



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:13 am GMT

PDB ID : 3NID  
Title : The Closed Headpiece of Integrin  $\alpha$ IIB  $\beta$ 3 and its Complex with an  $\alpha$ IIB  $\beta$ 3 -Specific Antagonist That Does Not Induce Opening  
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.  
Deposited on : 2010-06-15  
Resolution : 2.30 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](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.

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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 : trunk28683  
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) : recalc28949

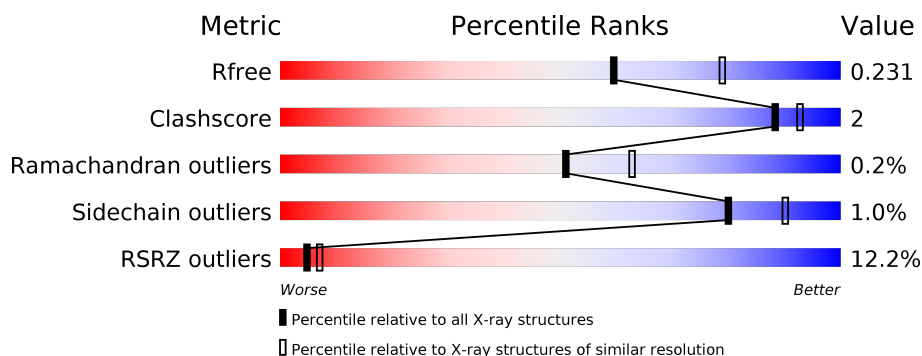
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	457	<div> <div></div> <div>94%</div> <div>5%</div> <div></div> </div>
1	C	457	<div> <div></div> <div>94%</div> <div>5%</div> <div></div> </div>
2	B	471	<div> <div>14%</div> <div>91%</div> <div>7%</div> <div></div> </div>
2	D	471	<div> <div>9%</div> <div>95%</div> <div>5%</div> <div></div> </div>
3	E	221	<div> <div>34%</div> <div>87%</div> <div>10%</div> <div></div> </div>
3	H	221	<div> <div>16%</div> <div>86%</div> <div>12%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
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	MAN	B	3322	X	-	-	-
12	MAN	D	3322	X	-	-	-
6	GOL	A	460	-	-	-	X
6	GOL	A	463	-	-	-	X
6	GOL	C	458	-	-	-	X
7	SO4	A	464	-	-	-	X
7	SO4	B	473	-	-	-	X
7	SO4	C	460	-	-	-	X
7	SO4	C	461	-	-	-	X
7	SO4	D	472	-	-	-	X
7	SO4	D	473	-	-	-	X
7	SO4	H	222	-	-	-	X
7	SO4	L	215	-	-	-	X
8	MG	D	2001	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22131 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 alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	5	0
			3504	2229	602	665	8			
1	C	453	Total	C	N	O	S	0	2	0
			3484	2214	600	662	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	4	2	0
			3601	2243	615	710	33			
2	D	471	Total	C	N	O	S	3	1	0
			3634	2265	620	715	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

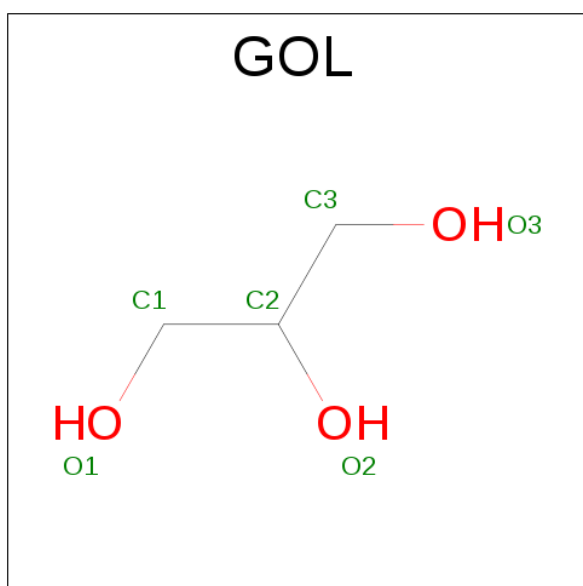
- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	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 GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

