



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:55 AM GMT

PDB ID : 3NIF
Title : The Closed Headpiece of Integrin IIb 3 and its Complex with an IIb 3 -Specific Antagonist That Does Not Induce Opening
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on : 2010-06-15
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

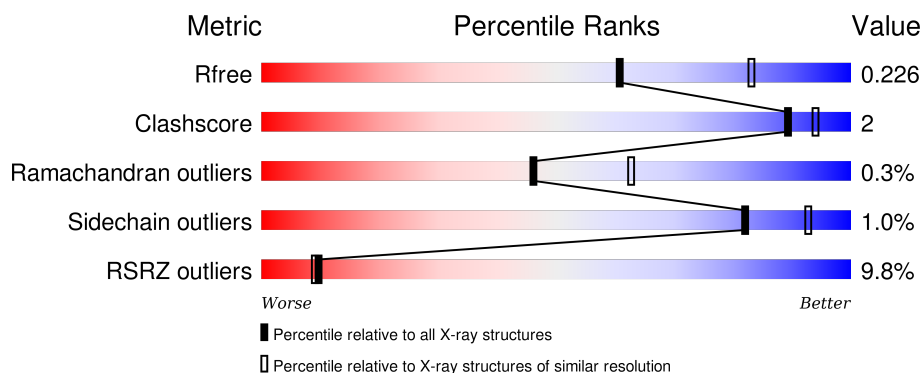
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	457	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
1	C	457	<div> <div style="width: 94%;"></div> <div>94%</div> <div style="width: 5%;"></div> <div>5%</div> </div>
2	B	471	<div> <div style="width: 8%;"></div> <div>8%</div> <div style="width: 92%;"></div> <div>92%</div> <div style="width: 7%;"></div> <div>7%</div> </div>
2	D	471	<div> <div style="width: 6%;"></div> <div>6%</div> <div style="width: 91%;"></div> <div>91%</div> <div style="width: 8%;"></div> <div>8%</div> </div>
3	E	221	<div> <div style="width: 35%;"></div> <div>35%</div> <div style="width: 87%;"></div> <div>87%</div> <div style="width: 11%;"></div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	

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
10	NAG	D	3099	X	-	-	-
11	MAN	B	3322	X	-	-	-
12	NAG	D	3371	X	-	-	-
13	MAN	D	3322	X	-	-	-
7	GOL	A	459	-	-	-	X
7	GOL	A	460	-	-	-	X
7	GOL	A	461	-	-	-	X
7	GOL	B	472	-	-	-	X
7	GOL	D	472	-	-	-	X
8	SO4	A	462	-	-	-	X
8	SO4	A	463	-	-	-	X
8	SO4	A	465	-	-	-	X
8	SO4	A	466	-	-	-	X
8	SO4	B	473	-	-	-	X
8	SO4	C	456	-	-	-	X
8	SO4	C	457	-	-	-	X
8	SO4	C	460	-	-	-	X
8	SO4	C	461	-	-	-	X
8	SO4	D	473	-	-	-	X
8	SO4	D	474	-	-	-	X
8	SO4	D	475	-	-	-	X
8	SO4	H	222	-	-	-	X
8	SO4	L	215	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 21915 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 Integrin alphaIIB beta3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	3	0
			3501	2225	605	663	8			
1	C	453	Total	C	N	O	S	0	1	0
			3481	2212	600	661	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	0	0	0
			3590	2236	613	708	33			
2	D	467	Total	C	N	O	S	0	2	0
			3615	2256	616	710	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	216	Total	C	N	O	S	0	0	0
			1638	1039	263	330	6			
3	H	219	Total	C	N	O	S	0	1	0
			1665	1055	270	334	6			

