



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:26 PM GMT

PDB ID : 3ZDY  
Title : Integrin alphaIIB beta3 headpiece and RGD peptide complex  
Authors : Zhu, J.H.; Zhu, J.Q.; Springer, T.A.  
Deposited on : 2012-12-03  
Resolution : 2.45 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 (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

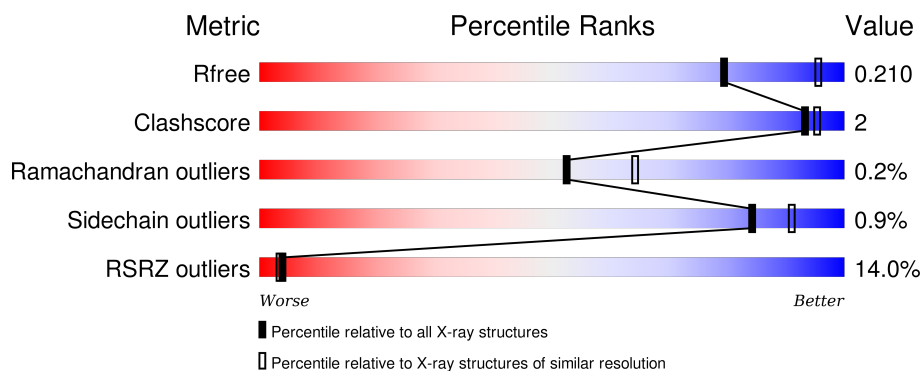
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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>3%</div> <div>95%</div> <div>..</div> </div>
1	C	457	<div> <div>2%</div> <div>95%</div> <div>...</div> </div>
2	B	472	<div> <div>11%</div> <div>94%</div> <div>..</div> </div>
2	D	472	<div> <div>11%</div> <div>94%</div> <div>...</div> </div>
3	E	221	<div> <div>45%</div> <div>93%</div> <div>5% .</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	I	6	
5	J	6	

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	SO4	A	1455	-	-	-	X
6	SO4	A	1457	-	-	-	X
6	SO4	A	1459	-	-	-	X
6	SO4	A	1462	-	-	X	-
6	SO4	A	1463	-	-	-	X
6	SO4	B	1467	-	-	-	X
6	SO4	B	1469	-	-	-	X
6	SO4	C	1454	-	-	-	X
6	SO4	C	1457	-	-	-	X
6	SO4	C	1458	-	-	-	X
6	SO4	L	1216	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 42366 atoms, of which 20280 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	1	7	0
			6862	2233	3352	602	667	8			
1	C	453	Total	C	H	N	O	S	1	3	0
			6809	2218	3319	601	663	8			

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	464	Total	C	H	N	O	S	7	5	0
			7131	2246	3525	615	711	34			
2	D	469	Total	C	H	N	O	S	11	1	0
			7154	2258	3531	618	713	34			

- Molecule 3 is a protein called 10E5 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3239	1041	1597	266	329	6			

- Molecule 4 is a protein called 10E5 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3187	1019	1550	268	341	9			

- Molecule 5 is a protein called RGD PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	3	0
			112	32	52	15	13			
5	J	5	Total	C	H	N	O	0	3	0
			97	27	45	14	11			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

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

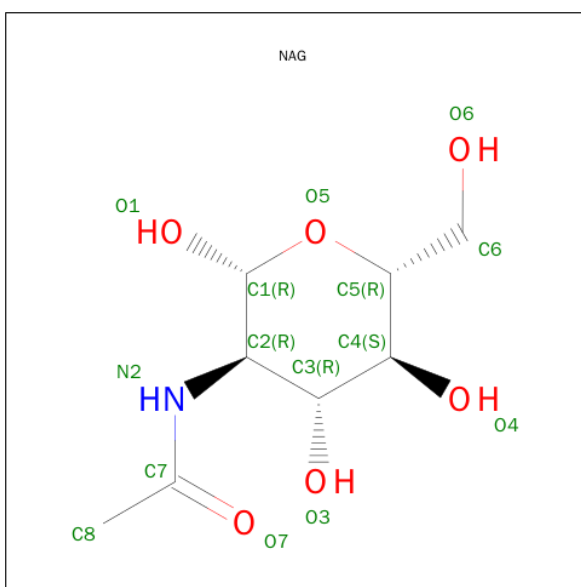
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- 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	H	N	O	0	0
			27	8	13	1	5		
9	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 10 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	4	Total	C	H	N	O	0	0
			93	28	43	2	20		
10	D	4	Total	C	H	N	O	0	0
			93	28	43	2	20		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
11	D	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	357	Total	O	0	2
			359	359		

