



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2017 – 08:18 PM EDT

PDB ID : 4Z7N
Title : Integrin alphaIIb beta3 in complex with AGDV peptide
Authors : Lin, F.-Y.; Zhu, J.; Springer, T.A.
Deposited on : unknown
Resolution : 2.60 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

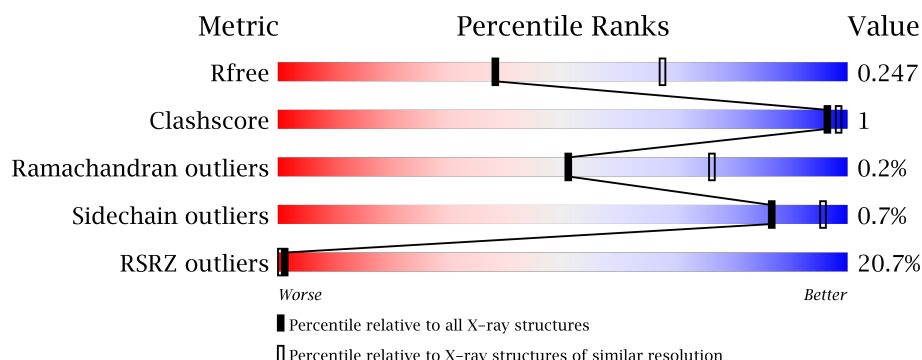
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



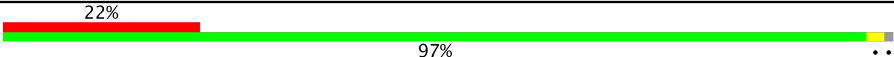
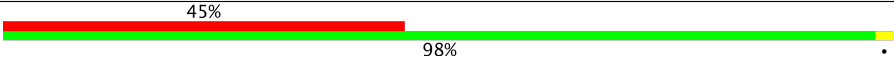
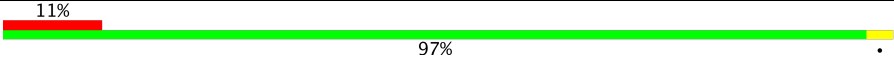
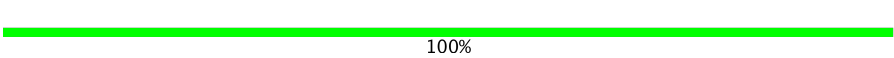

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	455	
1	C	455	
2	B	469	
2	D	469	
3	E	219	

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Mol	Chain	Length	Quality of chain
3	H	219	
4	F	214	
4	L	214	
5	G	4	
5	J	4	

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	SO4	A	505	-	-	-	X
7	SO4	A	508	-	-	-	X
9	MN	B	2002	-	-	-	X
9	MN	D	2003	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 41957 atoms, of which 20198 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	H	N	O	S	1	2	0
			6839	2223	3341	602	665	8			
1	C	453	Total	C	H	N	O	S	0	0	0
			6782	2207	3308	598	661	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	464	Total	C	H	N	O	S	4	0	0
			7075	2229	3496	611	706	33			
2	D	469	Total	C	H	N	O	S	10	0	0
			7140	2248	3528	617	713	34			

- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			

- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	1	0	0
			3190	1019	1553	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	268	341	9			

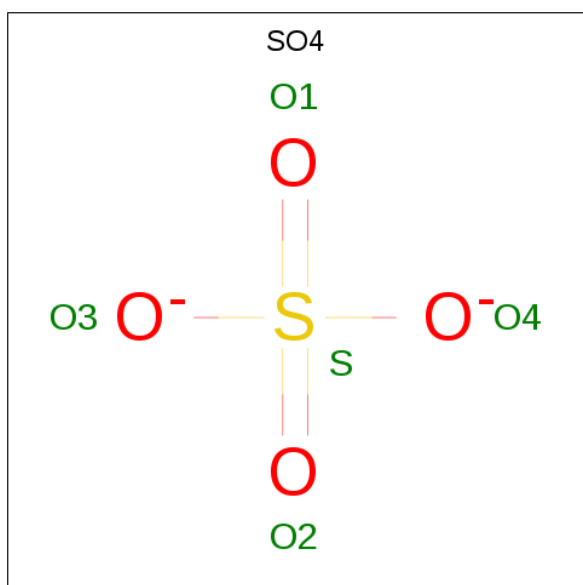
- Molecule 5 is a protein called Tetrapeptide ALA-GLY-ASP-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	4	Total	C	H	N	O	0	0	0
			45	14	20	4	7			
5	J	4	Total	C	H	N	O	0	0	0
			45	14	20	4	7			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Ca	0	0
			4	4		
6	C	4	Total	Ca	0	0
			4	4		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

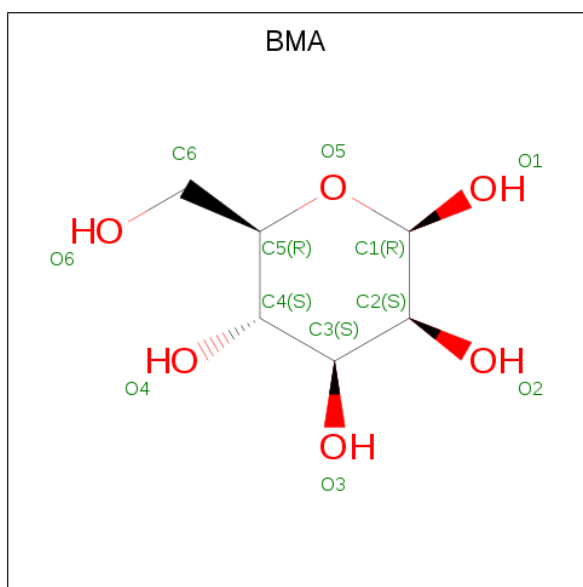
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	3	Total	Mn	0	0
			3	3		
9	D	3	Total	Mn	0	0
			3	3		

- Molecule 10 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



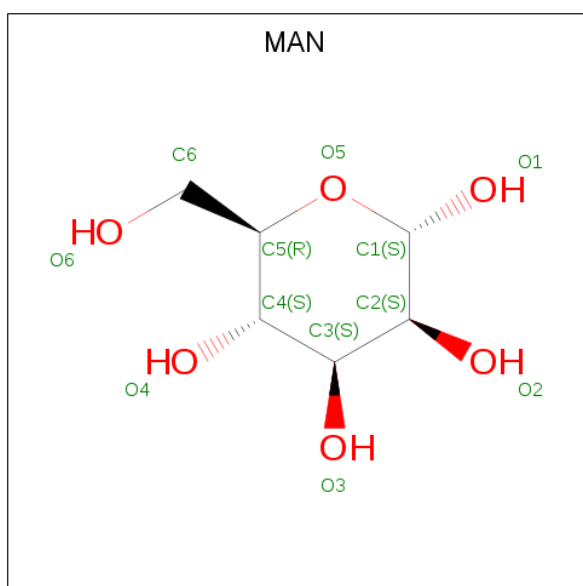
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
10	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
10	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
10	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	D	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
10	D	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
10	D	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
10	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 11 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	O	0	0
			19	6	8	5		
11	D	1	Total	C	H	O	0	0
			20	6	9	5		