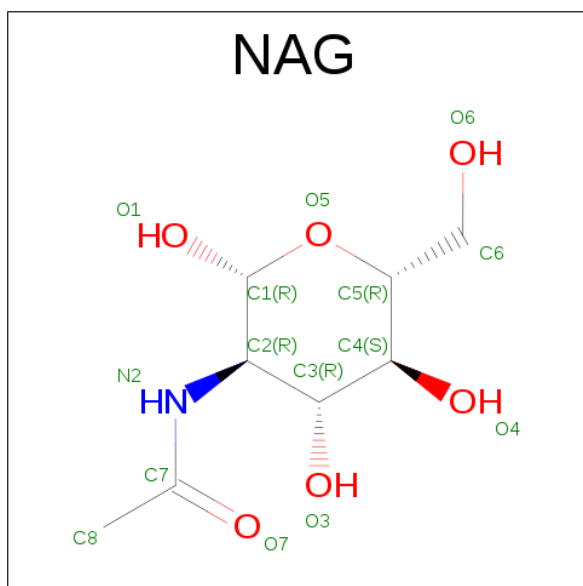


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 10 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

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

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

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 13 is water.

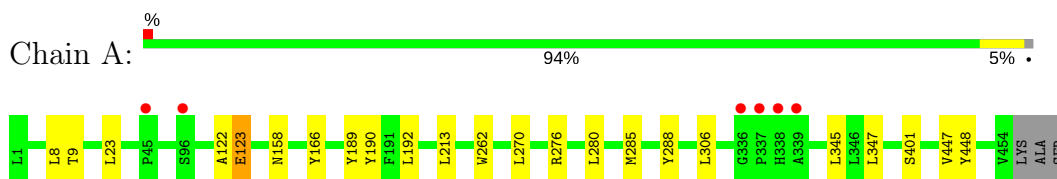
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	386	Total	O	0	0
			386	386		
13	B	192	Total	O	0	0
			192	192		
13	C	205	Total	O	0	0
			205	205		
13	D	182	Total	O	0	0
			182	182		
13	E	12	Total	O	0	0
			12	12		
13	F	12	Total	O	0	0
			12	12		
13	H	32	Total	O	0	0
			32	32		
13	L	38	Total	O	0	0
			38	38		



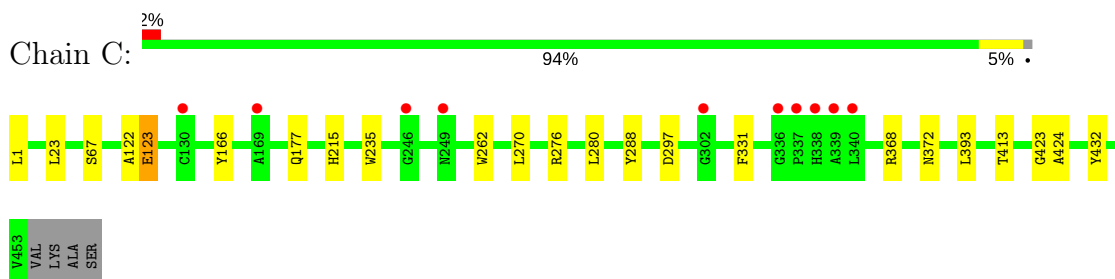
### 3 Residue-property plots [i](#)

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.