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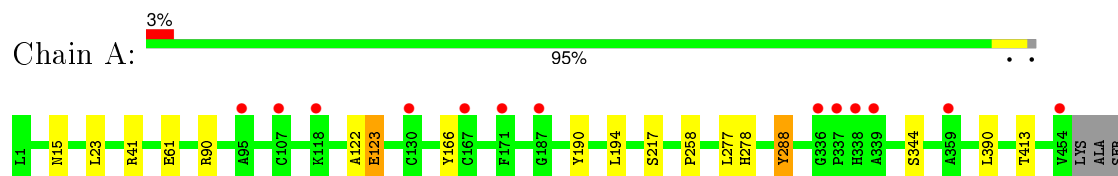
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	157	Total 157	O 157	0	0
12	C	192	Total 192	O 192	0	0
12	D	109	Total 109	O 109	0	0
12	E	10	Total 10	O 10	0	0
12	F	9	Total 9	O 9	0	0
12	H	25	Total 25	O 25	0	0
12	I	6	Total 6	O 6	0	0
12	J	1	Total 1	O 1	0	0
12	L	21	Total 21	O 21	0	0



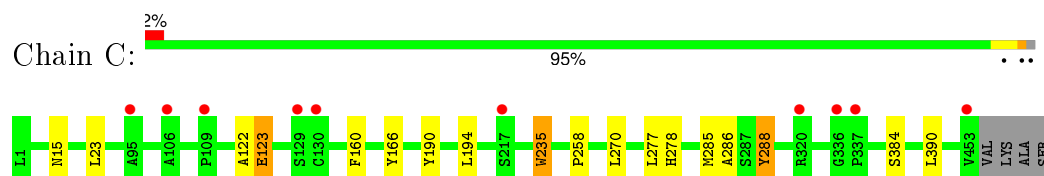
### 3 Residue-property plots [i](#)

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.