- Molecule 12 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	H	O	0	0
			21	6	10	5		
12	B	1	Total	C	H	O	0	0
			21	6	10	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	Cl	0	0
			1	1		

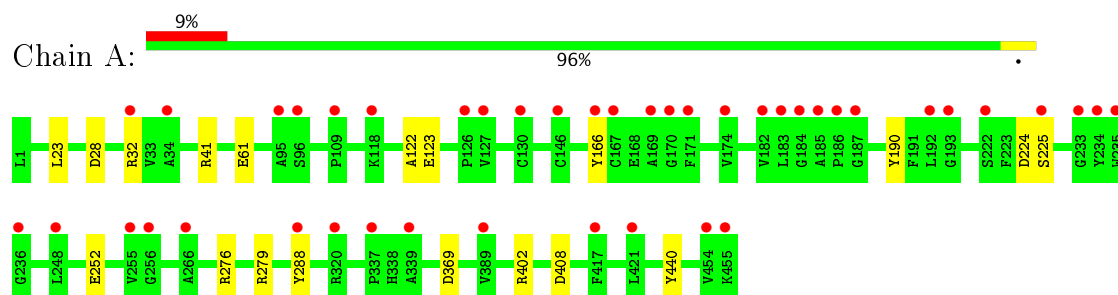
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	319	Total	O	0	0
			319	319		
14	B	144	Total	O	0	0
			144	144		
14	C	123	Total	O	0	0
			123	123		
14	D	75	Total	O	0	0
			75	75		
14	E	9	Total	O	0	0
			9	9		
14	F	9	Total	O	0	0
			9	9		
14	H	16	Total	O	0	0
			16	16		
14	L	28	Total	O	0	0
			28	28		
14	G	5	Total	O	0	0
			5	5		
14	J	4	Total	O	0	0
			4	4		

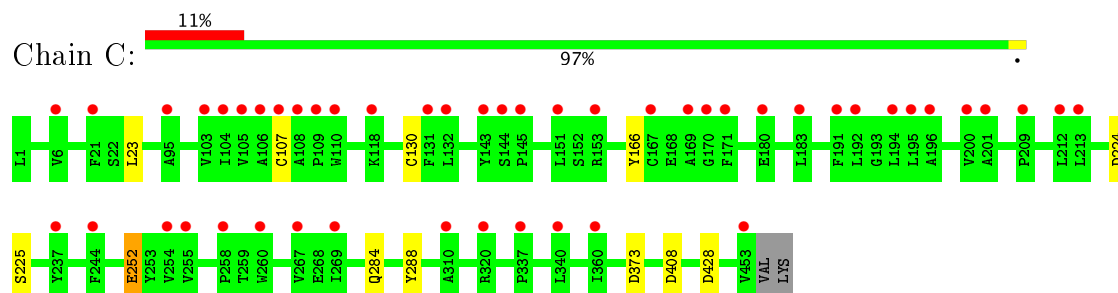
3 Residue-property plots [i](#)

