	0
All	All	7227	0	6665	38	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 (38) 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:346:PRO:HB3	1:A:372:PHE:HB3	1.71	0.72
1:D:297:ASN:O	1:D:298:SER:CB	2.43	0.67
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.83	0.59
2:E:290:LYS:HE3	2:E:305:VAL:HG21	1.84	0.58
2:B:242:LEU:HG	2:B:336:ILE:HG12	1.87	0.57
2:E:320:LYS:HD3	2:E:333:GLU:OE2	2.05	0.56
2:E:322:LYS:HG3	2:E:333:GLU:HG2	1.90	0.54
1:D:276:ASN:HB2	1:D:322:LYS:HB3	1.92	0.52
1:D:346:PRO:HB3	1:D:372:PHE:HB3	1.92	0.50
1:A:245:PRO:HD3	1:A:259:VAL:HG12	1.93	0.50
1:D:297:ASN:O	1:D:298:SER:HB3	2.12	0.49
1:D:318:GLU:HA	1:D:337:SER:HB3	1.95	0.49
2:B:274:LYS:HB3	2:B:324:SER:HB2	1.93	0.49
1:D:351:LEU:HB2	1:D:366:THR:HB	1.95	0.48
2:E:362:GLN:HG2	2:E:413:ASP:HA	1.95	0.47
1:A:424:SER:OG	1:A:440:SER:OG	2.31	0.47
2:E:246:LYS:HG2	7:E:506:GAL:O4	2.16	0.46
2:E:353:PRO:HA	10:E:616:HOH:O	2.16	0.46
1:A:246:LYS:O	1:A:247:PRO:C	2.55	0.45
2:E:261:CYS:HB2	2:E:277:TRP:CZ2	2.52	0.45
2:E:367:CYS:HB2	2:E:381:TRP:CZ2	2.51	0.45
1:D:443:LEU:C	10:D:644:HOH:O	2.54	0.45
1:D:238:PRO:HD2	1:D:328:LEU:HD13	1.99	0.44
2:E:379:VAL:HG21	2:E:406:LEU:HD11	1.99	0.44
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.99	0.44
2:E:366:VAL:HG22	2:E:409:PHE:CD2	2.53	0.44
2:B:238:PRO:HA	2:B:265:ASP:HB2	2.00	0.43
1:D:242:LEU:HG	1:D:336:ILE:HG12	2.00	0.43
1:D:295:GLN:OE1	4:D:501:NAG:H62	2.18	0.42
1:D:297:ASN:O	1:D:298:SER:HB2	2.19	0.42
1:A:238:PRO:HD2	1:A:328:LEU:HD13	2.01	0.42
1:A:322:LYS:HG3	1:A:333:GLU:HG2	2.02	0.41
2:E:373:TYR:CG	2:E:374:PRO:HA	2.55	0.41
1:A:406:LEU:C	1:A:406:LEU:HD12	2.41	0.41
2:B:391:TYR:HB3	2:B:410:LEU:HD12	2.03	0.41
1:A:257:PRO:HG2	1:A:308:VAL:O	2.21	0.40
1:D:356:GLU:O	1:D:359:THR:HG22	2.22	0.40
1:D:246:LYS:HG2	7:D:506:GAL:O4	2.22	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	205/227 (90%)	201 (98%)	4 (2%)	0	100	100
1	D	205/227 (90%)	200 (98%)	4 (2%)	1 (0%)	34	30
2	B	202/240 (84%)	195 (96%)	7 (4%)	0	100	100
2	E	205/240 (85%)	201 (98%)	4 (2%)	0	100	100
3	C	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
3	F	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
All	All	839/960 (87%)	817 (97%)	21 (2%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	298	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	188/209 (90%)	186 (99%)	2 (1%)	80	85
1	D	185/209 (88%)	183 (99%)	2 (1%)	80	85
2	B	172/219 (78%)	169 (98%)	3 (2%)	68	74
