



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 08:13 AM EDT

PDB ID : 4Z7Q  
Title : Integrin alphaIIb beta3 in complex with AGDV-NH2 peptide  
Authors : Lin, F.-Y.; Zhu, J.; Springer, T.A.  
Deposited on : 2015-04-07  
Resolution : 2.70 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](mailto: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-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

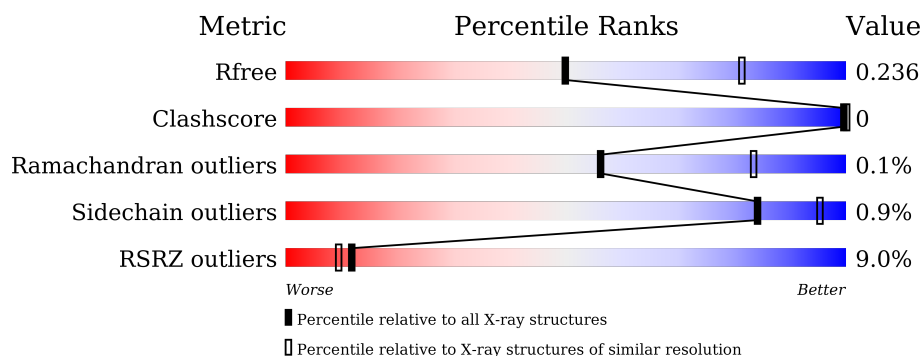
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



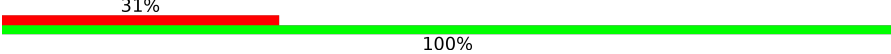

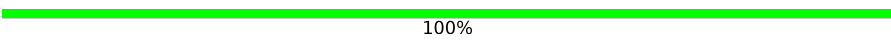
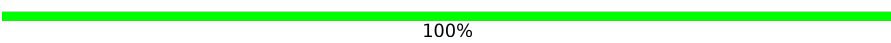
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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	454	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 98%; height: 10px; background-color: green;"></div> <div style="width: 98%; text-align: right;">98%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div>
1	C	454	<div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 98%; height: 10px; background-color: green;"></div> <div style="width: 98%; text-align: right;">98%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div>
2	B	471	<div> <div style="width: 9%; height: 10px; background-color: red;"></div> <div style="width: 97%; height: 10px; background-color: green;"></div> <div style="width: 97%; text-align: right;">97%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div>
2	D	471	<div> <div style="width: 7%; height: 10px; background-color: red;"></div> <div style="width: 98%; height: 10px; background-color: green;"></div> <div style="width: 98%; text-align: right;">98%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div>
3	E	219	<div> <div style="width: 32%; height: 10px; background-color: red;"></div> <div style="width: 98%; height: 10px; background-color: green;"></div> <div style="width: 98%; text-align: right;">98%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div>
3	H	219	<div> <div style="width: 8%; height: 10px; background-color: red;"></div> <div style="width: 98%; height: 10px; background-color: green;"></div> <div style="width: 98%; text-align: right;">98%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	F	214	
4	L	214	
5	G	5	
5	I	5	

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
6	CA	A	504	-	-	-	X
7	SO4	A	505	-	-	-	X
7	SO4	A	506	-	-	-	X
7	SO4	C	506	-	-	-	X
8	GOL	A	508	-	-	-	X
9	MN	B	2001	-	-	-	X
9	MN	B	2002	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 42446 atoms, of which 20326 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	454	Total	C	H	N	O	S	0	7	0
			6882	2236	3366	606	666	8			
1	C	453	Total	C	H	N	O	S	0	6	0
			6839	2224	3337	604	666	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	466	Total	C	H	N	O	S	6	8	0
			7178	2262	3546	620	717	33			
2	D	471	Total	C	H	N	O	S	10	2	0
			7182	2260	3551	620	716	35			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	214	Total	C	H	N	O	S	0	0	0
			3221	1035	1590	264	326	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	0	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			