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

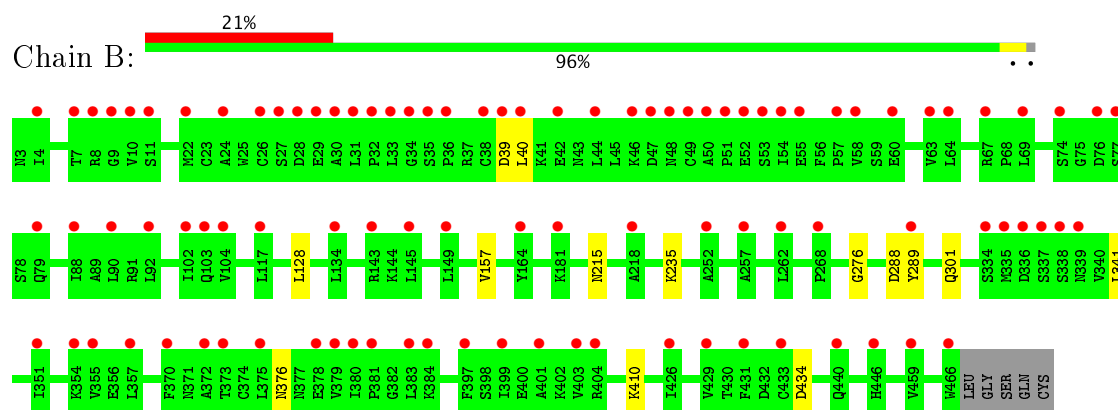
• Molecule 1: Integrin alpha-IIb



• Molecule 1: Integrin alpha-IIb

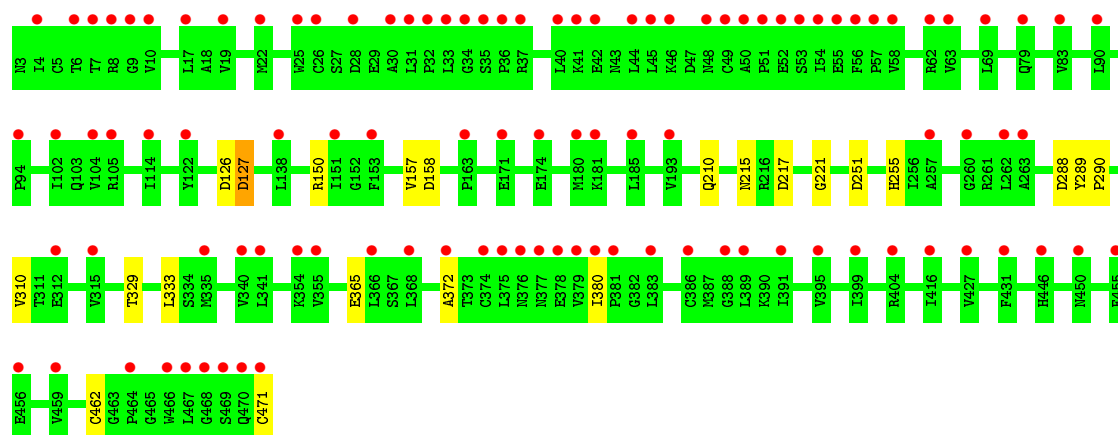


• Molecule 2: Integrin beta-3

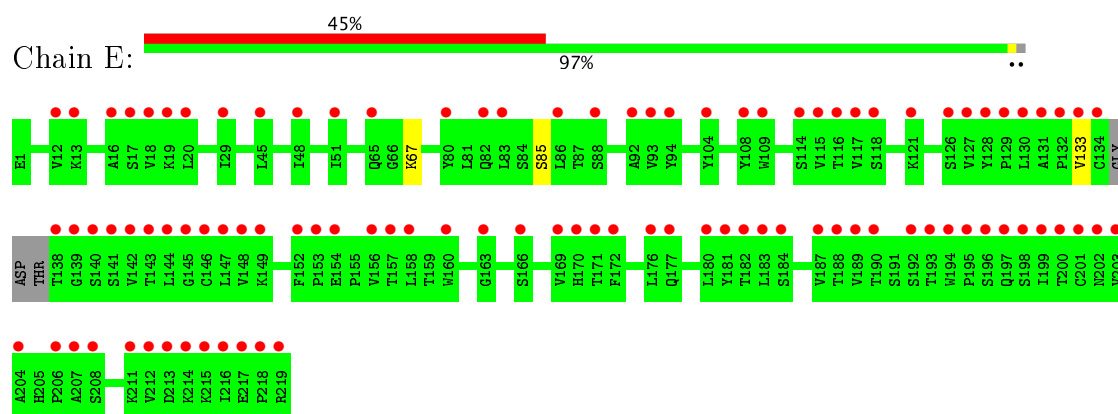


• Molecule 2: Integrin beta-3

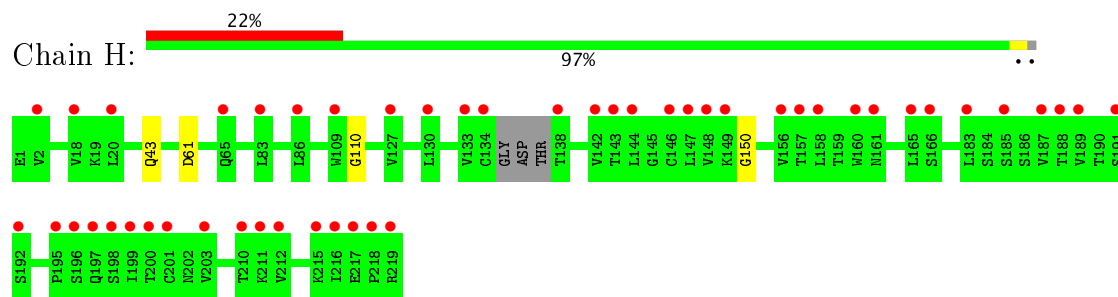




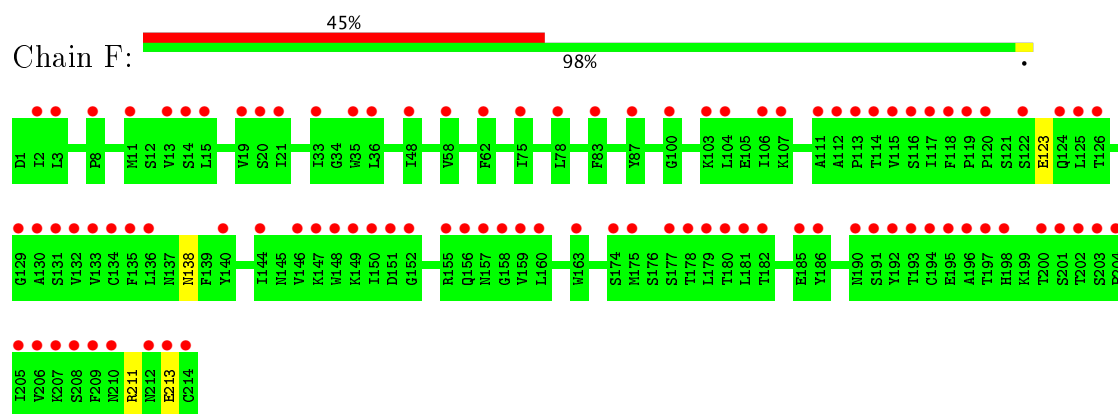
• Molecule 3: Monoclonal antibody 10E5 heavy chain



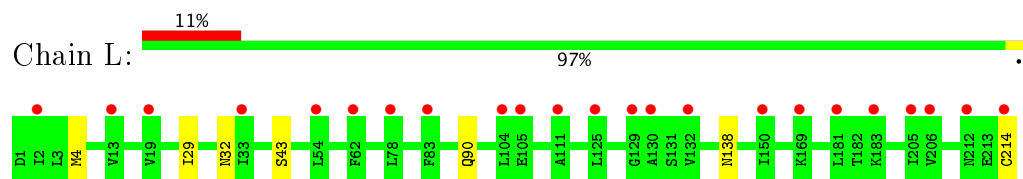
• Molecule 3: Monoclonal antibody 10E5 heavy chain



• Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 5: Tetrapeptide ALA-GLY-ASP-VAL



There are no outlier residues recorded for this chain.

- Molecule 5: Tetrapeptide ALA-GLY-ASP-VAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	256.88Å 144.37Å 104.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.60 49.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.19-2.60) 84.0 (49.19-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10pre_2104: ???)	Depositor
R, R_{free}	0.230 , 0.253 0.228 , 0.247	Depositor DCC
R_{free} test set	1708 reflections (1.69%)	DCC
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41957	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: GOL, BMA, NAG, CL, CA, MN, SO4, 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	0.30	0/3600	0.44	0/4905
1	C	0.27	0/3570	0.43	0/4865
2	B	0.25	0/3645	0.43	0/4942
2	D	0.25	0/3678	0.41	0/4986
3	E	0.25	0/1684	0.44	0/2305
3	H	0.25	0/1684	0.43	0/2305
4	F	0.24	0/1673	0.41	0/2269
4	L	0.24	0/1673	0.42	0/2269
5	G	0.19	0/24	0.45	0/30
5	J	0.21	0/24	0.37	0/30
All	All	0.26	0/21255	0.43	0/28906

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	341	LEU	Peptide

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	3498	3341	3341	13	0
1	C	3474	3308	3308	7	0
2	B	3579	3496	3496	5	0
2	D	3612	3528	3527	12	0
3	E	1642	1600	1600	1	0
3	H	1642	1600	1600	3	0
4	F	1637	1553	1553	2	0
4	L	1637	1553	1553	3	0
5	G	25	20	20	0	0
5	J	25	20	20	0	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
7	A	20	0	0	0	0
7	C	15	0	0	0	0
7	L	5	0	0	0	0
8	A	6	8	8	0	0
9	B	3	0	0	0	0
9	D	3	0	0	0	0
10	B	70	62	62	4	0
10	D	70	62	62	0	0
11	B	11	8	8	0	0
11	D	11	9	9	0	0
12	B	22	20	20	0	0
12	D	11	10	10	0	0
13	C	1	0	0	0	0
14	A	319	0	0	9	1
14	B	144	0	0	1	0
14	C	123	0	0	4	1
14	D	75	0	0	6	0
14	E	9	0	0	0	0
14	F	9	0	0	0	0
14	G	5	0	0	0	0
14	H	16	0	0	1	0
14	J	4	0	0	0	0
14	L	28	0	0	0	0
All	All	21759	20198	20197	49	1

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 1.