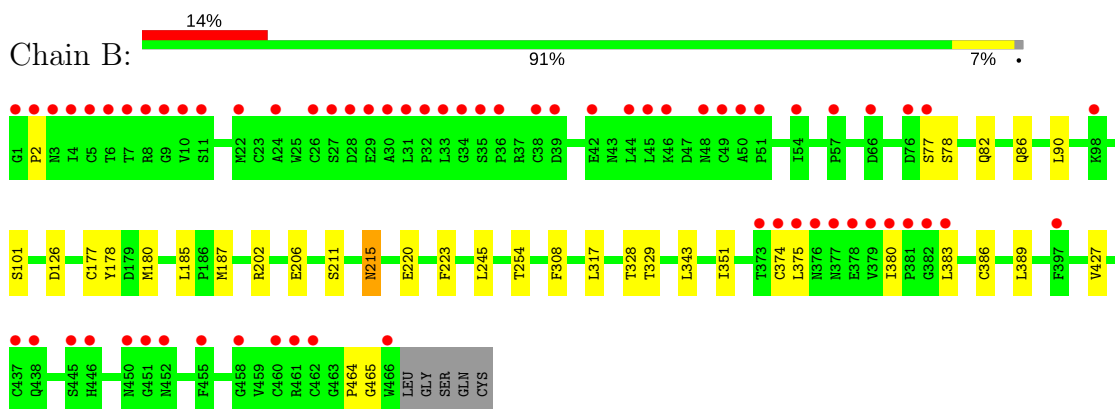
- Molecule 1: Integrin alpha-IIb



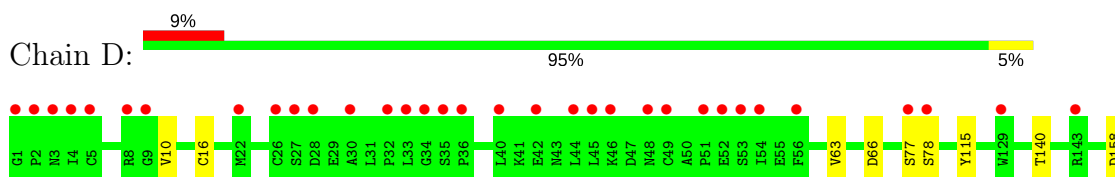
- Molecule 1: Integrin alpha-IIb



- Molecule 2: Integrin beta-3

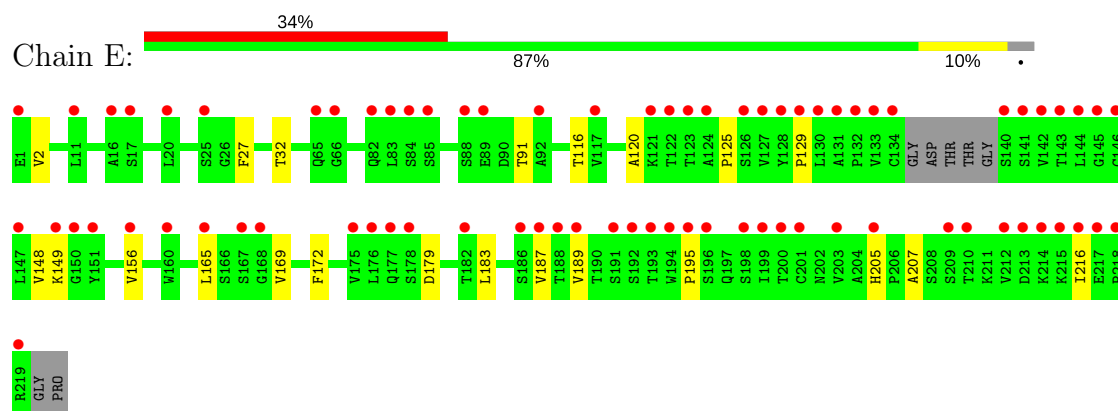


- Molecule 2: Integrin beta-3

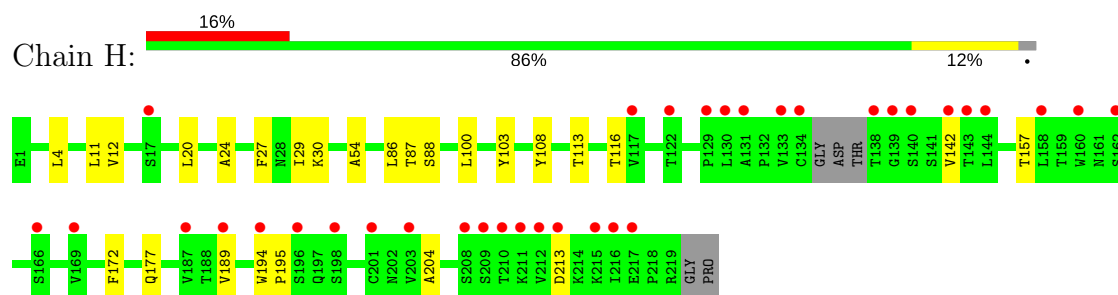




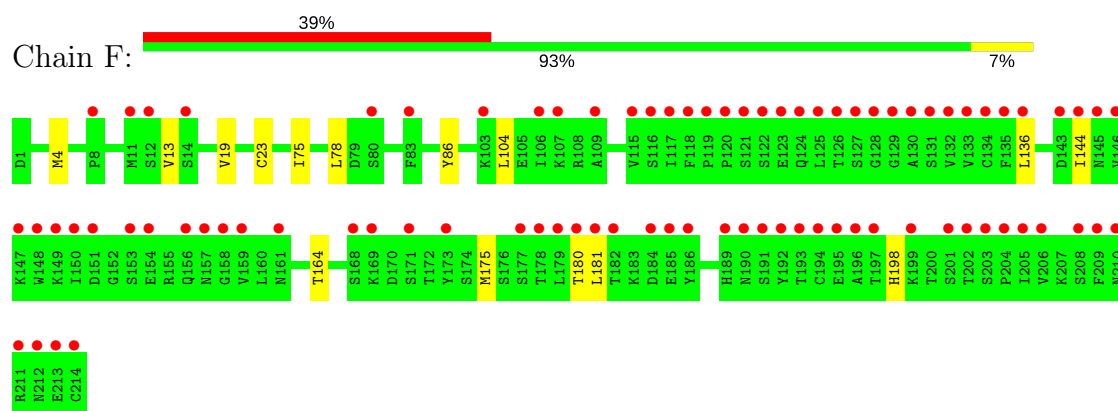
• Molecule 3: Monoclonal antibody 10E5 heavy chain



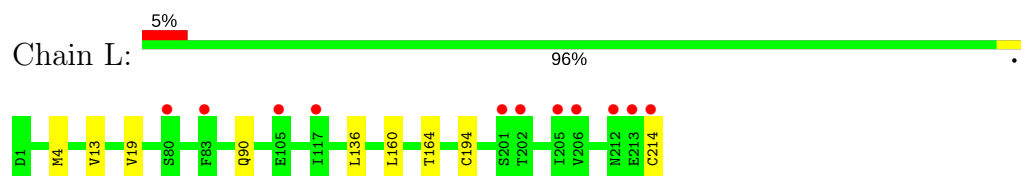
• Molecule 3: Monoclonal antibody 10E5 heavy chain



• Molecule 4: Monoclonal antibody 10E5 light chain



• Molecule 4: Monoclonal antibody 10E5 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	258.97Å 144.49Å 104.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 2.30 48.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.21-2.30) 97.8 (48.21-2.30)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	0.01	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.179 , 0.215 0.192 , 0.231	Depositor DCC
$R_{free}$ test set	1029 reflections (0.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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, 0.333 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, MG, NAG, CA, 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	0.44	0/3616	0.61	0/4929
1	C	0.38	0/3587	0.57	0/4888
2	B	0.38	0/3674	0.56	0/4982
2	D	0.37	0/3706	0.53	0/5026
3	E	0.31	0/1673	0.46	0/2290