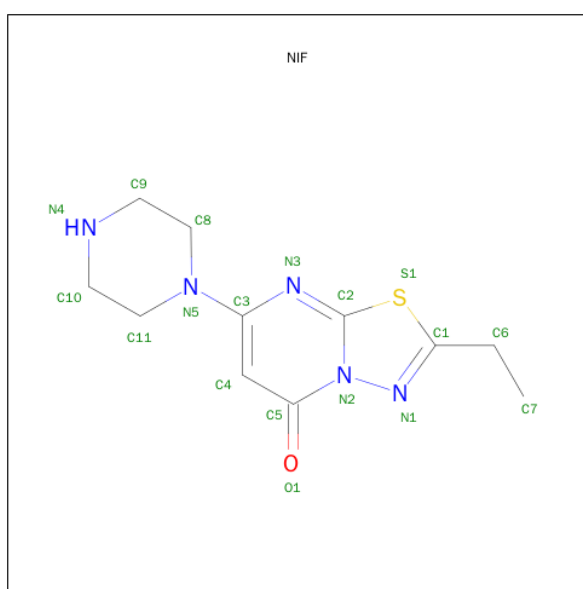
- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Ca 2 2	0	0
5	A	4	Total Ca 4 4	0	0
5	D	2	Total Ca 2 2	0	0
5	C	4	Total Ca 4 4	0	0

- Molecule 6 is 2-ETHYL-7-PIPERAZIN-1-YL-5H-[1,3,4]THIADIAZOLO[3,2-A]PYRIMIDIN-5-ONE (three-letter code: NIF) (formula: C₁₁H₁₅N₅OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 18 11 5 1 1	0	0
6	C	1	Total C N O S 18 11 5 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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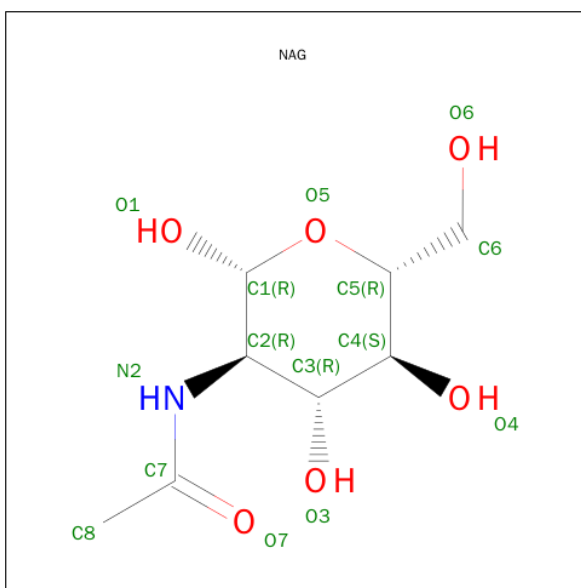
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 11 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 12 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	2	Total	C	N	O	0	0
			28	16	2	10		
12	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 13 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	D	3	Total	C	N	O	0	0
			39	22	2	15		

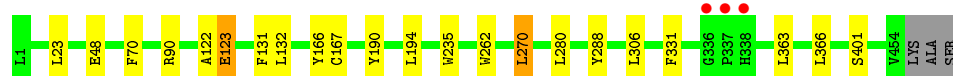
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	277	Total	O	0	0
			277	277		
14	B	175	Total	O	0	0
			175	175		
14	C	140	Total	O	0	0
			140	140		
14	D	110	Total	O	0	0
			110	110		
14	E	9	Total	O	0	0
			9	9		
14	F	6	Total	O	0	0
			6	6		
14	H	29	Total	O	0	0
			29	29		
14	L	44	Total	O	0	0
			44	44		

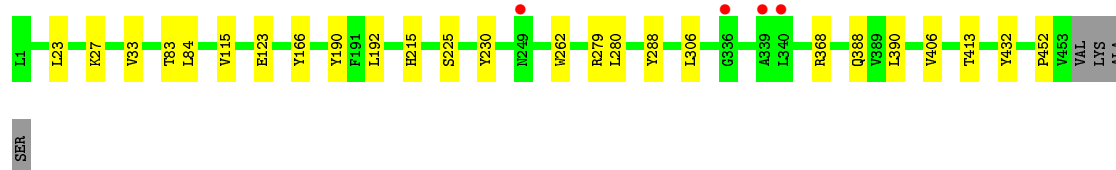
3 Residue-property plots [i](#)

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.