All (49) 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:276:ARG:NH1	14:A:604:HOH:O	2.17	0.78
1:A:369:ASP:OD2	14:A:601:HOH:O	2.02	0.77
2:B:235:LYS:NZ	2:B:276:GLY:O	2.24	0.71
1:C:408:ASP:OD2	14:C:601:HOH:O	2.10	0.69
10:B:2004:NAG:H3	10:B:2004:NAG:H83	1.73	0.69
1:A:276:ARG:NH1	14:A:612:HOH:O	2.26	0.69
1:C:428:ASP:OD2	14:C:602:HOH:O	2.14	0.64
2:D:462:CYS:SG	2:D:471:CYS:N	2.71	0.64
1:C:373:ASP:O	14:C:603:HOH:O	2.14	0.63
1:A:402:ARG:O	14:A:602:HOH:O	2.15	0.63
1:A:369:ASP:CG	14:A:601:HOH:O	2.37	0.61
1:C:284:GLN:OE1	14:C:604:HOH:O	2.17	0.57
1:A:190:TYR:O	14:A:606:HOH:O	2.18	0.56
1:A:408:ASP:OD2	14:A:605:HOH:O	2.17	0.56
10:B:2004:NAG:C8	10:B:2004:NAG:H3	2.37	0.55
1:C:252:GLU:N	1:C:252:GLU:OE2	2.39	0.55
2:D:288:ASP:OD1	2:D:289:TYR:N	2.40	0.55
1:A:440:TYR:OH	14:A:603:HOH:O	2.16	0.55
2:D:210:GLN:OE1	14:D:2101:HOH:O	2.18	0.54
4:F:211:ARG:O	4:F:213:GLU:N	2.41	0.53
10:B:2004:NAG:C3	10:B:2004:NAG:H83	2.41	0.51
1:C:224:ASP:OD1	1:C:225:SER:N	2.41	0.51
2:B:288:ASP:OD1	2:B:289:TYR:N	2.40	0.50
2:B:410:LYS:NZ	2:B:434:ASP:OD2	2.44	0.49
2:D:221:GLY:O	14:D:2102:HOH:O	2.19	0.49
3:H:61:ASP:OD1	14:H:301:HOH:O	2.19	0.49
2:D:217:ASP:OD2	2:D:255:HIS:NE2	2.43	0.49
4:F:123:GLU:OE1	4:F:123:GLU:N	2.43	0.48
2:D:290:PRO:O	14:D:2103:HOH:O	2.20	0.48
2:D:372:ALA:O	2:D:380:ILE:N	2.47	0.47
3:H:43:GLN:N	3:H:43:GLN:OE1	2.46	0.46
2:D:310:VAL:O	2:D:333:LEU:N	2.44	0.46
1:C:107:CYS:HA	1:C:130:CYS:HA	1.98	0.46
3:E:67:LYS:NZ	3:E:85:SER:O	2.50	0.44
1:A:122:ALA:O	1:A:123:GLU:HB2	2.18	0.44
4:L:4:MET:HE1	4:L:90:GLN:HB3	2.01	0.43
2:D:251:ASP:OD2	14:D:2104:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:NH2	14:A:634:HOH:O	2.44	0.42
1:A:224:ASP:OD1	1:A:225:SER:N	2.43	0.42
2:D:126:ASP:OD1	2:D:127:ASP:N	2.52	0.42
1:A:28:ASP:OD1	1:A:32:ARG:N	2.49	0.42
10:B:2004:NAG:C8	10:B:2004:NAG:C3	2.95	0.42
1:A:276:ARG:HD2	1:A:279:ARG:HB2	2.02	0.41
4:L:29:ILE:O	4:L:32:ASN:ND2	2.48	0.41
2:D:150:ARG:NH1	14:D:2111:HOH:O	2.45	0.41
2:B:301:GLN:NE2	14:B:2109:HOH:O	2.35	0.41
2:B:39:ASP:OD1	2:B:40:LEU:N	2.46	0.41
3:H:110:GLY:O	4:L:43:SER:OG	2.29	0.40
2:D:329:THR:N	14:D:2108:HOH:O	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:605:HOH:O	14:C:632:HOH:O[1_554]	2.13	0.07

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	455/455 (100%)	434 (95%)	21 (5%)	0	100	100
1	C	451/455 (99%)	432 (96%)	19 (4%)	0	100	100
2	B	462/469 (98%)	438 (95%)	23 (5%)	1 (0%)	51	76
2	D	467/469 (100%)	445 (95%)	21 (4%)	1 (0%)	51	76
3	E	212/219 (97%)	197 (93%)	14 (7%)	1 (0%)	32	58
3	H	212/219 (97%)	202 (95%)	9 (4%)	1 (0%)	32	58
4	F	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	32	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	32	58
5	G	2/4 (50%)	2 (100%)	0	0	100	100
5	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	2687/2722 (99%)	2559 (95%)	122 (4%)	6 (0%)	51	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	133	VAL
2	B	157	VAL
4	L	138	ASN
2	D	157	VAL
4	F	138	ASN
3	H	150	GLY

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	365/363 (101%)	360 (99%)	5 (1%)	71	89
1	C	361/363 (99%)	357 (99%)	4 (1%)	78	92
2	B	411/415 (99%)	408 (99%)	3 (1%)	87	96
2	D	415/415 (100%)	411 (99%)	4 (1%)	80	93
3	E	187/189 (99%)	187 (100%)	0	100	100
3	H	187/189 (99%)	187 (100%)	0	100	100
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	187 (100%)	1 (0%)	91	97
5	G	2/2 (100%)	2 (100%)	0	100	100
5	J	2/2 (100%)	2 (100%)	0	100	100
All	All	2306/2314 (100%)	2289 (99%)	17 (1%)	87	96

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	252	GLU
1	A	288	TYR
2	B	128	LEU
2	B	215	ASN
2	B	376	ASN
1	C	23	LEU
1	C	166	TYR
1	C	252	GLU
1	C	288	TYR
2	D	127	ASP
2	D	158	ASP
2	D	215	ASN
2	D	365	GLU
4	L	214	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