3	H	0.32	0/1684	0.49	0/2305
4	F	0.32	0/1673	0.46	0/2269
4	L	0.33	0/1673	0.51	0/2269
All	All	0.37	0/21286	0.54	0/28958

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
10	B	1	0
12	D	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	3322	MAN	C1
12	D	3322	MAN	C1

There are no planarity outliers.

## 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	3504	0	3351	14	0
1	C	3484	0	3320	11	0
2	B	3601	0	3525	19	0
2	D	3634	0	3551	14	0
3	E	1631	0	1590	14	0
3	H	1642	0	1600	16	0
4	F	1637	0	1553	10	0
4	L	1637	0	1553	6	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	36	0	48	1	0
6	B	6	0	8	0	0
6	C	12	0	16	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	20	0	0	0	0
7	D	10	0	0	0	0
7	H	5	0	0	0	0
7	L	5	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	14	0	13	0	0
9	D	14	0	13	0	0
10	B	61	0	52	0	0
11	B	28	0	25	0	0
11	D	28	0	25	1	0
12	D	39	0	34	0	0
13	A	386	0	0	1	0
13	B	192	0	0	1	0
13	C	205	0	0	1	0
13	D	182	0	0	1	0
13	E	12	0	0	0	0
13	F	12	0	0	0	0
13	H	32	0	0	0	0
13	L	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22131	0	20277	93	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 93 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)
4:L:13:VAL:HG11	4:L:19:VAL:HG11	1.73	0.70
3:E:165:LEU:HD23	3:E:187:VAL:HG21	1.74	0.69
2:B:90:LEU:HD13	2:B:427:VAL:HG13	1.78	0.64
3:E:169:VAL:HG22	3:E:187:VAL:HG23	1.80	0.61
1:A:276:ARG:NH1	13:A:931:HOH:O	2.34	0.61