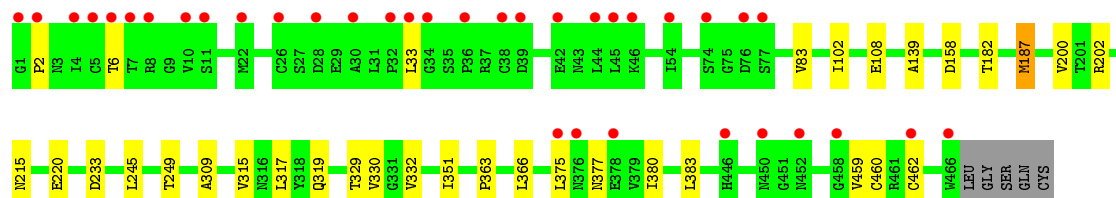
- Molecule 1: Integrin alphaIIB beta3



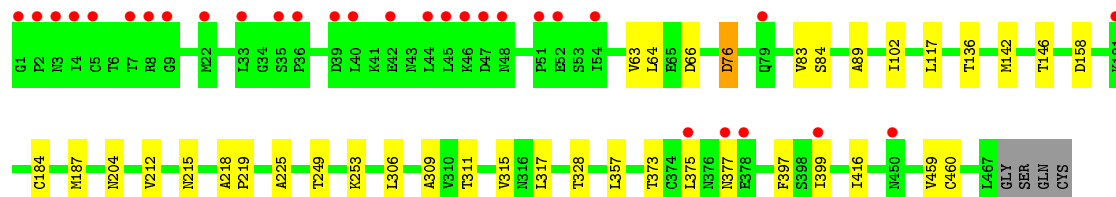
- Molecule 1: Integrin alphaIIB beta3



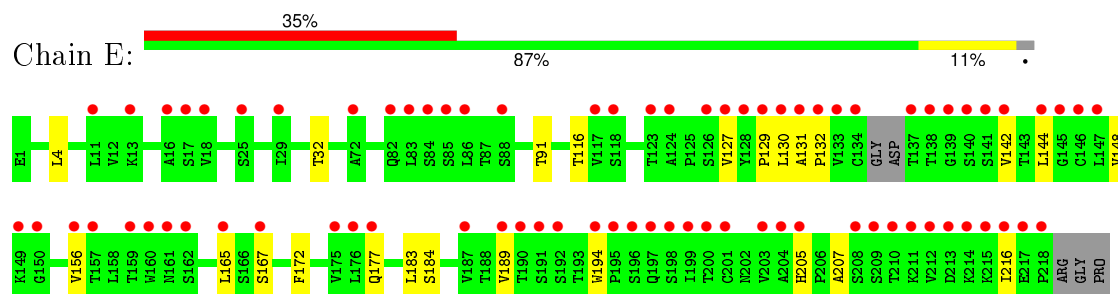
- Molecule 2: Integrin beta-3



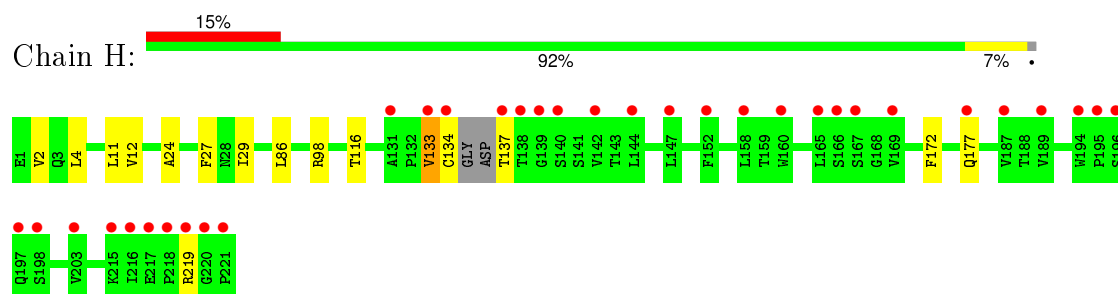
- Molecule 2: Integrin beta-3



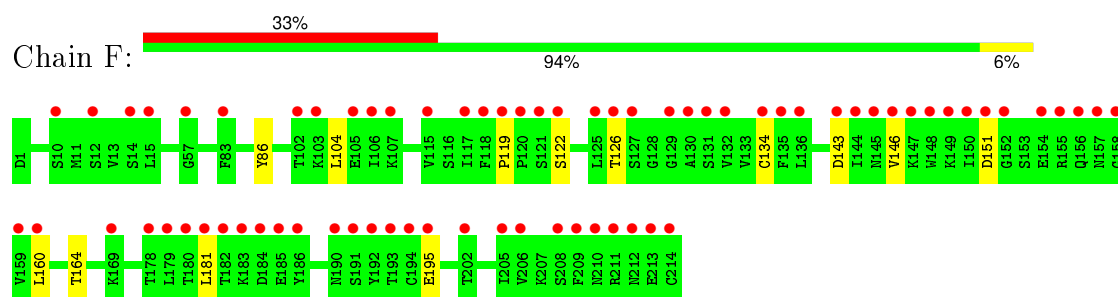
- Molecule 3: Monoclonal antibody 10E5 heavy chain



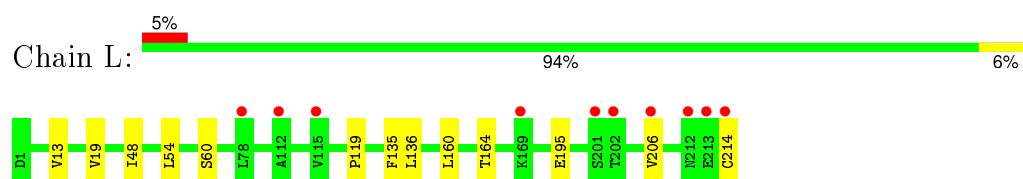
- Molecule 3: Monoclonal antibody 10E5 heavy chain



- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 4: Monoclonal antibody 10E5 light chain



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	259.53Å 144.28Å 104.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 2.40 45.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.21-2.40) 95.1 (45.89-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0093	Depositor
R, R_{free}	0.176 , 0.216 0.193 , 0.226	Depositor DCC
R_{free} test set	860 reflections (0.59%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 145844 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21915	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: GOL, MG, NAG, CA, NIF, 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	0.46	1/3607 (0.0%)	0.62	0/4915
1	C	0.40	0/3581	0.59	0/4880