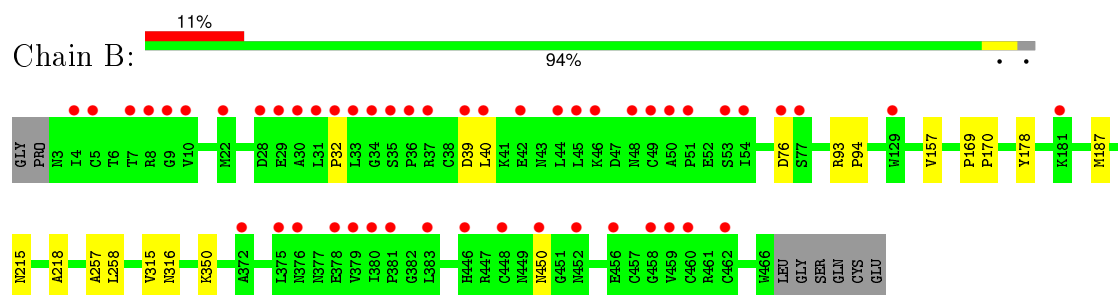
- Molecule 1: INTEGRIN ALPHA-IIB



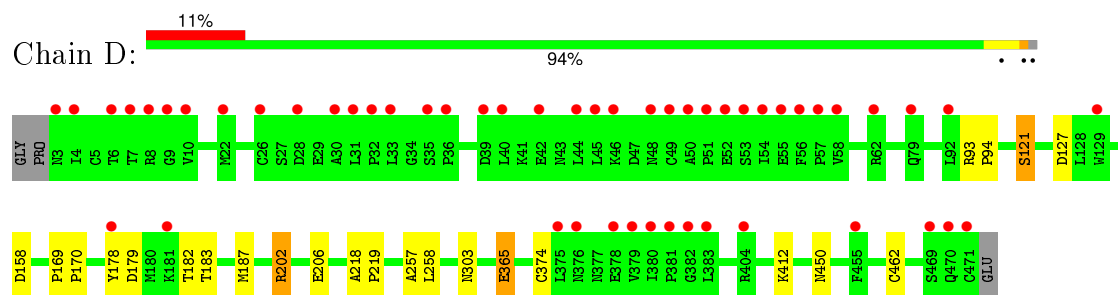
- Molecule 1: INTEGRIN ALPHA-IIB



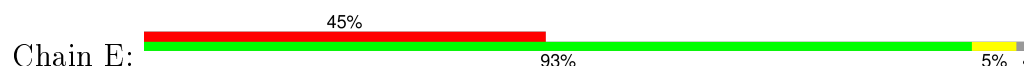
- Molecule 2: INTEGRIN BETA-3

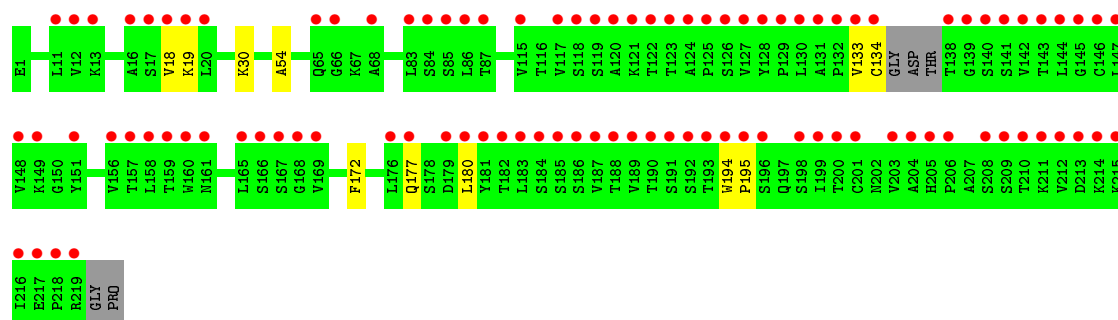


- Molecule 2: INTEGRIN BETA-3

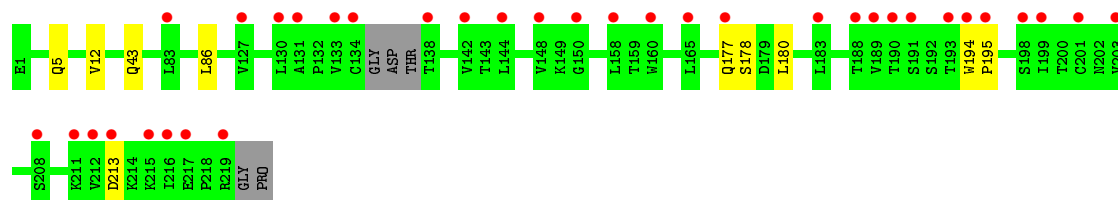


- Molecule 3: 10E5 FAB HEAVY CHAIN

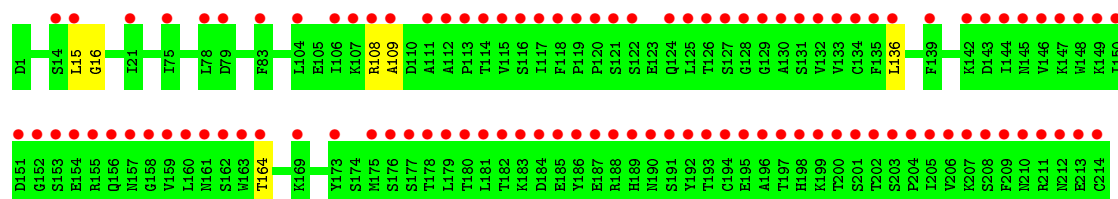




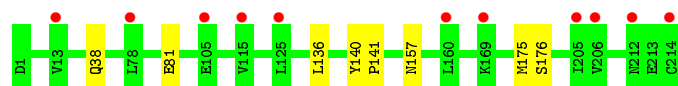
• Molecule 3: 10E5 FAB HEAVY CHAIN



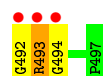
• Molecule 4: 10E5 FAB LIGHT CHAIN



• Molecule 4: 10E5 FAB LIGHT CHAIN

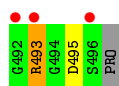


• Molecule 5: RGD PEPTIDE



• Molecule 5: RGD PEPTIDE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	257.76Å 145.25Å 106.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.45 49.15 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-2.45) 99.8 (49.15-2.45)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.182 , 0.216 0.175 , 0.210	Depositor DCC
$R_{free}$ test set	1009 reflections (0.69%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 64.1	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 146306 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	42366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, 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	0.22	0/3628	0.40	0/4945
1	C	0.22	0/3596	0.39	0/4900
2	B	0.21	0/3684	0.38	0/4994
2	D	0.21	0/3694	0.37	0/5009
3	E	0.20	0/1684	0.38	0/2305
3	H	0.21	0/1684	0.38	0/2305
4	F	0.21	0/1673	0.36	0/2269
4	L	0.21	0/1673	0.37	0/2269
5	I	0.20	0/60	0.43	0/76
5	J	0.21	0/51	0.37	0/64
All	All	0.21	0/21427	0.38	0/29136