2	E	172/219 (78%)	167 (97%)	5 (3%)	50	53
3	C	11/11 (100%)	11 (100%)	0	100	100
3	F	11/11 (100%)	11 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	739/878 (84%)	727 (98%)	12 (2%)	70	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	GLU
1	A	359	THR
2	B	370	LYS
2	B	418	GLN
2	B	440	SER
1	D	328	LEU
1	D	418	GLN
2	E	288	LYS
2	E	289	THR
2	E	328	LEU
2	E	382	GLU
2	E	443	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	418	GLN
1	D	389	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 33 ligands modelled in this entry, 1 is monoatomic - leaving 32 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	NAG	A	501	1,8,4	14,14,15	0.58	0	15,19,21	0.67	0
4	NAG	A	502	5,4	14,14,15	0.51	0	15,19,21	0.76	0
5	BMA	A	503	4,6	11,11,12	0.30	0	15,15,17	1.24	2 (13%)
6	MAN	A	504	5,4	11,11,12	0.59	0	15,15,17	1.25	2 (13%)
4	NAG	A	505	7,6	14,14,15	0.56	0	15,19,21	0.64	0
7	GAL	A	506	4	11,11,12	0.55	0	15,15,17	0.68	0
8	FUC	A	507	4	10,10,11	0.58	0	13,14,16	1.03	0
6	MAN	A	508	5	11,11,12	0.60	0	15,15,17	0.66	0
4	NAG	B	501	8,2,4	14,14,15	0.53	0	15,19,21	0.82	0
4	NAG	B	502	5,4	14,14,15	0.48	0	15,19,21	0.93	1 (6%)
5	BMA	B	503	4,6	11,11,12	0.60	0	15,15,17	1.69	3 (20%)
6	MAN	B	504	5,4	11,11,12	0.65	0	15,15,17	1.33	2 (13%)
4	NAG	B	505	7,6	14,14,15	0.59	0	15,19,21	0.98	1 (6%)
7	GAL	B	506	4	11,11,12	0.63	0	15,15,17	1.02	1 (6%)
6	MAN	B	507	5	11,11,12	0.52	0	15,15,17	2.16	5 (33%)
8	FUC	B	508	4	10,10,11	0.62	0	13,14,16	0.81	1 (7%)
4	NAG	D	501	1,8,4	14,14,15	0.58	0	15,19,21	0.70	0
4	NAG	D	502	5,4	14,14,15	0.64	0	15,19,21	1.02	0
5	BMA	D	503	4,6	11,11,12	0.26	0	15,15,17	1.09	1 (6%)
6	MAN	D	504	5,4	11,11,12	0.59	0	15,15,17	0.90	1 (6%)
4	NAG	D	505	7,6	14,14,15	0.66	0	15,19,21	0.77	0
7	GAL	D	506	4	11,11,12	0.65	0	15,15,17	1.13	1 (6%)
8	FUC	D	507	4	10,10,11	0.78	0	13,14,16	0.96	0
6	MAN	D	508	5	11,11,12	0.66	0	15,15,17	0.79	0
4	NAG	E	501	8,2,4	14,14,15	0.54	0	15,19,21	0.63	0
4	NAG	E	502	5,4	14,14,15	0.45	0	15,19,21	0.92	0
5	BMA	E	503	4,6	11,11,12	0.51	0	15,15,17	1.11	2 (13%)
6	MAN	E	504	5,4	11,11,12	0.62	0	15,15,17	0.92	0
4	NAG	E	505	7,6	14,14,15	0.58	0	15,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GAL	E	506	4	11,11,12	0.61	0	15,15,17	1.02	1 (6%)
6	MAN	E	507	5	11,11,12	0.56	0	15,15,17	1.01	1 (6%)
8	FUC	E	508	4	10,10,11	0.65	0	13,14,16	0.73	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	NAG	A	501	1,8,4	-	0/6/23/26	0/1/1/1