Of 39 ligands modelled in this entry, 15 are monoatomic - leaving 24 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
7	SO4	A	505	-	4,4,4	0.15	0	6,6,6	0.05	0
7	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.06	0
7	SO4	A	507	-	4,4,4	0.13	0	6,6,6	0.06	0
7	SO4	A	508	-	4,4,4	0.13	0	6,6,6	0.07	0
8	GOL	A	509	-	5,5,5	0.39	0	5,5,5	0.23	0
10	NAG	B	2004	2	14,14,15	0.45	0	15,19,21	1.48	2 (13%)
10	NAG	B	2005	10,2	14,14,15	0.29	0	15,19,21	0.47	0
10	NAG	B	2006	11,10	14,14,15	0.21	0	15,19,21	0.47	0
11	BMA	B	2007	10,12	11,11,12	0.79	1 (9%)	13,15,17	0.77	0
12	MAN	B	2008	11	11,11,12	0.68	0	13,15,17	1.14	2 (15%)
12	MAN	B	2009	11	11,11,12	0.68	0	13,15,17	1.13	2 (15%)
10	NAG	B	2010	10,2	14,14,15	0.31	0	15,19,21	0.39	0
10	NAG	B	2011	10	14,14,15	0.23	0	15,19,21	0.46	0
7	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.06	0
7	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.06	0
7	SO4	C	508	-	4,4,4	0.14	0	6,6,6	0.07	0
10	NAG	D	2004	2	14,14,15	0.24	0	15,19,21	0.43	0
10	NAG	D	2005	10,2	14,14,15	0.26	0	15,19,21	0.47	0
10	NAG	D	2006	11,10	14,14,15	0.23	0	15,19,21	0.46	0
11	BMA	D	2007	10,12	11,11,12	0.59	0	13,15,17	0.75	0
12	MAN	D	2008	11	11,11,12	0.72	0	13,15,17	1.09	2 (15%)
10	NAG	D	2009	10,2	14,14,15	0.40	0	15,19,21	0.39	0
10	NAG	D	2010	10	14,14,15	0.23	0	15,19,21	0.47	0
7	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.06	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
7	SO4	A	505	-	-	0/0/0/0	0/0/0/0
7	SO4	A	506	-	-	0/0/0/0	0/0/0/0
7	SO4	A	507	-	-	0/0/0/0	0/0/0/0
7	SO4	A	508	-	-	0/0/0/0	0/0/0/0
8	GOL	A	509	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
10	NAG	B	2005	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	2006	11,10	-	0/6/23/26	0/1/1/1
11	BMA	B	2007	10,12	-	0/2/19/22	0/1/1/1
12	MAN	B	2008	11	-	0/2/19/22	0/1/1/1
12	MAN	B	2009	11	-	0/2/19/22	0/1/1/1
10	NAG	B	2010	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	2011	10	-	0/6/23/26	0/1/1/1
7	SO4	C	501	-	-	0/0/0/0	0/0/0/0
7	SO4	C	507	-	-	0/0/0/0	0/0/0/0
7	SO4	C	508	-	-	0/0/0/0	0/0/0/0
10	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
10	NAG	D	2005	10,2	-	0/6/23/26	0/1/1/1
10	NAG	D	2006	11,10	-	0/6/23/26	0/1/1/1
11	BMA	D	2007	10,12	-	0/2/19/22	0/1/1/1
12	MAN	D	2008	11	-	0/2/19/22	0/1/1/1
10	NAG	D	2009	10,2	-	0/6/23/26	0/1/1/1
10	NAG	D	2010	10	-	0/6/23/26	0/1/1/1
7	SO4	L	301	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	2007	BMA	O5-C1	-2.05	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2008	MAN	O2-C2-C3	-2.47	105.33	110.17
12	D	2008	MAN	O2-C2-C3	-2.37	105.52	110.17
12	B	2009	MAN	O2-C2-C3	-2.31	105.65	110.17
12	B	2008	MAN	C1-O5-C5	2.05	115.00	112.17
12	D	2008	MAN	C1-O5-C5	2.09	115.05	112.17
12	B	2009	MAN	C1-O5-C5	2.27	115.30	112.17
10	B	2004	NAG	C1-O5-C5	2.63	115.79	112.17
10	B	2004	NAG	C2-N2-C7	3.88	128.60	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	2004	NAG	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	455/455 (100%)	1.00	43 (9%) 9 5	43, 58, 83, 169	1 (0%)
1	C	453/455 (99%)	0.98	49 (10%) 6 4	52, 76, 104, 137	0
2	B	464/469 (98%)	1.35	97 (20%) 1 0	47, 89, 159, 185	1 (0%)
2	D	469/469 (100%)	1.25	104 (22%) 1 0	58, 98, 147, 177	1 (0%)
3	E	216/219 (98%)	2.60	99 (45%) 0 0	86, 135, 218, 243	0
3	H	216/219 (98%)	1.27	49 (22%) 1 0	69, 113, 158, 181	0
4	F	214/214 (100%)	2.70	96 (44%) 0 0	93, 135, 219, 252	1 (0%)
4	L	214/214 (100%)	0.86	23 (10%) 7 4	70, 101, 124, 160	0
5	G	4/4 (100%)	1.04	0 100 100	54, 64, 67, 68	0
5	J	4/4 (100%)	2.18	2 (50%) 0 0	80, 81, 81, 86	0
All	All	2709/2722 (99%)	1.37	562 (20%) 1 0	43, 92, 170, 252	4 (0%)

All (562) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	179	LEU	15.1
3	E	198	SER	14.8
3	E	144	LEU	13.8
4	F	193	THR	13.0
3	E	131	ALA	12.8
4	F	194	CYS	12.2
4	F	130	ALA	12.2
3	E	142	VAL	11.5
3	E	132	PRO	11.4
4	F	195	GLU	10.9
3	E	133	VAL	10.8
4	F	148	TRP	10.6
3	H	216	ILE	10.3