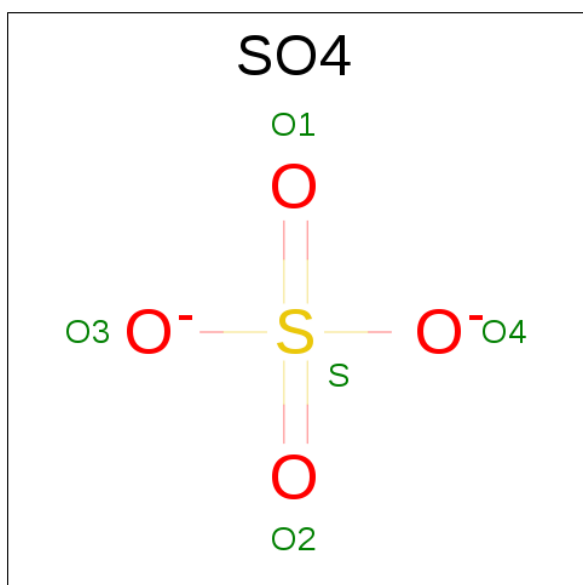
- Molecule 5 is a protein called Tetrapeptide AGDV-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	5	Total	C	H	N	O	0	0	1
			45	14	20	5	6			
5	I	5	Total	C	H	N	O	0	0	1
			45	14	20	5	6			

- 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: O<sub>4</sub>S).



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	C	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		

*Continued on next page...*

Continued from previous page...

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

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

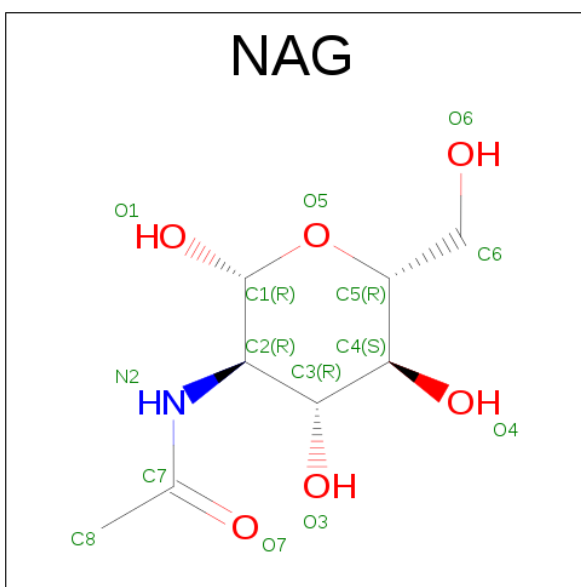


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

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

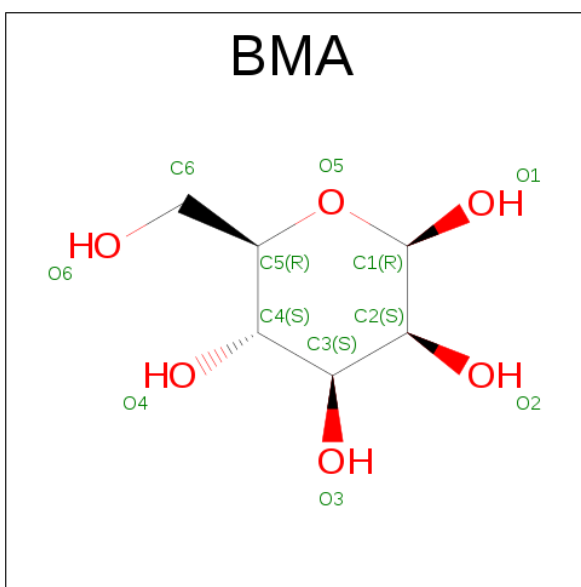
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	3	Total	Mn	0	0
			3	3		
9	D	3	Total	Mn	0	0
			3	3		

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



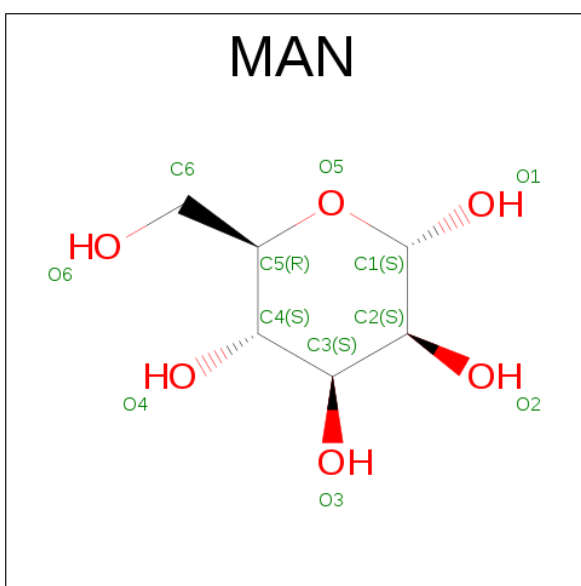
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
10	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
10	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
10	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 11 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	O	0	0
			20	6	9	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: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	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		