4	NAG	A	502	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	503	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	504	5,4	-	0/2/19/22	0/1/1/1
4	NAG	A	505	7,6	-	0/6/23/26	0/1/1/1
7	GAL	A	506	4	-	0/2/19/22	0/1/1/1
8	FUC	A	507	4	-	0/0/17/20	0/1/1/1
6	MAN	A	508	5	-	0/2/19/22	0/1/1/1
4	NAG	B	501	8,2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	502	5,4	-	0/6/23/26	0/1/1/1
5	BMA	B	503	4,6	-	0/2/19/22	0/1/1/1
6	MAN	B	504	5,4	-	0/2/19/22	0/1/1/1
4	NAG	B	505	7,6	-	0/6/23/26	0/1/1/1
7	GAL	B	506	4	-	0/2/19/22	0/1/1/1
6	MAN	B	507	5	-	0/2/19/22	0/1/1/1
8	FUC	B	508	4	-	0/0/17/20	0/1/1/1
4	NAG	D	501	1,8,4	-	0/6/23/26	0/1/1/1
4	NAG	D	502	5,4	-	0/6/23/26	0/1/1/1
5	BMA	D	503	4,6	-	0/2/19/22	0/1/1/1
6	MAN	D	504	5,4	-	0/2/19/22	0/1/1/1
4	NAG	D	505	7,6	-	0/6/23/26	0/1/1/1
7	GAL	D	506	4	-	0/2/19/22	0/1/1/1
8	FUC	D	507	4	-	0/0/17/20	0/1/1/1
6	MAN	D	508	5	-	0/2/19/22	0/1/1/1
4	NAG	E	501	8,2,4	-	0/6/23/26	0/1/1/1
4	NAG	E	502	5,4	-	0/6/23/26	0/1/1/1
5	BMA	E	503	4,6	-	0/2/19/22	0/1/1/1
6	MAN	E	504	5,4	-	0/2/19/22	0/1/1/1
4	NAG	E	505	7,6	-	0/6/23/26	0/1/1/1
7	GAL	E	506	4	-	0/2/19/22	0/1/1/1
6	MAN	E	507	5	-	0/2/19/22	0/1/1/1
8	FUC	E	508	4	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	NAG	C2-N2-C7	-2.52	119.83	123.11
6	A	504	MAN	O2-C2-C3	-2.20	105.74	110.19
5	B	503	BMA	O6-C6-C5	-2.05	104.46	111.30
6	D	504	MAN	C1-O5-C5	2.03	115.12	112.14
6	B	507	MAN	C1-C2-C3	2.06	112.05	109.55
4	B	505	NAG	C1-O5-C5	2.16	115.32	112.14
6	E	507	MAN	C1-C2-C3	2.18	112.20	109.55
6	B	504	MAN	C3-C4-C5	2.24	114.23	110.23
8	B	508	FUC	O5-C5-C6	2.25	110.31	106.28
5	A	503	BMA	C1-C2-C3	2.27	112.30	109.55
6	B	507	MAN	O5-C5-C6	2.31	112.29	107.34
5	E	503	BMA	C1-O5-C5	2.32	115.55	112.14
7	B	506	GAL	C1-C2-C3	2.42	112.48	109.55
6	B	504	MAN	C1-O5-C5	2.44	115.73	112.14
5	D	503	BMA	C1-O5-C5	2.72	116.14	112.14
5	E	503	BMA	C1-C2-C3	2.73	112.86	109.55
7	D	506	GAL	C1-C2-C3	2.77	112.90	109.55
5	B	503	BMA	C1-O5-C5	3.00	116.56	112.14
5	A	503	BMA	C1-O5-C5	3.02	116.58	112.14
7	E	506	GAL	C1-C2-C3	3.08	113.28	109.55
6	A	504	MAN	C1-O5-C5	3.10	116.70	112.14
6	B	507	MAN	C3-C4-C5	3.18	115.89	110.23
6	B	507	MAN	O5-C1-C2	3.52	116.53	110.89
5	B	503	BMA	C1-C2-C3	4.62	115.15	109.55
6	B	507	MAN	C1-O5-C5	5.35	120.01	112.14

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	D	501	NAG	1	0
7	D	506	GAL	1	0
7	E	506	GAL	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	207/227 (91%)	0.04	0	100	100	23, 36, 48, 67	0