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

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	3510	3352	3361	16	0
1	C	3490	3319	3328	10	0
2	B	3606	3525	3530	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3623	3531	3537	12	0
3	E	1642	1597	1600	6	0
3	H	1642	1597	1600	6	0
4	F	1637	1550	1553	4	0
4	L	1637	1550	1553	6	0
5	I	60	52	51	5	0
5	J	52	45	44	5	0
6	A	45	0	0	4	2
6	B	15	0	0	0	0
6	C	25	0	0	1	0
6	D	5	0	0	0	0
6	L	10	0	0	0	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
7	C	4	0	0	0	0
7	D	2	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	14	13	13	0	0
9	D	14	13	13	0	0
10	B	50	43	43	0	0
10	D	50	43	43	0	0
11	B	28	25	25	0	0
11	D	28	25	25	0	0
12	A	359	0	0	17	1
12	B	157	0	0	1	0
12	C	192	0	0	3	3
12	D	109	0	0	0	0
12	E	10	0	0	0	0
12	F	9	0	0	0	0
12	H	25	0	0	1	0
12	I	6	0	0	1	0
12	J	1	0	0	0	0
12	L	21	0	0	1	0
All	All	22086	20280	20319	79	3

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 79 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)
12:A:3159:HOH:O	5:I:492[B]:GLY:N	1.99	0.95
12:A:3155:HOH:O	5:I:493[A]:ARG:NH1	2.09	0.84
6:A:1462:SO4:S	12:A:3332:HOH:O	2.36	0.83
12:A:3155:HOH:O	5:I:493[B]:ARG:NH2	2.13	0.81
6:A:1462:SO4:O4	12:A:3331:HOH:O	2.06	0.72

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1462:SO4:O2	12:C:3163:HOH:O[1_554]	2.04	0.16
6:A:1462:SO4:O2	12:C:3175:HOH:O[1_554]	2.06	0.14
12:A:3352:HOH:O	12:C:3174:HOH:O[1_554]	2.12	0.08

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/457 (100%)	440 (96%)	18 (4%)	1 (0%)	52	64
1	C	454/457 (99%)	440 (97%)	13 (3%)	1 (0%)	52	64
2	B	467/472 (99%)	445 (95%)	20 (4%)	2 (0%)	39	49
2	D	468/472 (99%)	449 (96%)	18 (4%)	1 (0%)	52	64
3	E	212/221 (96%)	197 (93%)	15 (7%)	0	100	100
3	H	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	34	41
4	F	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
4	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
5	I	6/6 (100%)	3 (50%)	3 (50%)	0	100	100
5	J	5/6 (83%)	3 (60%)	2 (40%)	0	100	100
All	All	2707/2740 (99%)	2579 (95%)	122 (4%)	6 (0%)	52	64

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	76	ASP
1	C	123	GLU
3	H	178	SER
2	B	32	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	369/364 (101%)	364 (99%)	5 (1%)	74	85
1	C	364/364 (100%)	358 (98%)	6 (2%)	70	83
2	B	416/417 (100%)	414 (100%)	2 (0%)	92	95
2	D	416/417 (100%)	410 (99%)	6 (1%)	74	85
3	E	187/190 (98%)	187 (100%)	0	100	100
3	H	187/190 (98%)	187 (100%)	0	100	100
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
5	I	5/4 (125%)	3 (60%)	2 (40%)	0	0
5	J	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	2324/2326 (100%)	2301 (99%)	23 (1%)	84	89

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	190	TYR
1	C	288	TYR
5	J	493[A]	ARG
1	C	235	TRP
2	D	121	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such



sidechains are listed below:

Mol	Chain	Res	Type
2	B	3	ASN
2	D	3	ASN
2	D	82	GLN
3	E	202	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 ⓘ