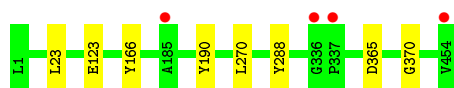
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	369	Total	O	0	0
			369	369		
14	B	183	Total	O	0	0
			183	183		
14	C	165	Total	O	0	0
			165	165		
14	D	141	Total	O	0	0
			141	141		
14	E	18	Total	O	0	0
			18	18		
14	F	19	Total	O	0	0
			19	19		
14	H	36	Total	O	0	0
			36	36		
14	L	54	Total	O	0	0
			54	54		
14	G	3	Total	O	0	0
			3	3		
14	I	3	Total	O	0	0
			3	3		

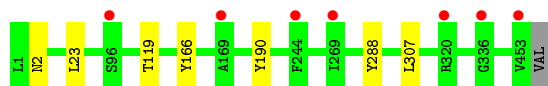
### 3 Residue-property plots [i](#)

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.

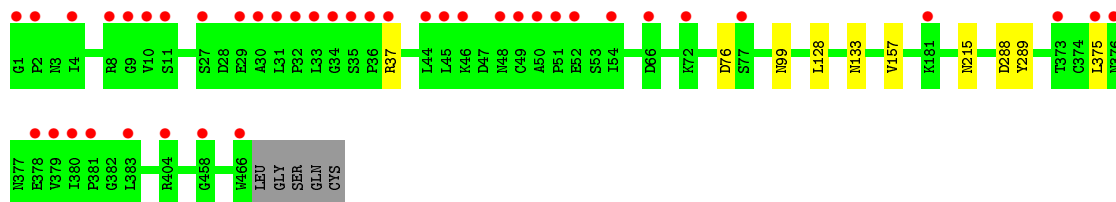
- Molecule 1: Integrin alpha-IIb



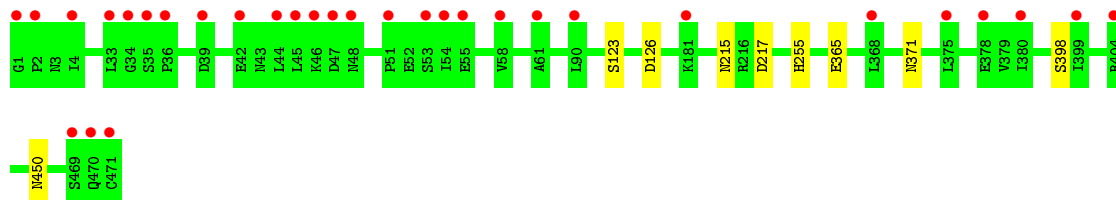
- Molecule 1: Integrin alpha-IIb



- Molecule 2: Integrin beta-3

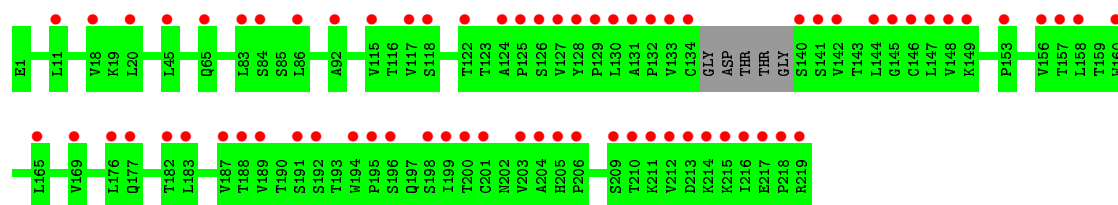


- Molecule 2: Integrin beta-3

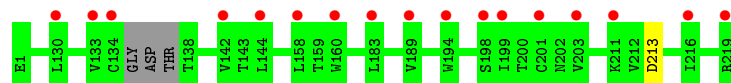


- Molecule 3: Monoclonal antibody 10E5 heavy chain

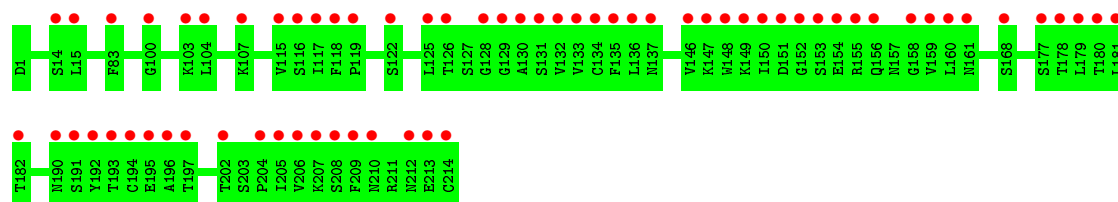




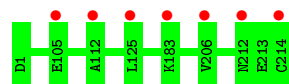
- Molecule 3: Monoclonal antibody 10E5 heavy chain



- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 4: Monoclonal antibody 10E5 light chain



- Molecule 5: Tetrapeptide AGDV-NH2



There are no outlier residues recorded for this chain.

- Molecule 5: Tetrapeptide AGDV-NH2



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.44Å 144.24Å 104.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.70 48.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.94-2.70) 99.6 (48.94-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9 _1692	Depositor
R, $R_{free}$	0.188 , 0.236 0.187 , 0.236	Depositor DCC
$R_{free}$ test set	1077 reflections (1.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 107768 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	42446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, BMA, NAG, CL, CA, MN, SO4, NH2, 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	0.22	0/3633	0.40	0/4951
1	C	0.22	0/3618	0.38	0/4930
2	B	0.22	0/3728	0.39	0/5057
2	D	0.22	0/3710	0.38	0/5029
3	E	0.21	0/1673	0.37	0/2290
3	H	0.21	0/1684	0.38	0/2305