2	B	0.40	0/3657	0.57	0/4959
2	D	0.38	0/3690	0.54	0/5005
3	E	0.31	0/1680	0.46	0/2301
3	H	0.32	0/1711	0.50	0/2343
4	F	0.31	0/1673	0.45	0/2269
4	L	0.33	0/1673	0.52	0/2269
All	All	0.39	1/21272 (0.0%)	0.55	0/28941

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
11	B	1	0
12	D	1	0
13	D	1	0
All	All	3	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	CYS	CB-SG	-5.12	1.73	1.81

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	B	3322	MAN	C1
13	D	3322	MAN	C1
12	D	3371	NAG	C1

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	3501	0	3343	12	0
1	C	3481	0	3316	17	0
2	B	3590	0	3511	15	0
2	D	3615	0	3540	19	0
3	E	1638	0	1594	19	0
3	H	1665	0	1623	10	0
4	F	1637	0	1553	6	0
4	L	1637	0	1553	9	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	4	0	0	0	0
5	D	2	0	0	0	0
6	A	18	0	15	0	0
6	C	18	0	15	3	0
7	A	36	0	48	1	0
7	B	6	0	8	0	0
7	D	6	0	8	0	0
8	A	25	0	0	0	0
8	B	5	0	0	0	0
8	C	30	0	0	0	0
8	D	15	0	0	0	0
8	H	5	0	0	0	0
8	L	10	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	B	50	0	43	0	0
12	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	28	0	25	0	0
13	D	39	0	34	0	0
14	A	277	0	0	0	0
14	B	175	0	0	1	0
14	C	140	0	0	1	0
14	D	110	0	0	0	0
14	E	9	0	0	0	0
14	F	6	0	0	0	0
14	H	29	0	0	0	0
14	L	44	0	0	0	0
All	All	21915	0	20280	98	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 2.