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Mol	Chain	Res	Type	RSRZ
4	F	181	LEU	10.3
4	F	206	VAL	10.2
4	F	214	CYS	10.1
3	E	183	LEU	9.9
3	E	194	TRP	9.4
3	E	219	ARG	9.3
3	E	130	LEU	9.0
4	F	205	ILE	8.9
3	E	148	VAL	8.8
3	E	216	ILE	8.7
4	F	208	SER	8.7
4	F	180	THR	8.4
3	E	200	THR	8.3
4	F	209	PHE	8.3
2	D	375	LEU	8.2
3	E	189	VAL	8.1
4	F	126	THR	8.0
2	B	33	LEU	7.9
4	F	132	VAL	7.9
4	F	135	PHE	7.8
3	E	199	ILE	7.8
4	F	160	LEU	7.7
4	F	117	ILE	7.5
4	L	214	CYS	7.4
4	F	125	LEU	7.3
1	A	455	LYS	7.3
4	F	178	THR	7.2
4	F	118	PHE	7.2
2	D	471	CYS	7.2
2	B	338	SER	7.1
2	B	36	PRO	7.0
4	F	115	VAL	7.0
3	E	147	LEU	7.0
3	H	158	LEU	6.9
4	F	192	TYR	6.9
4	F	159	VAL	6.9
4	F	116	SER	6.9
2	B	51	PRO	6.9
3	E	146	CYS	6.7
2	B	337	SER	6.7
3	H	144	LEU	6.6
3	E	195	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
4	F	119	PRO	6.5
2	D	44	LEU	6.5
2	B	339	ASN	6.4
4	F	120	PRO	6.4
4	F	134	CYS	6.4
1	A	454	VAL	6.4
3	E	160	TRP	6.4
3	E	218	PRO	6.4
3	E	134	CYS	6.4
3	E	207	ALA	6.3
2	D	54	ILE	6.3
4	F	204	PRO	6.2
3	E	127	VAL	6.2
4	F	104	LEU	6.2
2	B	10	VAL	6.1
3	E	176	LEU	6.1
4	F	157	ASN	6.1
4	F	133	VAL	6.0
2	B	46	LYS	6.0
4	F	207	LYS	6.0
3	E	129	PRO	5.9
2	D	380	ILE	5.8
3	E	190	THR	5.8
2	D	9	GLY	5.8
3	E	187	VAL	5.7
2	B	54	ILE	5.7
2	D	33	LEU	5.7
4	F	155	ARG	5.7
4	F	147	LYS	5.7
3	E	145	GLY	5.7
2	B	336	ASP	5.7
4	F	136	LEU	5.5
4	F	196	ALA	5.5
2	B	380	ILE	5.4
3	E	201	CYS	5.4
2	B	30	ALA	5.4
5	J	411	VAL	5.4
2	B	440	GLN	5.4
2	B	44	LEU	5.3
2	D	468	GLY	5.3
2	B	53	SER	5.3
3	E	217	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
3	H	138	THR	5.2
4	F	144	ILE	5.2
3	H	133	VAL	5.2
3	E	138	THR	5.1
2	D	36	PRO	5.1
3	E	128	TYR	5.1
4	F	78	LEU	5.1
2	B	181	LYS	5.1
3	E	139	GLY	5.0
3	E	12	VAL	5.0
3	E	83	LEU	5.0
3	E	188	THR	4.9
3	H	198	SER	4.9
4	F	150	ILE	4.9
2	B	92	LEU	4.8
3	E	215	LYS	4.8
3	H	134	CYS	4.8
3	H	160	TRP	4.8
3	H	142	VAL	4.8
3	E	115	VAL	4.8
3	E	212	VAL	4.8
4	F	151	ASP	4.8
2	D	379	VAL	4.7
4	F	129	GLY	4.7
3	H	201	CYS	4.7
4	F	212	ASN	4.7
3	E	181	TYR	4.7
3	E	211	LYS	4.7
3	E	86	LEU	4.7
3	E	143	THR	4.6
3	H	189	VAL	4.6
3	H	203	VAL	4.6
2	B	8	ARG	4.6
2	B	28	ASP	4.6
3	E	156	VAL	4.5
1	C	453	VAL	4.5
4	F	149	LYS	4.5
2	B	34	GLY	4.5
2	B	375	LEU	4.5
2	B	76	ASP	4.5
4	L	104	LEU	4.5
4	L	212	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	35	SER	4.4
4	F	131	SER	4.4
4	F	146	VAL	4.4
4	F	202	THR	4.4
4	F	87	TYR	4.4
2	D	51	PRO	4.4
2	B	48	ASN	4.4
3	E	157	THR	4.3
2	B	49	CYS	4.3
2	B	9	GLY	4.3
3	E	204	ALA	4.2
4	F	83	PHE	4.2
3	H	197	GLN	4.2
4	F	113	PRO	4.2
2	D	450	ASN	4.2
3	E	197	GLN	4.1
2	B	466	TRP	4.1
4	L	129	GLY	4.1
2	B	4	ILE	4.1
4	F	21	ILE	4.1
2	D	48	ASN	4.1
3	H	215	LYS	4.0
2	D	34	GLY	4.0
4	F	158	GLY	4.0
1	C	320	ARG	4.0
2	D	381	PRO	4.0
4	F	124	GLN	4.0
3	H	219	ARG	4.0
2	D	376	ASN	3.9
4	F	191	SER	3.9
2	D	58	VAL	3.9
2	D	404	ARG	3.9
4	F	15	LEU	3.9
3	E	18	VAL	3.8
1	A	337	PRO	3.8
2	D	8	ARG	3.8
3	E	140	SER	3.8
4	F	11	MET	3.8
2	B	69	LEU	3.8
4	L	206	VAL	3.7
3	E	184	SER	3.7
2	D	378	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	17	LEU	3.7
3	H	212	VAL	3.7
2	D	181	LYS	3.7
2	B	459	VAL	3.7
2	B	88	ILE	3.7
3	E	19	LYS	3.7
2	B	381	PRO	3.6
4	F	33	ILE	3.6
4	F	106	ILE	3.6
2	D	31	LEU	3.6
3	E	149	LYS	3.6
1	C	337	PRO	3.6
3	E	182	THR	3.6
3	H	188	THR	3.6
3	E	126	SER	3.6
2	D	63	VAL	3.6
4	L	183	LYS	3.5
4	F	182	THR	3.5
3	E	48	ILE	3.5
2	D	90	LEU	3.5
3	E	203	VAL	3.5
4	F	186	TYR	3.5
2	B	370	PHE	3.5
2	D	30	ALA	3.5
2	D	466	TRP	3.4
4	F	107	LYS	3.4
3	E	196	SER	3.4
2	B	90	LEU	3.4
2	D	377	ASN	3.4
3	H	210	THR	3.4
4	L	111	ALA	3.4
2	D	40	LEU	3.4
3	E	16	ALA	3.4
2	D	83	VAL	3.4
3	E	193	THR	3.3
3	E	172	PHE	3.3
2	B	373	THR	3.3
1	A	417	PHE	3.3
2	B	50	ALA	3.3
4	F	122	SER	3.3
4	F	175	MET	3.3
2	B	383	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	10	VAL	3.2
2	B	26	CYS	3.2
3	H	200	THR	3.2
2	D	22	MET	3.2
2	D	56	PHE	3.2
2	B	117	LEU	3.2
4	F	20	SER	3.2
3	E	65	GLN	3.2
3	H	166	SER	3.2
3	H	217	GLU	3.2