4	F	0.21	0/1673	0.36	0/2269
4	L	0.22	0/1673	0.37	0/2269
5	G	0.16	0/23	0.32	0/30
5	I	0.31	0/23	0.53	0/30
All	All	0.22	0/21438	0.38	0/29160

There are no bond length outliers.

There are no bond angle outliers.

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	3516	3366	3361	1	0
1	C	3502	3337	3320	1	0
2	B	3632	3546	3516	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3631	3551	3539	4	0
3	E	1631	1590	1590	0	0
3	H	1642	1600	1600	0	0
4	F	1637	1553	1553	0	0
4	L	1637	1553	1553	0	0
5	G	25	20	20	0	0
5	I	25	20	20	0	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
7	A	15	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	67	62	0	0
10	D	70	67	61	0	0
11	B	11	9	8	0	0
11	D	11	9	9	0	0
12	B	22	20	20	0	0
12	C	11	10	10	0	0
13	C	1	0	0	0	0
14	A	369	0	0	0	0
14	B	183	0	0	0	0
14	C	165	0	0	0	0
14	D	141	0	0	0	0
14	E	18	0	0	0	0
14	F	19	0	0	0	0
14	G	3	0	0	0	0
14	H	36	0	0	0	0
14	I	3	0	0	0	0
14	L	54	0	0	0	0
All	All	22120	20326	20250	7	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 0.

All (7) 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)
2:B:288:ASP:OD1	2:B:289:TYR:N	2.43	0.52

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:371:ASN:HB2	2:D:398:SER:HB3	2.00	0.43
2:D:126:ASP:N	2:D:126:ASP:OD1	2.53	0.42
2:D:217:ASP:OD2	2:D:255:HIS:NE2	2.53	0.41
1:A:365:ASP:OD2	1:A:370:GLY:N	2.47	0.41
2:D:450:ASN:O	2:D:450:ASN:ND2	2.53	0.40
1:C:2:ASN:OD1	1:C:2:ASN:N	2.53	0.40

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	459/454 (101%)	439 (96%)	19 (4%)	1 (0%)	52	80
1	C	457/454 (101%)	437 (96%)	20 (4%)	0	100	100
2	B	472/471 (100%)	449 (95%)	21 (4%)	2 (0%)	39	69
2	D	471/471 (100%)	454 (96%)	17 (4%)	0	100	100
3	E	210/219 (96%)	197 (94%)	13 (6%)	0	100	100
3	H	212/219 (97%)	196 (92%)	16 (8%)	0	100	100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
4	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
5	G	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
5	I	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	2711/2726 (99%)	2575 (95%)	133 (5%)	3 (0%)	56	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	375	LEU
2	B	157	VAL