1	D	207/227 (91%)	0.01	0	100	100	23, 36, 48, 62	1 (0%)
2	B	206/240 (85%)	0.36	8 (3%)	43	52	26, 46, 87, 103	0
2	E	207/240 (86%)	0.28	10 (4%)	34	43	26, 48, 83, 98	0
3	C	13/13 (100%)	0.24	1 (7%)	16	22	29, 40, 53, 70	0
3	F	13/13 (100%)	0.15	0	100	100	33, 45, 63, 68	0
All	All	853/960 (88%)	0.17	19 (2%)	65	71	23, 40, 76, 103	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	417	TRP	4.7
2	E	354	SER	3.9
2	E	443	LEU	3.6
2	B	417	TRP	3.5
2	E	412	VAL	3.4
2	B	412	VAL	3.2
2	E	361	ASN	3.2
2	B	362	GLN	3.0
2	E	359	THR	3.0
2	B	443	LEU	2.9
2	E	362	GLN	2.5
2	E	441	LEU	2.3
2	E	420	GLY	2.3
2	B	354	SER	2.2
3	C	13	THR	2.2
2	B	419	GLN	2.2
2	B	300	TYR	2.2
2	E	422	VAL	2.1
2	B	363	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	GAL	A	506	11/12	0.81	0.20	5.55	43,63,75,77	0
7	GAL	B	506	11/12	0.84	0.23	1.87	56,62,73,75	0
7	GAL	E	506	11/12	0.93	0.18	1.43	50,61,69,72	0
9	IOD	D	509	1/1	1.00	0.13	0.37	35,35,35,35	0
4	NAG	D	502	14/15	0.95	0.12	-0.66	31,38,47,51	0
4	NAG	A	505	14/15	0.93	0.13	-0.79	33,41,49,60	0
4	NAG	A	502	14/15	0.94	0.13	-0.86	38,43,53,54	0
4	NAG	B	502	14/15	0.90	0.13	-1.00	47,59,72,73	0
4	NAG	B	505	14/15	0.94	0.10	-1.17	46,54,70,70	0
7	GAL	D	506	11/12	0.88	0.12	-1.23	46,52,65,76	0
4	NAG	E	505	14/15	0.93	0.11	-1.50	44,51,60,62	0
4	NAG	D	505	14/15	0.95	0.11	-1.72	27,40,52,55	0
6	MAN	D	504	11/12	0.94	0.11	-	31,44,56,58	0
6	MAN	E	504	11/12	0.88	0.15	-	50,62,75,76	0
6	MAN	A	504	11/12	0.94	0.10	-	30,41,50,51	0
6	MAN	B	507	11/12	0.76	0.14	-	72,83,88,92	0
6	MAN	D	508	11/12	0.86	0.13	-	58,68,75,85	0
5	BMA	B	503	11/12	0.85	0.09	-	48,59,65,70	0
4	NAG	A	501	14/15	0.93	0.12	-	37,43,55,57	0
5	BMA	E	503	11/12	0.93	0.08	-	51,57,67,71	0
5	BMA	D	503	11/12	0.97	0.09	-	41,46,53,61	0
6	MAN	E	507	11/12	0.67	0.17	-	78,84,88,89	0
8	FUC	E	508	10/11	0.81	0.22	-	75,82,97,98	0
6	MAN	B	504	11/12	0.89	0.11	-	42,63,70,72	0
5	BMA	A	503	11/12	0.96	0.09	-	35,40,49,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	E	501	14/15	0.92	0.12	-	53,61,79,82	0
4	NAG	E	502	14/15	0.91	0.11	-	43,58,65,69	0
4	NAG	B	501	14/15	0.93	0.12	-	58,64,78,78	0
8	FUC	A	507	10/11	0.92	0.15	-	47,50,59,60	0
4	NAG	D	501	14/15	0.94	0.13	-	34,40,44,51	0
6	MAN	A	508	11/12	0.83	0.14	-	53,61,66,85	0
8	FUC	D	507	10/11	0.93	0.12	-	36,43,45,48	0
8	FUC	B	508	10/11	0.87	0.15	-	74,86,93,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.