The worst 5 of 98 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)
3:H:133:VAL:HG21	4:L:119:PRO:HG2	1.71	0.72
3:E:144:LEU:HD22	3:E:216:ILE:HG21	1.74	0.70
1:A:235:TRP:CZ2	1:A:270:LEU:HD21	2.27	0.68
3:E:129:PRO:HB2	3:E:216:ILE:HD13	1.80	0.63
4:L:13:VAL:HG11	4:L:19:VAL:HG11	1.79	0.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	455/457 (100%)	441 (97%)	13 (3%)	1 (0%)	52 69
1	C	452/457 (99%)	437 (97%)	14 (3%)	1 (0%)	52 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	464/471 (98%)	442 (95%)	20 (4%)	2 (0%)	39	56
2	D	467/471 (99%)	448 (96%)	16 (3%)	3 (1%)	30	43
3	E	212/221 (96%)	191 (90%)	20 (9%)	1 (0%)	34	48
3	H	216/221 (98%)	203 (94%)	12 (6%)	1 (0%)	34	48
4	F	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
4	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	2690/2726 (99%)	2570 (96%)	111 (4%)	9 (0%)	46	63

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	C	123	GLU
2	D	375	LEU
2	D	76	ASP
3	E	167	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	365/364 (100%)	360 (99%)	5 (1%)	74	88
1	C	362/364 (100%)	358 (99%)	4 (1%)	80	92
2	B	412/416 (99%)	405 (98%)	7 (2%)	68	85
2	D	415/416 (100%)	412 (99%)	3 (1%)	88	95
3	E	187/190 (98%)	187 (100%)	0	100	100
3	H	190/190 (100%)	190 (100%)	0	100	100
4	F	188/188 (100%)	184 (98%)	4 (2%)	61	80
4	L	188/188 (100%)	187 (100%)	1 (0%)	92	97
All	All	2307/2316 (100%)	2283 (99%)	24 (1%)	82	93

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	233	ASP
1	C	166	TYR
4	F	181	LEU
2	B	462	CYS
1	C	23	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	301	GLN
3	E	161	ASN
3	H	170	HIS
4	L	138	ASN
4	L	190	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 ⓘ