4	F	8	PRO	3.1
2	D	45	LEU	3.1
3	H	127	VAL	3.1
3	H	165	LEU	3.1
3	E	177	GLN	3.1
4	L	83	PHE	3.1
2	D	470	GLN	3.1
3	E	180	LEU	3.1
2	D	354	LYS	3.1
1	A	339	ALA	3.1
4	L	181	LEU	3.1
2	B	289	TYR	3.1
2	B	32	PRO	3.0
2	D	171	GLU	3.0
2	D	62	ARG	3.0
2	D	46	LYS	3.0
4	F	197	THR	3.0
3	E	29	ILE	3.0
2	B	29	GLU	3.0
2	B	42	GLU	3.0
4	F	156	GLN	3.0
2	D	26	CYS	3.0
3	E	141	SER	3.0
2	D	459	VAL	3.0
1	C	131	PHE	3.0
2	D	52	GLU	3.0
4	F	13	VAL	3.0
3	H	192	SER	3.0
4	F	201	SER	3.0
2	D	7	THR	3.0
1	A	320	ARG	3.0
2	D	57	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
4	L	205	ILE	2.9
1	C	143	TYR	2.9
2	B	145	LEU	2.9
2	D	37	ARG	2.9
3	E	45	LEU	2.9
3	E	214	LYS	2.9
2	D	469	SER	2.9
3	E	202	ASN	2.9
3	E	116	THR	2.9
2	B	7	THR	2.9
3	H	130	LEU	2.9
3	E	169	VAL	2.9
1	C	269	ILE	2.9
2	D	391	ILE	2.9
3	H	199	ILE	2.9
2	D	456	GLU	2.9
3	E	171	THR	2.9
2	D	42	GLU	2.9
1	A	183	LEU	2.9
5	J	408	ALA	2.9
2	B	35	SER	2.8
3	H	196	SER	2.8
3	H	147	LEU	2.8
4	F	198	HIS	2.8
2	D	174	GLU	2.8
2	B	399	ILE	2.8
4	L	33	ILE	2.8
4	L	62	PHE	2.8
2	B	52	GLU	2.8
2	D	185	LEU	2.8
2	B	39	ASP	2.8
3	E	88	SER	2.8
1	C	255	VAL	2.8
4	F	35	TRP	2.8
1	C	200	VAL	2.8
2	B	384	LYS	2.8
2	D	455	PHE	2.8
1	C	106	ALA	2.8
4	F	200	THR	2.8
2	B	357	LEU	2.8
2	B	77	SER	2.8
2	B	149	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	429	VAL	2.8
2	B	74	SER	2.8
3	E	117	VAL	2.7
4	F	100	GLY	2.7
1	C	340	LEU	2.7
4	F	14	SER	2.7
2	B	104	VAL	2.7
2	B	334	SER	2.7
2	B	79	GLN	2.7
4	F	213	GLU	2.7
2	B	102	ILE	2.7
3	H	83	LEU	2.7
4	F	2	ILE	2.7
1	A	185	ALA	2.7
2	B	38	CYS	2.7
4	F	177	SER	2.7
2	B	378	GLU	2.6
2	B	27	SER	2.6
3	E	13	LYS	2.6
3	E	93	VAL	2.6
3	H	18	VAL	2.6
3	H	191	SER	2.6
3	E	92	ALA	2.6
2	D	467	LEU	2.6
3	E	163	GLY	2.6
1	C	109	PRO	2.6
4	L	105	GLU	2.6
3	H	218	PRO	2.6
2	D	69	LEU	2.6
3	H	86	LEU	2.6
2	B	397	PHE	2.6
1	C	167	CYS	2.6
2	B	143	ARG	2.6
2	D	431	PHE	2.6
2	D	427	VAL	2.6
4	F	75	ILE	2.6
1	A	32	ARG	2.6
2	D	28	ASP	2.6
1	C	196	ALA	2.5
1	C	105	VAL	2.5
2	D	79	GLN	2.5
1	C	244	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	255	VAL	2.5
1	C	183	LEU	2.5
3	E	20	LEU	2.5
1	C	171	PHE	2.5
1	A	192	LEU	2.5
1	A	248	LEU	2.5
2	B	403	VAL	2.5
2	D	340	VAL	2.5
2	D	341	LEU	2.5
1	A	187	GLY	2.5
2	B	55	GLU	2.5
3	H	146	CYS	2.5
2	B	24	ALA	2.5
1	C	267	VAL	2.5
2	B	31	LEU	2.5
4	F	152	GLY	2.5
2	B	11	SER	2.5
2	B	67	ARG	2.5
1	A	118	LYS	2.5
1	C	95	ALA	2.5
1	C	192	LEU	2.5
2	B	134	LEU	2.5
1	A	96	SER	2.5
3	E	192	SER	2.5
4	F	62	PHE	2.4
1	A	256	GLY	2.4
3	E	121	LYS	2.4
3	E	158	LEU	2.4
1	C	103	VAL	2.4
2	D	53	SER	2.4
2	B	354	LYS	2.4
4	F	3	LEU	2.4
3	E	17	SER	2.4
1	A	235	TRP	2.4
1	A	236	GLY	2.4
2	D	464	PRO	2.4
1	C	144	SER	2.4
3	E	118	SER	2.4
1	A	182	VAL	2.4
2	B	58	VAL	2.4
3	H	148	VAL	2.4
2	D	260	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	145	PRO	2.4
1	A	266	ALA	2.4
1	C	107	CYS	2.4
1	A	109	PRO	2.4
1	C	237	TYR	2.4
1	C	153	ARG	2.4
2	D	372	ALA	2.4
3	E	114	SER	2.4
2	D	368	LEU	2.4
2	D	386	CYS	2.4
3	H	183	LEU	2.4
2	D	104	VAL	2.3
3	E	108	TYR	2.3
3	H	143	THR	2.3
1	C	110	TRP	2.3
2	D	19	VAL	2.3
2	D	114	ILE	2.3
2	D	263	ALA	2.3
1	A	222	SER	2.3
2	D	138	LEU	2.3
3	E	213	ASP	2.3
2	D	399	ILE	2.3
2	D	50	ALA	2.3
4	L	130	ALA	2.3
2	D	6	THR	2.3
4	L	125	LEU	2.3
1	A	389	VAL	2.3
2	D	25	TRP	2.3
1	A	184	GLY	2.3
1	A	233	GLY	2.3
3	E	104	TYR	2.3
1	A	186	PRO	2.3
2	B	63	VAL	2.3
2	B	379	VAL	2.3
1	C	260	TRP	2.3
2	B	401	ALA	2.3
3	H	195	PRO	2.3
2	B	404	ARG	2.3
2	D	395	VAL	2.3
3	H	211	LYS	2.3
2	D	4	ILE	2.3
2	D	416	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	111	ALA	2.3
4	F	163	TRP	2.3
2	D	389	LEU	2.3
4	L	54	LEU	2.3
2	D	374	CYS	2.3
3	H	161	ASN	2.2
2	D	335	MET	2.2
3	E	152	PHE	2.2
3	H	157	THR	2.2
2	D	366	LEU	2.2
2	D	122	TYR	2.2
2	B	57	PRO	2.2
1	A	130	CYS	2.2
2	B	433	CYS	2.2
2	D	49	CYS	2.2
1	A	127	VAL	2.2
1	C	108	ALA	2.2
2	B	426	ILE	2.2
1	C	195	LEU	2.2
2	B	40	LEU	2.2
2	B	64	LEU	2.2
2	D	41	LYS	2.2
2	D	315	VAL	2.2
3	E	166	SER	2.2
1	A	34	ALA	2.2
1	C	201	ALA	2.2
1	C	360	ILE	2.2