### 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	368/362 (102%)	363 (99%)	5 (1%)	74	92
1	C	366/362 (101%)	360 (98%)	6 (2%)	70	91
2	B	420/416 (101%)	413 (98%)	7 (2%)	68	90
2	D	418/416 (100%)	415 (99%)	3 (1%)	88	96
3	E	186/189 (98%)	186 (100%)	0	100	100
3	H	187/189 (99%)	186 (100%)	1 (0%)	92	98
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
5	G	2/2 (100%)	2 (100%)	0	100	100
5	I	2/2 (100%)	2 (100%)	0	100	100
All	All	2325/2314 (100%)	2303 (99%)	22 (1%)	84	95

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	37	ARG
2	B	76	ASP
2	B	99	ASN
2	B	128	LEU
2	B	133[A]	ASN
2	B	133[B]	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	215	ASN
1	C	23	LEU
1	C	119	THR
1	C	166	TYR
1	C	190	TYR
1	C	288	TYR
1	C	307	LEU
2	D	123	SER
2	D	215	ASN
2	D	365	GLU
3	H	213	ASP

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 15 are monoatomic - leaving 23 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	0.24	0	6,6,6	0.06	0
7	SO4	A	506	-	4,4,4	0.25	0	6,6,6	0.07	0
7	SO4	A	507	-	4,4,4	0.25	0	6,6,6	0.07	0
8	GOL	A	508	-	5,5,5	0.35	0	5,5,5	0.17	0
10	NAG	B	2004	2	14,14,15	0.18	0	15,19,21	0.35	0
10	NAG	B	2005	10,2	14,14,15	0.33	0	15,19,21	0.32	0
10	NAG	B	2006	11,10	14,14,15	0.34	0	15,19,21	0.41	0
11	BMA	B	2007	10,12	11,11,12	0.91	1 (9%)	15,15,17	0.96	0
12	MAN	B	2008	11	11,11,12	0.72	0	15,15,17	1.08	2 (13%)
12	MAN	B	2009	11	11,11,12	0.94	0	15,15,17	1.13	1 (6%)
10	NAG	B	2010	10,2	14,14,15	0.28	0	15,19,21	0.31	0
10	NAG	B	2011	10	14,14,15	0.20	0	15,19,21	0.43	0
12	MAN	C	505	-	11,11,12	0.65	0	15,15,17	1.05	2 (13%)
7	SO4	C	506	-	4,4,4	0.25	0	6,6,6	0.08	0
7	SO4	C	507	-	4,4,4	0.25	0	6,6,6	0.06	0
7	SO4	C	508	-	4,4,4	0.25	0	6,6,6	0.06	0
10	NAG	D	503	2	14,14,15	0.55	0	15,19,21	0.44	0
10	NAG	D	504	10,2	14,14,15	0.15	0	15,19,21	0.39	0
10	NAG	D	505	11,10	14,14,15	0.31	0	15,19,21	0.30	0
11	BMA	D	506	10	11,11,12	0.62	0	15,15,17	0.73	0
10	NAG	D	507	10,2	14,14,15	0.21	0	15,19,21	0.36	0
10	NAG	D	508	10	14,14,15	0.52	0	15,19,21	0.46	0
7	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.07	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
8	GOL	A	508	-	-	0/4/4/4	0/0/0/0
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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	C	505	-	-	0/2/19/22	0/1/1/1
7	SO4	C	506	-	-	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	503	2	-	0/6/23/26	0/1/1/1
10	NAG	D	504	10,2	-	0/6/23/26	0/1/1/1
10	NAG	D	505	11,10	-	0/6/23/26	0/1/1/1