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	0.59	0
10	NAG	B	3321	10	14,14,15	0.56	0	15,19,21	0.71	0
10	BMA	B	3322	10	11,11,12	0.62	0	14,15,17	0.85	1 (7%)
10	MAN	B	3323	10	11,11,12	0.60	0	14,15,17	0.71	0
11	NAG	B	3371	11,2	14,14,15	0.53	0	15,19,21	0.68	0
11	NAG	B	3372	11	14,14,15	0.49	0	15,19,21	0.60	0
10	NAG	D	3320	10,2	14,14,15	0.50	0	15,19,21	0.63	0
10	NAG	D	3321	10	14,14,15	0.54	0	15,19,21	0.65	0
10	BMA	D	3322	10	11,11,12	0.63	0	14,15,17	0.97	1 (7%)
10	MAN	D	3323	10	11,11,12	0.61	0	14,15,17	0.66	0
11	NAG	D	3371	11,2	14,14,15	0.54	0	15,19,21	0.62	0
11	NAG	D	3372	11	14,14,15	0.49	0	15,19,21	0.65	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	BMA	B	3322	10	-	0/2/19/22	0/1/1/1
10	MAN	B	3323	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
10	NAG	D	3320	10,2	-	0/6/23/26	0/1/1/1
10	NAG	D	3321	10	-	0/6/23/26	0/1/1/1
10	BMA	D	3322	10	-	0/2/19/22	0/1/1/1
10	MAN	D	3323	10	-	0/2/19/22	0/1/1/1
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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	3322	BMA	C1-C2-C3	2.34	112.31	109.54
10	D	3322	BMA	C1-C2-C3	3.07	113.18	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 36 ligands modelled in this entry, 14 are monoatomic - leaving 22 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	SO4	A	1455	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	A	1456	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	A	1457	-	4,4,4	0.23	0	6,6,6	0.06	0
6	SO4	A	1458	-	4,4,4	0.22	0	6,6,6	0.08	0
6	SO4	A	1459	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	A	1460	-	4,4,4	0.25	0	6,6,6	0.10	0
6	SO4	A	1461	-	4,4,4	0.22	0	6,6,6	0.09	0
6	SO4	A	1462	-	4,4,4	0.23	0	6,6,6	0.10	0
6	SO4	A	1463	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	B	1467	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	B	1468	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	B	1469	-	4,4,4	0.24	0	6,6,6	0.08	0
9	NAG	B	3319	2	14,14,15	0.50	0	15,19,21	0.72	0
6	SO4	C	1454	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	C	1455	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	C	1456	-	4,4,4	0.22	0	6,6,6	0.08	0
6	SO4	C	1457	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	C	1458	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	D	1472	-	4,4,4	0.23	0	6,6,6	0.09	0
9	NAG	D	3319	2	14,14,15	0.49	0	15,19,21	0.60	0
6	SO4	L	1215	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	L	1216	-	4,4,4	0.23	0	6,6,6	0.08	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	SO4	A	1455	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1456	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1457	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1458	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1459	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1460	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1461	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1462	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1463	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1467	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1468	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1469	-	-	0/0/0/0	0/0/0/0
9	NAG	B	3319	2	-	0/6/23/26	0/1/1/1
6	SO4	C	1454	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	C	1455	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1456	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1457	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1458	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1472	-	-	0/0/0/0	0/0/0/0
9	NAG	D	3319	2	-	0/6/23/26	0/1/1/1
6	SO4	L	1215	-	-	0/0/0/0	0/0/0/0
6	SO4	L	1216	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1462	SO4	4	2
6	C	1458	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.56	13 (2%) 55 58	19, 32, 62, 132	2 (0%)
1	C	453/457 (99%)	0.40	10 (2%) 65 68	27, 46, 80, 121	1 (0%)
2	B	464/472 (98%)	0.80	50 (10%) 8 7	20, 56, 137, 181	2 (0%)
2	D	469/472 (99%)	0.61	52 (11%) 7 7	30, 60, 128, 179	3 (0%)
3	E	216/221 (97%)	2.79	99 (45%) 0 0	56, 116, 214, 250	0
3	H	216/221 (97%)	0.79	35 (16%) 3 2	38, 90, 145, 182	0
4	F	214/214 (100%)	2.75	103 (48%) 0 0	57, 123, 220, 256	1 (0%)
4	L	214/214 (100%)	0.51	11 (5%) 32 35	38, 75, 110, 212	0
5	I	6/6 (100%)	1.96	3 (50%) 0 0	75, 80, 91, 97	0
5	J	5/6 (83%)	2.68	3 (60%) 0 0	83, 90, 105, 121	0
All	All	2711/2740 (98%)	0.95	379 (13%) 4 3	19, 61, 157, 256	9 (0%)