4	L	150	ILE	2.2
3	E	206	PRO	2.2
2	D	388	GLY	2.2
1	A	174	VAL	2.2
2	D	257	ALA	2.2
2	D	312	GLU	2.2
1	C	151	LEU	2.2
1	C	213	LEU	2.2
4	F	36	LEU	2.2
3	E	80	TYR	2.2
2	D	180	MET	2.2
4	F	58	VAL	2.2
2	B	257	ALA	2.2
2	D	151	ILE	2.2
3	E	94	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	335	MET	2.2
2	B	446	HIS	2.2
1	C	310	ALA	2.2
4	F	112	ALA	2.2
1	C	104	ILE	2.2
1	A	171	PHE	2.2
1	A	193	GLY	2.2
2	D	383	LEU	2.2
4	L	78	LEU	2.2
2	B	60	GLU	2.2
3	E	208	SER	2.2
2	B	22	MET	2.1
2	B	355	VAL	2.1
3	E	109	TRP	2.1
3	H	187	VAL	2.1
4	L	132	VAL	2.1
1	A	169	ALA	2.1
2	B	103	GLN	2.1
4	F	174	SER	2.1
3	E	170	HIS	2.1
1	A	288	TYR	2.1
1	C	170	GLY	2.1
2	D	55	GLU	2.1
2	D	163	PRO	2.1
2	D	262	LEU	2.1
4	F	185	GLU	2.1
4	F	210	ASN	2.1
1	A	167	CYS	2.1
4	L	13	VAL	2.1
3	E	153	PRO	2.1
3	H	65	GLN	2.1
1	C	132	LEU	2.1
1	C	212	LEU	2.1
2	D	446	HIS	2.1
4	L	169	LYS	2.1
1	A	95	ALA	2.1
1	A	166	TYR	2.1
3	H	156	VAL	2.1
4	F	140	TYR	2.1
2	D	94	PRO	2.1
1	C	191	PHE	2.1
2	D	153	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	154	GLU	2.1
1	C	254	VAL	2.1
2	D	193	VAL	2.1
4	F	19	VAL	2.1
4	F	114	THR	2.1
2	B	351	ILE	2.1
4	L	2	ILE	2.1
1	A	146	CYS	2.1
4	F	190	ASN	2.1
3	E	82	GLN	2.1
2	B	218	ALA	2.1
2	B	372	ALA	2.1
4	L	19	VAL	2.1
3	E	51	ILE	2.1
1	C	21	PHE	2.1
2	B	262	LEU	2.1
1	C	118	LYS	2.1
2	D	105	ARG	2.1
1	C	169	ALA	2.0
2	B	47	ASP	2.0
2	B	164	TYR	2.0
1	A	421	LEU	2.0
3	H	20	LEU	2.0
3	H	149	LYS	2.0
3	H	109	TRP	2.0
2	B	252	ALA	2.0
2	B	268	PRO	2.0
3	H	2	VAL	2.0
3	H	185	SER	2.0
4	F	48	ILE	2.0
4	F	103	LYS	2.0
4	F	203	SER	2.0
1	A	234	TYR	2.0
2	D	102	ILE	2.0
1	A	126	PRO	2.0
1	C	180	GLU	2.0
1	C	209	PRO	2.0
1	A	170	GLY	2.0
1	A	225	SER	2.0
1	C	6	VAL	2.0
2	D	355	VAL	2.0
1	C	194	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	431	PHE	2.0
1	C	258	PRO	2.0
2	D	32	PRO	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	SO4	A	505	5/5	0.79	0.36	5.56	125,126,127,132	0
7	SO4	A	508	5/5	0.89	0.30	4.23	99,103,110,111	0
9	MN	D	2003	1/1	0.80	0.31	3.48	143,143,143,143	0
9	MN	B	2002	1/1	0.59	0.32	2.58	145,145,145,145	0
9	MN	D	2001	1/1	0.91	0.29	1.94	109,109,109,109	0
6	CA	C	506	1/1	0.90	0.20	1.78	75,75,75,75	0
9	MN	D	2002	1/1	0.70	0.33	1.74	247,247,247,247	0
10	NAG	B	2004	14/15	0.88	0.33	1.68	72,92,108,110	0
8	GOL	A	509	6/6	0.85	0.28	1.47	70,84,91,94	0
6	CA	A	503	1/1	0.94	0.23	1.19	53,53,53,53	0
10	NAG	D	2004	14/15	0.78	0.25	1.06	70,91,107,107	0
10	NAG	B	2010	14/15	0.75	0.33	0.96	72,89,105,105	0
10	NAG	D	2009	14/15	0.85	0.28	0.35	70,88,104,105	0
6	CA	C	503	1/1	0.74	0.19	0.28	141,141,141,141	0
6	CA	A	501	1/1	0.88	0.17	0.09	84,84,84,84	0
6	CA	C	505	1/1	0.93	0.15	0.05	73,73,73,73	0
9	MN	B	2001	1/1	0.96	0.23	0.04	46,46,46,46	0
7	SO4	C	501	5/5	0.86	0.24	-0.45	134,134,135,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	SO4	C	507	5/5	0.86	0.19	-0.55	124,125,126,131	0
7	SO4	A	506	5/5	0.95	0.21	-0.57	110,113,114,115	0
6	CA	A	502	1/1	0.95	0.16	-0.61	46,46,46,46	0
6	CA	C	504	1/1	0.74	0.14	-0.70	123,123,123,123	0
7	SO4	L	301	5/5	0.85	0.14	-1.02	123,123,124,125	0
10	NAG	B	2005	14/15	0.93	0.17	-1.25	51,69,94,100	0
6	CA	A	504	1/1	0.98	0.16	-1.41	53,53,53,53	0
10	NAG	D	2005	14/15	0.94	0.13	-1.85	59,78,93,94	0
9	MN	B	2003	1/1	0.88	0.17	-3.19	65,65,65,65	0
11	BMA	D	2007	11/12	0.79	0.28	-	85,91,109,109	0
10	NAG	B	2011	14/15	0.83	0.30	-	88,101,122,122	0
12	MAN	B	2009	11/12	0.65	0.37	-	85,99,119,121	0
11	BMA	B	2007	11/12	0.79	0.19	-	76,89,110,110	0
10	NAG	B	2006	14/15	0.86	0.17	-	75,87,101,106	0
12	MAN	D	2008	11/12	0.87	0.30	-	82,92,110,111	0
12	MAN	B	2008	11/12	0.87	0.21	-	79,87,104,106	0
7	SO4	A	507	5/5	0.94	0.16	-	102,102,102,108	0
7	SO4	C	508	5/5	0.85	0.21	-	108,116,120,122	0
10	NAG	D	2010	14/15	0.83	0.30	-	83,100,117,125	0
10	NAG	D	2006	14/15	0.84	0.28	-	79,94,113,113	0
13	CL	C	502	1/1	0.95	0.40	-	95,95,95,95	0

6.5 Other polymers

There are no such residues in this entry.