11 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	NAG	B	3320	11,2	14,14,15	0.61	0	15,19,21	0.95	1 (6%)
11	NAG	B	3321	11	14,14,15	0.60	0	15,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	B	3322	11	11,11,12	0.60	0	14,15,17	1.00	2 (14%)
11	MAN	B	3323	11	11,11,12	0.52	0	14,15,17	0.78	0
12	NAG	B	3371	12,2	14,14,15	0.60	0	15,19,21	1.22	2 (13%)
12	NAG	B	3372	12	14,14,15	0.50	0	15,19,21	1.05	0
13	NAG	D	3320	13,2	14,14,15	0.46	0	15,19,21	0.91	1 (6%)
13	NAG	D	3321	13	14,14,15	0.59	0	15,19,21	0.95	0
13	MAN	D	3322	13	11,11,12	0.53	0	14,15,17	1.92	2 (14%)
12	NAG	D	3371	12,2	14,14,15	0.42	0	15,19,21	0.93	1 (6%)
12	NAG	D	3372	12	14,14,15	0.44	0	15,19,21	0.98	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
11	NAG	B	3320	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	3321	11	-	0/6/23/26	0/1/1/1
11	MAN	B	3322	11	1/1/4/5	0/2/19/22	0/1/1/1
11	MAN	B	3323	11	-	0/2/19/22	0/1/1/1
12	NAG	B	3371	12,2	-	0/6/23/26	0/1/1/1
12	NAG	B	3372	12	-	0/6/23/26	0/1/1/1
13	NAG	D	3320	13,2	-	0/6/23/26	0/1/1/1
13	NAG	D	3321	13	-	0/6/23/26	0/1/1/1
13	MAN	D	3322	13	1/1/4/5	0/2/19/22	1/1/1/1
12	NAG	D	3371	12,2	1/1/5/7	0/6/23/26	0/1/1/1
12	NAG	D	3372	12	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	3322	MAN	O5-C1-C2	-2.19	107.30	110.86
11	B	3320	NAG	C2-N2-C7	-2.09	120.36	123.04
12	B	3371	NAG	C4-C3-C2	2.37	114.92	111.23
11	B	3322	MAN	C3-C4-C5	2.45	114.47	110.20
13	D	3320	NAG	C1-O5-C5	2.78	115.77	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	B	3322	MAN	C1
13	D	3322	MAN	C1
12	D	3371	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	3322	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 14 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NIF	A	455	-	15,20,20	4.35	8 (53%)	13,28,28	2.37	4 (30%)
7	GOL	A	456	-	5,5,5	0.30	0	5,5,5	0.30	0
7	GOL	A	457	-	5,5,5	0.31	0	5,5,5	0.29	0
7	GOL	A	458	-	5,5,5	0.36	0	5,5,5	0.26	0
7	GOL	A	459	-	5,5,5	0.34	0	5,5,5	0.69	0
7	GOL	A	460	-	5,5,5	0.27	0	5,5,5	0.58	0
7	GOL	A	461	-	5,5,5	0.30	0	5,5,5	0.77	0
8	SO4	A	462	-	4,4,4	0.16	0	6,6,6	0.07	0
8	SO4	A	463	-	4,4,4	0.14	0	6,6,6	0.26	0
8	SO4	A	464	-	4,4,4	0.20	0	6,6,6	0.19	0
8	SO4	A	465	-	4,4,4	0.18	0	6,6,6	0.14	0
8	SO4	A	466	-	4,4,4	0.25	0	6,6,6	0.10	0
10	NAG	B	3099	2	14,14,15	0.49	0	15,19,21	0.88	0
7	GOL	B	472	-	5,5,5	0.35	0	5,5,5	0.17	0
8	SO4	B	473	-	4,4,4	0.19	0	6,6,6	0.18	0
6	NIF	C	455	-	15,20,20	4.50	8 (53%)	13,28,28	1.98	4 (30%)
8	SO4	C	456	-	4,4,4	0.13	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	C	457	-	4,4,4	0.14	0	6,6,6	0.35	0
8	SO4	C	458	-	4,4,4	0.16	0	6,6,6	0.16	0
8	SO4	C	459	-	4,4,4	0.19	0	6,6,6	0.06	0
8	SO4	C	460	-	4,4,4	0.20	0	6,6,6	0.12	0