The worst 5 of 379 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	133	VAL	18.7
4	F	181	LEU	16.9
4	F	179	LEU	15.1
4	F	214	CYS	14.8
3	E	199	ILE	14.8

### 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	0.83	0.27	1.21	86,108,128,132	0
10	NAG	D	3320	14/15	0.93	0.15	0.67	48,64,89,91	0
11	NAG	B	3371	14/15	0.90	0.26	0.55	87,104,120,125	0
10	NAG	B	3320	14/15	0.95	0.14	-3.70	26,53,72,78	0
11	NAG	B	3372	14/15	0.92	0.34	-	106,129,155,157	0
10	MAN	B	3323	11/12	0.77	0.28	-	136,140,166,168	0
10	BMA	D	3322	11/12	0.84	0.38	-	134,142,170,170	0
10	NAG	B	3321	14/15	0.92	0.15	-	76,93,106,112	0
10	NAG	D	3321	14/15	0.89	0.32	-	92,115,141,144	0
11	NAG	D	3372	14/15	0.86	0.35	-	114,138,165,167	0
10	BMA	B	3322	11/12	0.77	0.22	-	120,135,160,162	0
10	MAN	D	3323	11/12	0.74	0.30	-	124,133,158,159	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
6	SO4	C	1457	5/5	0.86	0.34	7.36	150,151,152,152	0
6	SO4	A	1455	5/5	0.88	0.30	6.93	123,125,126,128	0
6	SO4	B	1469	5/5	0.83	0.29	4.78	163,163,164,164	0
6	SO4	C	1458	5/5	0.93	0.24	4.38	133,135,135,137	0
6	SO4	L	1216	5/5	0.78	0.26	4.31	140,140,143,144	0
6	SO4	A	1457	5/5	0.90	0.22	4.23	125,125,127,128	0
6	SO4	B	1467	5/5	0.72	0.32	4.10	141,142,143,145	0
6	SO4	C	1454	5/5	0.81	0.24	3.52	133,134,135,137	0
6	SO4	A	1463	5/5	0.91	0.27	3.28	116,119,120,122	0
6	SO4	A	1459	5/5	0.77	0.50	2.81	161,161,162,162	0
6	SO4	D	1472	5/5	0.86	0.20	1.88	128,130,131,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CA	D	2003	1/1	1.00	0.23	1.84	37,37,37,37	0
9	NAG	D	3319	14/15	0.85	0.30	1.50	82,102,122,126	0
7	CA	A	2006	1/1	0.98	0.21	1.47	25,25,25,25	0
7	CA	A	2007	1/1	0.99	0.21	1.42	26,26,26,26	0
7	CA	B	2003	1/1	0.99	0.26	1.41	28,28,28,28	0
6	SO4	A	1458	5/5	0.91	0.21	1.23	94,107,109,112	0
6	SO4	A	1462	5/5	0.97	0.19	1.04	83,92,97,100	0
7	CA	C	2007	1/1	0.96	0.16	0.79	39,39,39,39	0
6	SO4	A	1461	5/5	0.91	0.21	0.59	91,91,97,101	0
7	CA	C	2006	1/1	0.97	0.15	0.47	49,49,49,49	0
7	CA	A	2005	1/1	0.98	0.15	0.44	32,32,32,32	0
8	MG	B	2001	1/1	0.99	0.20	0.02	33,33,33,33	0
6	SO4	A	1460	5/5	0.98	0.16	-0.54	76,76,80,83	0
7	CA	D	2002	1/1	0.96	0.15	-0.55	53,53,53,53	0
7	CA	A	2004	1/1	0.98	0.08	-1.72	43,43,43,43	0
7	CA	B	2002	1/1	0.91	0.09	-1.83	67,67,67,67	0
6	SO4	C	1455	5/5	0.93	0.10	-2.21	104,106,106,107	0
8	MG	D	2001	1/1	0.95	0.10	-2.52	50,50,50,50	0
7	CA	C	2005	1/1	0.99	0.04	-2.78	55,55,55,55	0
7	CA	C	2004	1/1	0.92	0.04	-3.72	66,66,66,66	0
6	SO4	A	1456	5/5	0.88	0.19	-	117,121,123,124	0
6	SO4	L	1215	5/5	0.92	0.23	-	115,116,116,118	0
6	SO4	C	1456	5/5	0.82	0.18	-	134,135,137,138	0
6	SO4	B	1468	5/5	0.80	0.31	-	153,154,154,154	0
9	NAG	B	3319	14/15	0.82	0.36	-	104,123,147,151	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.