11	BMA	D	506	10	-	0/2/19/22	0/1/1/1
10	NAG	D	507	10,2	-	0/6/23/26	0/1/1/1
10	NAG	D	508	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	-2.12	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	505	MAN	O2-C2-C3	-2.45	105.26	110.19
12	B	2009	MAN	O2-C2-C3	-2.36	105.42	110.19
12	B	2008	MAN	O2-C2-C3	-2.31	105.52	110.19
12	C	505	MAN	C1-O5-C5	2.47	115.78	112.14
12	B	2008	MAN	C1-O5-C5	2.77	116.22	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	454/454 (100%)	0.38	4 (0%) 85 86	35, 52, 89, 158	0
1	C	453/454 (99%)	0.32	7 (1%) 76 76	44, 73, 117, 171	0
2	B	466/471 (98%)	0.61	41 (8%) 12 10	35, 90, 180, 211	1 (0%)
2	D	471/471 (100%)	0.41	31 (6%) 22 20	47, 93, 161, 251	1 (0%)
3	E	214/219 (97%)	1.72	71 (33%) 0 0	80, 153, 227, 280	0
3	H	216/219 (98%)	0.52	17 (7%) 15 13	52, 116, 179, 204	0
4	F	214/214 (100%)	1.46	66 (30%) 1 0	77, 143, 211, 250	0
4	L	214/214 (100%)	0.34	7 (3%) 50 50	57, 102, 141, 204	0
5	G	4/5 (80%)	0.74	0 100 100	59, 64, 67, 76	0
5	I	4/5 (80%)	0.47	0 100 100	81, 87, 92, 102	0
All	All	2710/2726 (99%)	0.61	244 (9%) 12 9	35, 89, 181, 280	2 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	193	THR	11.5
3	E	212	VAL	9.9
3	E	194	TRP	9.4
3	E	147	LEU	9.1
3	E	216	ILE	8.5
3	E	183	LEU	8.0
2	D	469	SER	7.7
3	E	215	LYS	7.2
3	E	196	SER	7.1
3	E	201	CYS	6.9
4	F	117	ILE	6.9
3	E	210	THR	6.8
3	E	133	VAL	6.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	F	206	VAL	6.6
3	E	148	VAL	6.6
4	F	214	CYS	6.5
2	B	33	LEU	6.5
4	F	181	LEU	6.4
4	F	115	VAL	6.3
3	E	129	PRO	6.2
2	B	2	PRO	6.1
4	F	180	THR	6.0
3	E	144	LEU	5.8
3	E	134	CYS	5.8
3	E	199	ILE	5.6
3	E	187	VAL	5.6
3	E	195	PRO	5.5
4	F	134	CYS	5.4
3	E	156	VAL	5.4
3	E	219	ARG	5.3
4	F	209	PHE	5.2
3	H	203	VAL	5.1
3	E	198	SER	5.0
3	E	145	GLY	4.9
4	F	130	ALA	4.8
2	B	1	GLY	4.8
3	E	127	VAL	4.7
4	F	116	SER	4.7
4	F	154	GLU	4.7
3	E	169	VAL	4.7
2	D	44	LEU	4.7
2	B	27	SER	4.7
4	F	192	TYR	4.7
3	E	205	HIS	4.7
2	B	46	LYS	4.5
2	D	1	GLY	4.5
3	E	131	ALA	4.4
3	E	142	VAL	4.4
3	H	144	LEU	4.4
2	B	36	PRO	4.3
3	E	200	THR	4.2
3	H	198	SER	4.2
4	F	135	PHE	4.2
4	F	194	CYS	4.1
4	F	147	LYS	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	E	132	PRO	4.0
4	F	156	GLN	4.0
3	E	160	TRP	4.0
3	H	189	VAL	4.0
3	H	130	LEU	4.0
3	E	176	LEU	4.0
3	H	199	ILE	3.9
2	B	375	LEU	3.9
4	F	132	VAL	3.9
3	E	217	GLU	3.9
3	E	130	LEU	3.8
2	B	49	CYS	3.8
2	D	54	ILE	3.8
4	F	104	LEU	3.7
2	B	34	GLY	3.7
4	F	210	ASN	3.7
3	E	45	LEU	3.7
3	E	158	LEU	3.7
4	F	125	LEU	3.7
4	F	148	TRP	3.7