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	457/457 (100%)	444 (97%)	12 (3%)	1 (0%)	51	63
1	C	453/457 (99%)	440 (97%)	12 (3%)	1 (0%)	51	63
2	B	466/471 (99%)	451 (97%)	13 (3%)	2 (0%)	38	47
2	D	470/471 (100%)	457 (97%)	13 (3%)	0	100	100
3	E	210/221 (95%)	200 (95%)	9 (4%)	1 (0%)	32	39
3	H	212/221 (96%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
4	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	2692/2726 (99%)	2608 (97%)	79 (3%)	5 (0%)	51	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	375	LEU
1	C	123	GLU
2	B	2	PRO
3	E	195	PRO

### 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	367/364 (101%)	362 (99%)	5 (1%)	71	85
1	C	363/364 (100%)	358 (99%)	5 (1%)	71	85
2	B	414/416 (100%)	408 (99%)	6 (1%)	71	85
2	D	417/416 (100%)	413 (99%)	4 (1%)	80	90
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	91	96
4	F	188/188 (100%)	187 (100%)	1 (0%)	91	96
4	L	188/188 (100%)	186 (99%)	2 (1%)	78	89
All	All	2310/2316 (100%)	2286 (99%)	24 (1%)	80	90

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

Mol	Chain	Res	Type
2	B	374	CYS
1	C	166	TYR
4	L	194	CYS
1	C	23	LEU
1	C	67	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	177	GLN
4	L	138	ASN
4	F	124	GLN
1	C	15	ASN
3	H	170	HIS

### 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 ⓘ

12 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	$\# Z  > 2$
10	NAG	B	3320	10,2	14,14,15	0.49	0	15,19,21	1.11	2 (13%)
10	NAG	B	3321	10	14,14,15	0.57	0	15,19,21	1.18	2 (13%)
10	MAN	B	3322	10	11,11,12	0.57	0	13,15,17	1.47	2 (15%)
10	MAN	B	3323	10	11,11,12	0.55	0	13,15,17	0.65	0
10	MAN	B	3324	10	11,11,12	0.63	0	13,15,17	1.24	2 (15%)
11	NAG	B	3371	11,2	14,14,15	0.58	0	15,19,21	0.76	0
11	NAG	B	3372	11	14,14,15	0.48	0	15,19,21	1.06	1 (6%)
12	NAG	D	3320	12,2	14,14,15	0.48	0	15,19,21	1.29	2 (13%)
12	NAG	D	3321	12	14,14,15	0.56	0	15,19,21	0.83	0
12	MAN	D	3322	12	11,11,12	0.47	0	13,15,17	1.55	1 (7%)
11	NAG	D	3371	11,2	14,14,15	0.55	0	15,19,21	0.84	0
11	NAG	D	3372	11	14,14,15	0.49	0	15,19,21	0.83	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
10	NAG	B	3320	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	3321	10	-	0/6/23/26	0/1/1/1
10	MAN	B	3322	10	1/1/4/5	0/2/19/22	0/1/1/1
10	MAN	B	3323	10	-	0/2/19/22	0/1/1/1
10	MAN	B	3324	10	-	0/2/19/22	0/1/1/1
11	NAG	B	3371	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	3372	11	-	0/6/23/26	0/1/1/1
12	NAG	D	3320	12,2	-	0/6/23/26	0/1/1/1
12	NAG	D	3321	12	-	0/6/23/26	0/1/1/1
12	MAN	D	3322	12	1/1/4/5	0/2/19/22	1/1/1/1
11	NAG	D	3371	11,2	-	0/6/23/26	0/1/1/1
11	NAG	D	3372	11	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3324	MAN	O5-C1-C2	-2.89	106.26	110.79
10	B	3320	NAG	O5-C1-C2	-2.66	107.77	111.47
12	D	3320	NAG	O5-C1-C2	-2.60	107.86	111.47
11	B	3372	NAG	O5-C1-C2	-2.29	108.29	111.47
10	B	3322	MAN	O5-C1-C2	-2.13	107.45	110.79

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	3322	MAN	C1
12	D	3322	MAN	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