8	SO4	C	461	-	4,4,4	0.15	0	6,6,6	0.14	0
10	NAG	D	3099	2	14,14,15	0.44	0	15,19,21	0.71	0
7	GOL	D	472	-	5,5,5	0.32	0	5,5,5	0.26	0
8	SO4	D	473	-	4,4,4	0.19	0	6,6,6	0.25	0
8	SO4	D	474	-	4,4,4	0.20	0	6,6,6	0.17	0
8	SO4	D	475	-	4,4,4	0.19	0	6,6,6	0.21	0
8	SO4	H	222	-	4,4,4	0.18	0	6,6,6	0.11	0
8	SO4	L	215	-	4,4,4	0.18	0	6,6,6	0.18	0
8	SO4	L	216	-	4,4,4	0.19	0	6,6,6	0.10	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
6	NIF	A	455	-	-	0/4/14/14	0/2/3/3
7	GOL	A	456	-	-	0/4/4/4	0/0/0/0
7	GOL	A	457	-	-	0/4/4/4	0/0/0/0
7	GOL	A	458	-	-	0/4/4/4	0/0/0/0
7	GOL	A	459	-	-	0/4/4/4	0/0/0/0
7	GOL	A	460	-	-	0/4/4/4	0/0/0/0
7	GOL	A	461	-	-	0/4/4/4	0/0/0/0
8	SO4	A	462	-	-	0/0/0/0	0/0/0/0
8	SO4	A	463	-	-	0/0/0/0	0/0/0/0
8	SO4	A	464	-	-	0/0/0/0	0/0/0/0
8	SO4	A	465	-	-	0/0/0/0	0/0/0/0
8	SO4	A	466	-	-	0/0/0/0	0/0/0/0
10	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
7	GOL	B	472	-	-	0/4/4/4	0/0/0/0
8	SO4	B	473	-	-	0/0/0/0	0/0/0/0
6	NIF	C	455	-	-	0/4/14/14	0/2/3/3
8	SO4	C	456	-	-	0/0/0/0	0/0/0/0
8	SO4	C	457	-	-	0/0/0/0	0/0/0/0
8	SO4	C	458	-	-	0/0/0/0	0/0/0/0
8	SO4	C	459	-	-	0/0/0/0	0/0/0/0
8	SO4	C	460	-	-	0/0/0/0	0/0/0/0
8	SO4	C	461	-	-	0/0/0/0	0/0/0/0
10	NAG	D	3099	2	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	D	472	-	-	0/4/4/4	0/0/0/0
8	SO4	D	473	-	-	0/0/0/0	0/0/0/0
8	SO4	D	474	-	-	0/0/0/0	0/0/0/0
8	SO4	D	475	-	-	0/0/0/0	0/0/0/0
8	SO4	H	222	-	-	0/0/0/0	0/0/0/0
8	SO4	L	215	-	-	0/0/0/0	0/0/0/0
8	SO4	L	216	-	-	0/0/0/0	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	455	NIF	C4-C3	-3.55	1.34	1.40
6	C	455	NIF	C4-C3	-3.52	1.34	1.40
6	C	455	NIF	C11-N5	-3.50	1.41	1.46
6	A	455	NIF	C11-N5	-3.45	1.41	1.46
6	A	455	NIF	C2-N3	-2.70	1.30	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	455	NIF	N3-C3-N5	-3.15	113.19	116.75
6	C	455	NIF	C4-C3-N3	-2.70	118.12	122.53
6	A	455	NIF	C4-C3-N3	-2.23	118.89	122.53
6	C	455	NIF	C5-C4-C3	2.51	119.47	116.33
6	C	455	NIF	C4-C3-N5	3.53	126.44	122.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	D	3099	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	457	GOL	1	0
6	C	455	NIF	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	454/457 (99%)	0.05	3 (0%) 89 88	12, 21, 47, 84	0
1	C	453/457 (99%)	0.08	4 (0%) 85 85	19, 35, 64, 102	0
2	B	466/471 (98%)	0.46	36 (7%) 16 16	12, 45, 134, 189	0
2	D	467/471 (99%)	0.16	30 (6%) 23 23	20, 48, 109, 151	0
3	E	216/221 (97%)	1.80	77 (35%) 0 0	45, 120, 192, 220	0
3	H	219/221 (99%)	0.58	33 (15%) 3 3	27, 73, 143, 166	1 (0%)
4	F	214/214 (100%)	1.54	71 (33%) 0 1	44, 102, 170, 248	1 (0%)
4	L	214/214 (100%)	0.14	10 (4%) 35 36	30, 60, 100, 147	1 (0%)
All	All	2703/2726 (99%)	0.45	264 (9%) 10 9	12, 48, 148, 248	3 (0%)