3	H	133	VAL	3.6
4	F	159	VAL	3.6
3	E	83	LEU	3.6
4	F	182	THR	3.6
4	F	146	VAL	3.6
2	D	55	GLU	3.6
3	E	128	TYR	3.6
3	E	204	ALA	3.6
2	B	32	PRO	3.5
2	B	72	LYS	3.5
4	L	214	CYS	3.5
4	F	122	SER	3.5
3	E	218	PRO	3.5
2	D	46	LYS	3.5
4	F	136	LEU	3.5
4	F	151	ASP	3.5
4	F	103	LYS	3.5
4	F	208	SER	3.5
3	E	203	VAL	3.5
2	B	35	SER	3.5
4	F	133	VAL	3.4
4	L	212	ASN	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	375	LEU	3.4
2	D	36	PRO	3.4
3	H	134	CYS	3.4
4	F	160	LEU	3.4
2	B	29	GLU	3.4
2	B	44	LEU	3.3
4	F	213	GLU	3.3
3	E	209	SER	3.3
2	B	48	ASN	3.3
4	F	155	ARG	3.3
1	A	454	VAL	3.3
2	B	8	ARG	3.3
2	B	378	GLU	3.2
1	A	337	PRO	3.2
3	H	160	TRP	3.2
3	H	142	VAL	3.2
4	F	179	LEU	3.2
4	F	212	ASN	3.2
4	F	207	LYS	3.2
2	B	4	ILE	3.2
2	D	51	PRO	3.1
2	B	181	LYS	3.1
3	H	216	ILE	3.1
4	F	178	THR	3.1
3	E	157	THR	3.0
4	F	15	LEU	3.0
3	E	84	SER	3.0
3	E	126	SER	3.0
2	D	35	SER	3.0
3	E	188	THR	3.0
2	D	34	GLY	3.0
4	L	125	LEU	3.0
4	F	100	GLY	3.0
2	B	52	GLU	3.0
2	B	30	ALA	3.0
2	B	381	PRO	3.0
4	F	118	PHE	2.9
4	L	105	GLU	2.9
2	B	10	VAL	2.9
3	E	213	ASP	2.9
3	E	149	LYS	2.9
4	F	131	SER	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	F	119	PRO	2.8
2	D	33	LEU	2.8
4	F	195	GLU	2.8
3	E	141	SER	2.8
3	E	177	GLN	2.8
2	D	380	ILE	2.8
1	A	336	GLY	2.8
3	E	118	SER	2.8
2	B	383	LEU	2.8
3	H	201	CYS	2.8
2	B	458	GLY	2.8
3	E	140	SER	2.7
2	B	466	TRP	2.7
4	F	190	ASN	2.7
2	B	54	ILE	2.7
4	F	149	LYS	2.7
2	D	378	GLU	2.7
2	B	45	LEU	2.7
3	H	211	LYS	2.7
2	B	51	PRO	2.7
2	D	181	LYS	2.7
3	E	214	LYS	2.7
4	F	152	GLY	2.6
2	D	471	CYS	2.6
4	F	205	ILE	2.6
1	C	269	ILE	2.5
4	F	177	SER	2.5
2	B	404	ARG	2.5
3	E	86	LEU	2.5
3	E	65	GLN	2.5
4	F	126	THR	2.5
3	E	11	LEU	2.5
2	D	42	GLU	2.5
3	H	158	LEU	2.5
2	D	368	LEU	2.4
3	E	146	CYS	2.4
4	F	158	GLY	2.4
4	F	150	ILE	2.4
3	E	117	VAL	2.4
3	H	219	ARG	2.4
2	B	9	GLY	2.4
3	E	165	LEU	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	244	PHE	2.4
4	F	83	PHE	2.4
4	F	14	SER	2.4
4	F	197	THR	2.4
4	F	204	PRO	2.3
3	E	191	SER	2.3
2	D	399	ILE	2.3
2	B	379	VAL	2.3
2	D	470	GLN	2.3
2	B	380	ILE	2.3
3	E	20	LEU	2.3
3	E	92	ALA	2.3
3	E	192	SER	2.3
3	H	194	TRP	2.3
2	D	90	LEU	2.3
2	D	45	LEU	2.2
2	D	48	ASN	2.2
3	E	124	ALA	2.2
4	F	153	SER	2.2
3	E	206	PRO	2.2
3	E	211	LYS	2.2
4	F	191	SER	2.2
2	D	58	VAL	2.2
2	B	31	LEU	2.2
4	F	128	GLY	2.2
2	D	404	ARG	2.2
2	D	53	SER	2.2
4	L	112	ALA	2.2
2	B	50	ALA	2.2
1	C	320	ARG	2.2
4	F	107	LYS	2.1
3	E	189	VAL	2.1
4	L	206	VAL	2.1
2	D	61	ALA	2.1
3	E	182	THR	2.1
2	B	376	ASN	2.1
1	A	185	ALA	2.1
3	E	125	PRO	2.1