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

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	3371	NAG	1	0

## 5.6 Ligand geometry

Of 35 ligands modelled in this entry, 14 are monoatomic - leaving 21 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	GOL	A	458	-	5,5,5	0.35	0	5,5,5	0.29	0
6	GOL	A	459	-	5,5,5	0.38	0	5,5,5	0.22	0
6	GOL	A	460	-	5,5,5	0.33	0	5,5,5	0.45	0
6	GOL	A	461	-	5,5,5	0.22	0	5,5,5	0.38	0
6	GOL	A	462	-	5,5,5	0.34	0	5,5,5	0.16	0
6	GOL	A	463	-	5,5,5	0.34	0	5,5,5	0.21	0
7	SO4	A	464	-	4,4,4	0.18	0	6,6,6	0.05	0
9	NAG	B	3099	2	14,14,15	0.57	0	15,19,21	0.90	1 (6%)
6	GOL	B	472	-	5,5,5	0.30	0	5,5,5	0.25	0
7	SO4	B	473	-	4,4,4	0.16	0	6,6,6	0.17	0
6	GOL	C	458	-	5,5,5	0.23	0	5,5,5	0.35	0
6	GOL	C	459	-	5,5,5	0.38	0	5,5,5	0.22	0
7	SO4	C	460	-	4,4,4	0.17	0	6,6,6	0.26	0
7	SO4	C	461	-	4,4,4	0.16	0	6,6,6	0.25	0
7	SO4	C	462	-	4,4,4	0.17	0	6,6,6	0.10	0
7	SO4	C	463	-	4,4,4	0.15	0	6,6,6	0.12	0
9	NAG	D	3099	2	14,14,15	0.59	0	15,19,21	0.87	0
7	SO4	D	472	-	4,4,4	0.18	0	6,6,6	0.13	0
7	SO4	D	473	-	4,4,4	0.15	0	6,6,6	0.10	0
7	SO4	H	222	-	4,4,4	0.16	0	6,6,6	0.06	0
7	SO4	L	215	-	4,4,4	0.15	0	6,6,6	0.11	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	GOL	A	458	-	-	0/4/4/4	0/0/0/0
6	GOL	A	459	-	-	0/4/4/4	0/0/0/0
6	GOL	A	460	-	-	0/4/4/4	0/0/0/0
6	GOL	A	461	-	-	0/4/4/4	0/0/0/0
6	GOL	A	462	-	-	0/4/4/4	0/0/0/0
6	GOL	A	463	-	-	0/4/4/4	0/0/0/0
7	SO4	A	464	-	-	0/0/0/0	0/0/0/0
9	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
6	GOL	B	472	-	-	0/4/4/4	0/0/0/0
7	SO4	B	473	-	-	0/0/0/0	0/0/0/0
6	GOL	C	458	-	-	0/4/4/4	0/0/0/0
6	GOL	C	459	-	-	0/4/4/4	0/0/0/0
7	SO4	C	460	-	-	0/0/0/0	0/0/0/0
7	SO4	C	461	-	-	0/0/0/0	0/0/0/0
7	SO4	C	462	-	-	0/0/0/0	0/0/0/0
7	SO4	C	463	-	-	0/0/0/0	0/0/0/0
9	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
7	SO4	D	472	-	-	0/0/0/0	0/0/0/0
7	SO4	D	473	-	-	0/0/0/0	0/0/0/0
7	SO4	H	222	-	-	0/0/0/0	0/0/0/0
7	SO4	L	215	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	3099	NAG	C1-O5-C5	2.18	115.17	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	458	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	454/457 (99%)	0.38	6 (1%) 77 81	9, 20, 49, 89	0
1	C	453/457 (99%)	0.24	10 (2%) 62 69	15, 32, 63, 106	0
2	B	466/471 (98%)	0.86	65 (13%) 3 5	10, 44, 127, 170	1 (0%)
2	D	471/471 (100%)	0.54	43 (9%) 10 14	16, 41, 101, 142	1 (0%)
3	E	214/221 (96%)	1.88	76 (35%) 0 0	41, 96, 147, 161	0
3	H	216/221 (97%)	0.66	35 (16%) 2 3	24, 73, 143, 176	0
4	F	214/214 (100%)	1.85	84 (39%) 0 0	41, 91, 143, 170	1 (0%)
4	L	214/214 (100%)	0.30	11 (5%) 29 36	26, 57, 104, 194	1 (0%)
All	All	2702/2726 (99%)	0.72	330 (12%) 5 7	9, 44, 128, 194	4 (0%)