The worst 5 of 264 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	212	VAL	15.7
3	E	137	THR	14.2
4	F	214	CYS	12.7
3	H	221	PRO	12.3
3	E	134	CYS	11.1

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

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

6.3 Carbohydrates ⓘ

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
12	NAG	B	3371	14/15	0.87	0.26	1.40	71,88,99,109	0
12	NAG	D	3371	14/15	0.92	0.25	1.05	63,85,96,106	0
13	NAG	D	3320	14/15	0.93	0.15	0.26	36,52,61,64	0
12	NAG	D	3372	14/15	0.83	0.31	-	112,115,120,123	0
11	MAN	B	3322	11/12	0.78	0.29	-	76,98,105,108	0
13	NAG	D	3321	14/15	0.86	0.25	-	52,77,92,102	0
11	NAG	B	3321	14/15	0.92	0.12	-	44,58,70,80	0
13	MAN	D	3322	11/12	0.56	0.27	-	98,111,116,118	0
11	MAN	B	3323	11/12	0.77	0.22	-	80,95,99,100	0
12	NAG	B	3372	14/15	0.80	0.32	-	109,116,117,118	0
11	NAG	B	3320	14/15	0.96	0.10	-	21,34,49,49	0

6.4 Ligands ⓘ

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	GOL	A	461	6/6	0.81	0.38	15.50	48,52,60,62	0
8	SO4	L	215	5/5	0.84	0.36	13.41	80,90,101,102	0
7	GOL	A	459	6/6	0.72	0.31	7.87	67,71,79,81	0
8	SO4	D	474	5/5	0.85	0.29	7.70	115,120,123,123	0
8	SO4	H	222	5/5	0.84	0.32	6.93	95,105,107,108	0
8	SO4	A	466	5/5	0.82	0.36	6.56	137,139,139,142	0
8	SO4	A	463	5/5	0.84	0.23	5.90	77,89,96,98	0
8	SO4	A	462	5/5	0.69	0.24	5.65	114,115,120,121	0
8	SO4	C	456	5/5	0.91	0.21	5.13	56,76,81,84	0
8	SO4	D	475	5/5	0.75	0.22	5.13	123,123,125,126	0
8	SO4	A	465	5/5	0.89	0.22	5.01	90,95,96,99	0
8	SO4	B	473	5/5	0.76	0.25	4.51	107,110,116,119	0
8	SO4	C	460	5/5	0.80	0.29	4.41	93,102,107,114	0
7	GOL	B	472	6/6	0.92	0.23	3.60	75,76,78,79	0
8	SO4	C	461	5/5	0.89	0.29	3.60	98,99,101,104	0
8	SO4	C	457	5/5	0.84	0.23	3.52	63,71,86,88	0
7	GOL	D	472	6/6	0.86	0.29	3.42	44,55,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	GOL	A	460	6/6	0.94	0.23	2.33	34,47,61,71	0
8	SO4	D	473	5/5	0.85	0.24	2.29	101,106,109,109	0
7	GOL	A	458	6/6	0.94	0.17	1.83	31,47,57,60	0
7	GOL	A	456	6/6	0.92	0.18	1.72	20,42,44,46	0
9	MG	D	2001	1/1	0.95	0.17	1.66	82,82,82,82	0
5	CA	A	2006	1/1	1.00	0.17	1.08	19,19,19,19	0
5	CA	C	2007	1/1	0.81	0.13	0.63	39,39,39,39	0
5	CA	C	2006	1/1	0.98	0.13	0.47	38,38,38,38	0
5	CA	D	2003	1/1	0.98	0.16	-0.13	26,26,26,26	0
6	NIF	C	455	18/18	0.96	0.13	-0.50	31,35,43,44	0
6	NIF	A	455	18/18	0.98	0.17	-0.54	19,23,29,30	0
5	CA	A	2007	1/1	0.99	0.12	-0.64	18,18,18,18	0
5	CA	A	2005	1/1	0.99	0.12	-0.84	24,24,24,24	0
9	MG	B	2001	1/1	0.96	0.13	-1.77	53,53,53,53	0
5	CA	B	2003	1/1	1.00	0.18	-1.91	14,14,14,14	0
5	CA	C	2004	1/1	0.95	0.04	-2.19	55,55,55,55	0
5	CA	C	2005	1/1	0.96	0.09	-2.28	44,44,44,44	0
5	CA	A	2004	1/1	0.99	0.06	-2.64	33,33,33,33	0
5	CA	B	2002	1/1	0.96	0.07	-2.94	36,36,36,36	0
5	CA	D	2002	1/1	0.95	0.08	-3.79	36,36,36,36	0
8	SO4	L	216	5/5	0.92	0.29	-	91,93,94,96	0
10	NAG	D	3099	14/15	0.79	0.33	-	90,101,104,106	0
8	SO4	A	464	5/5	0.79	0.22	-	82,94,97,97	0
10	NAG	B	3099	14/15	0.88	0.33	-	87,97,105,105	0
8	SO4	C	458	5/5	0.89	0.18	-	78,89,92,93	0
7	GOL	A	457	6/6	0.89	0.17	-	33,47,55,57	0
8	SO4	C	459	5/5	0.78	0.19	-	109,116,117,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.