4	F	196	ALA	2.1
2	B	11	SER	2.1
1	C	453	VAL	2.1
3	H	183	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	L	183	LYS	2.1
2	D	39	ASP	2.1
3	E	115	VAL	2.1
2	D	2	PRO	2.1
1	C	169	ALA	2.1
4	F	137	ASN	2.1
1	C	96	SER	2.1
2	D	47	ASP	2.1
2	B	77	SER	2.0
2	B	373	THR	2.0
3	E	122	THR	2.0
4	F	202	THR	2.0
2	B	37	ARG	2.0
2	D	4	ILE	2.0
4	F	161	ASN	2.0
2	B	66	ASP	2.0
4	F	129	GLY	2.0
4	F	168	SER	2.0
3	E	18	VAL	2.0
3	E	153	PRO	2.0
1	C	336	GLY	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	MN	B	2002	1/1	0.71	0.32	13.07	341,341,341,341	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	C	506	5/5	0.87	0.29	5.52	145,159,162,164	0
7	SO4	A	505	5/5	0.92	0.35	5.35	135,139,148,160	0
7	SO4	A	506	5/5	0.96	0.29	4.26	115,126,130,141	0
6	CA	A	504	1/1	0.99	0.28	2.80	65,65,65,65	0
8	GOL	A	508	6/6	0.91	0.27	2.75	69,95,115,117	0
9	MN	B	2001	1/1	1.00	0.26	2.41	49,49,49,49	0
6	CA	A	503	1/1	0.98	0.23	1.86	47,47,47,47	0
6	CA	C	504	1/1	0.95	0.20	1.21	76,76,76,76	0
9	MN	D	501	1/1	0.79	0.24	1.10	373,373,373,373	0
10	NAG	D	507	14/15	0.90	0.28	0.39	82,124,151,154	0
6	CA	A	502	1/1	0.92	0.17	0.33	58,58,58,58	0
6	CA	C	503	1/1	0.97	0.16	0.28	75,75,75,75	0
10	NAG	D	503	14/15	0.87	0.24	-0.12	90,120,136,151	0
10	NAG	B	2010	14/15	0.89	0.25	-0.19	84,118,145,145	0
7	SO4	C	508	5/5	0.96	0.15	-0.30	128,134,137,137	0
7	SO4	C	507	5/5	0.86	0.18	-0.56	142,142,158,159	0
10	NAG	D	504	14/15	0.94	0.15	-0.84	73,96,114,118	0
6	CA	A	501	1/1	0.93	0.10	-1.19	65,65,65,65	0
10	NAG	B	2005	14/15	0.97	0.17	-1.39	55,78,103,103	0
9	MN	B	2003	1/1	0.92	0.19	-1.84	74,74,74,74	0
6	CA	C	502	1/1	0.95	0.07	-2.23	77,77,77,77	0
9	MN	D	502	1/1	0.98	0.15	-2.32	81,81,81,81	0
6	CA	C	501	1/1	0.96	0.05	-2.48	116,116,116,116	0
9	MN	D	509	1/1	0.94	0.14	-2.97	126,126,126,126	0
7	SO4	L	301	5/5	0.95	0.11	-3.20	119,121,128,136	0
10	NAG	B	2006	14/15	0.94	0.18	-	97,116,143,144	0
12	MAN	B	2009	11/12	0.76	0.17	-	94,122,147,152	0
13	CL	C	509	1/1	0.92	0.34	-	100,100,100,100	0
11	BMA	B	2007	11/12	0.86	0.17	-	88,134,166,170	0
10	NAG	B	2011	14/15	0.88	0.38	-	117,140,165,168	0
12	MAN	B	2008	11/12	0.93	0.15	-	92,117,131,143	0
10	NAG	D	505	14/15	0.91	0.21	-	104,125,153,155	0
7	SO4	A	507	5/5	0.98	0.15	-	88,93,107,118	0
10	NAG	B	2004	14/15	0.87	0.37	-	112,139,164,168	0
10	NAG	D	508	14/15	0.89	0.28	-	116,135,154,159	0
12	MAN	C	505	11/12	0.89	0.27	-	105,127,152,153	0
11	BMA	D	506	11/12	0.88	0.22	-	97,124,146,149	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.