The worst 5 of 330 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	212	VAL	13.5
4	F	214	CYS	12.6
3	E	133	VAL	11.8
2	B	33	LEU	11.3
3	E	201	CYS	11.0

### 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 ⓘ

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
11	NAG	D	3371	14/15	0.86	0.26	1.98	55,84,97,112	0
11	NAG	B	3371	14/15	0.86	0.25	0.46	58,87,99,110	0
12	NAG	D	3320	14/15	0.94	0.13	-	25,41,53,57	0
10	NAG	B	3320	14/15	0.97	0.11	-	17,28,41,46	0
10	MAN	B	3324	11/12	0.67	0.24	-	106,113,118,118	0
12	NAG	D	3321	14/15	0.88	0.26	-	57,71,87,101	0
10	NAG	B	3321	14/15	0.90	0.12	-	40,53,63,76	0
10	MAN	B	3322	11/12	0.79	0.26	-	52,93,109,113	0
12	MAN	D	3322	11/12	0.51	0.31	-	100,108,110,110	0
11	NAG	B	3372	14/15	0.84	0.31	-	108,117,121,123	0
11	NAG	D	3372	14/15	0.73	0.45	-	118,126,130,131	0
10	MAN	B	3323	11/12	0.69	0.23	-	64,77,88,90	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, 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
8	MG	D	2001	1/1	0.87	0.72	21.72	41,41,41,41	1
7	SO4	L	215	5/5	0.81	0.44	11.63	101,106,112,115	0
7	SO4	D	473	5/5	0.72	0.39	9.70	131,133,136,137	0
6	GOL	C	458	6/6	0.83	0.30	8.64	45,61,71,79	0
6	GOL	A	463	6/6	0.73	0.30	7.75	77,79,83,84	0
6	GOL	A	460	6/6	0.81	0.27	6.14	68,70,78,84	0
7	SO4	H	222	5/5	0.83	0.36	5.69	112,116,118,123	0
7	SO4	C	461	5/5	0.88	0.26	5.64	55,75,85,87	0
7	SO4	B	473	5/5	0.76	0.30	4.50	90,98,103,108	0
7	SO4	C	460	5/5	0.90	0.19	3.61	39,53,83,84	0
7	SO4	A	464	5/5	0.86	0.17	3.09	97,98,107,112	0
7	SO4	D	472	5/5	0.79	0.25	2.66	73,92,98,108	0
6	GOL	A	461	6/6	0.92	0.18	1.49	28,50,57,71	0
6	GOL	B	472	6/6	0.83	0.17	1.43	65,70,72,77	0
5	CA	A	2006	1/1	0.99	0.15	0.56	16,16,16,16	0
8	MG	B	2001	1/1	0.97	0.16	0.22	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	C	2007	1/1	0.97	0.14	0.17	36,36,36,36	0
5	CA	A	2005	1/1	0.99	0.12	-0.41	19,19,19,19	0
5	CA	C	2006	1/1	0.97	0.11	-0.51	34,34,34,34	0
5	CA	B	2003	1/1	0.99	0.17	-0.65	13,13,13,13	0
5	CA	A	2007	1/1	1.00	0.13	-0.70	16,16,16,16	0
5	CA	D	2003	1/1	0.99	0.16	-0.89	22,22,22,22	0
7	SO4	C	463	5/5	0.93	0.12	-1.14	84,91,98,98	0
5	CA	A	2004	1/1	0.99	0.06	-1.84	29,29,29,29	0
5	CA	D	2002	1/1	0.95	0.12	-2.05	31,31,31,31	0
5	CA	C	2004	1/1	0.97	0.04	-2.22	45,45,45,45	0
5	CA	C	2005	1/1	0.99	0.05	-3.76	38,38,38,38	0
5	CA	B	2002	1/1	0.96	0.05	-4.01	35,35,35,35	0
6	GOL	A	458	6/6	0.86	0.20	-	28,51,56,58	0
6	GOL	A	459	6/6	0.93	0.16	-	42,45,58,58	0
6	GOL	C	459	6/6	0.79	0.27	-	52,67,73,74	0
6	GOL	A	462	6/6	0.84	0.21	-	47,61,65,70	0
9	NAG	B	3099	14/15	0.88	0.38	-	85,98,104,106	0
9	NAG	D	3099	14/15	0.79	0.29	-	76,90,95,96	0
7	SO4	C	462	5/5	0.85	0.18	-	110,113,117,118	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.