W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:26 PM GMT

PDB ID	:	3ZE1
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	:	3.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

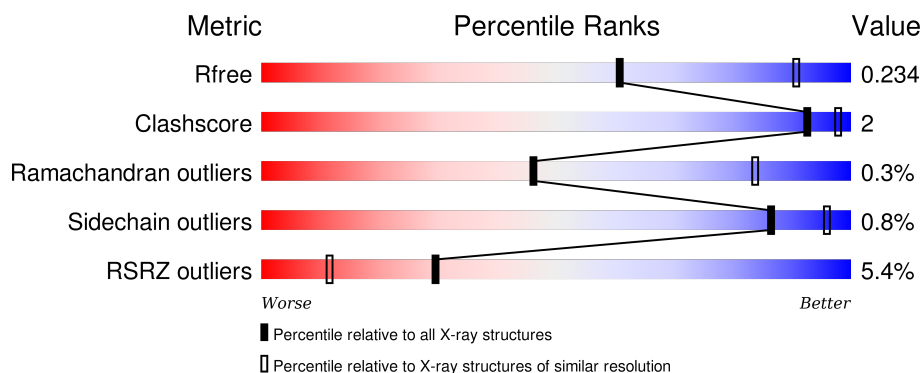|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.00 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		2
Ramachandran outliers		0.3%
Sidechain outliers		0.8%
RSRZ outliers		5.4%

Worse　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	95% ·
1	C	457	93% 6% ·
2	B	472	4% / 90% 7% ·
2	D	472	7% / 92% 7% ·
3	E	221	13% / 93% 5% ·

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Mol	Chain	Length	Quality of chain
3	H	221	5% ... 91% ... 6% •
4	F	214	22% ... 96% ... •
4	L	214	% ... 97% ... •
5	I	6	83% ... 17%
5	J	6	17% ... 100%

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	1457	-	-	-	X
9	NAG	D	3099	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 41577 atoms, of which 20215 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called INTEGRIN ALPHA-IIB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	H	N	O	S	1	4	0
			6860	2233	3350	604	665	8			
1	C	453	Total	C	H	N	O	S	0	3	0
			6807	2218	3317	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	6	1	0
			7083	2233	3498	612	707	33			
2	D	469	Total	C	H	N	O	S	10	2	0
			7146	2253	3526	618	715	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	0	0
			75	22	34	9	10			
5	J	6	Total	C	H	N	O	0	0	0
			75	22	34	9	10			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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	L	1	Total	O	S	0	0
			5	4	1		

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

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

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

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

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

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

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

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

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	161	Total 161	O 161	0	0
13	B	61	Total 61	O 61	0	0
13	C	50	Total 50	O 50	0	0
13	D	16	Total 16	O 16	0	0
13	E	2	Total 2	O 2	0	0
13	H	5	Total 5	O 5	0	0
13	I	1	Total 1	O 1	0	0
13	J	1	Total 1	O 1	0	0
13	L	6	Total 6	O 6	0	0

3 Residue-property plots ⓘ

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.
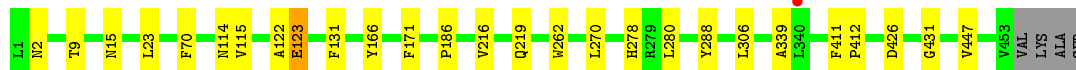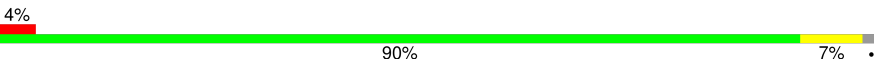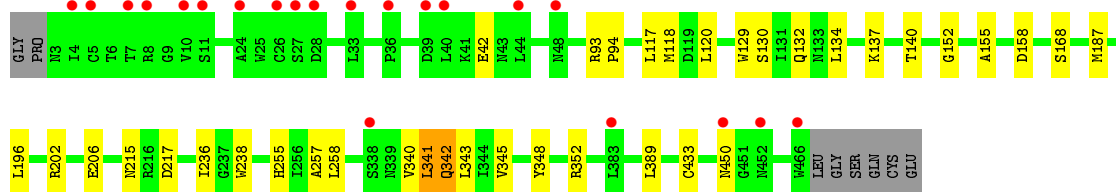
- Molecule 1: INTEGRIN ALPHA-IIB

Chain A:

- Molecule 1: INTEGRIN ALPHA-IIB

Chain C:
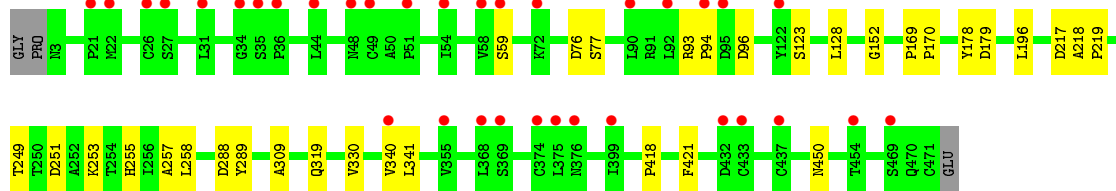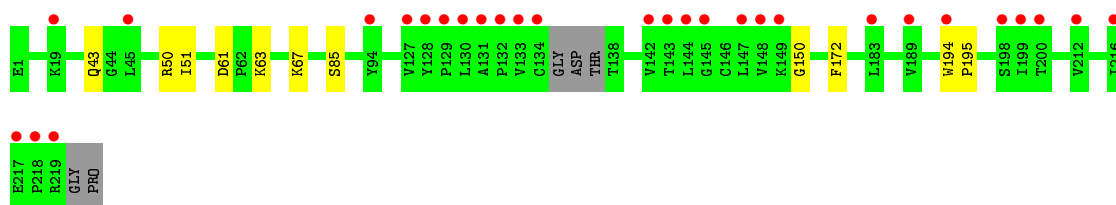

- Molecule 2: INTEGRIN BETA-3
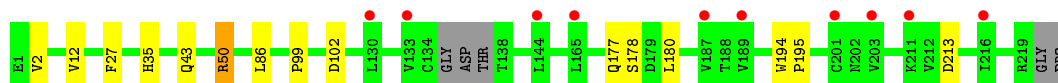
Chain B:

- Molecule 2: INTEGRIN BETA-3

Chain D:

- Molecule 3: 10E5 FAB HEAVY CHAIN

Chain E:

E19 K19 Q43 G44 L45 R50 I51 D61 P62 K63 K67 S85 Y94 V127 Y128 P129 L130 A131 P132 V133 C134 GLY ASP THR T138 V142 T143 L144 G145 C146 L147 K148 K149 G150 F172 L183 V189 W194 P195 S198 I199 T200 V212 I216

E217 P218 R219 GLY PRO

● Molecule 3: 10E5 FAB HEAVY CHAIN

Chain H:

5%
91%   6%

E1 V2 V12 F27 H35 Q43 R50 L86 P99 D102 L130 V133 C134 GLY ASP THR T138 L144 L165 Q177 S178 D179 L180 V187 T188 V189 W194 P195 C201 N202 V203 K211 V212 D213 I216 R219 GLY PRO

● Molecule 4: 10E5 FAB LIGHT CHAIN

Chain F:

22%
96%

D1 M11 S12 V13 W35 I48 Y49 S77 L78 C88 K103 L104 E105 V115 F118 P119 P120 L125 T126 G129 A130 S131 V132 V133 C134 F135 L136 N137 N138 K142 V146 K147 W148 K149 I150 S153 E154 R155 Q156 N157 G158 V159 T164 T178 L179

T180 L181 T182 Y186 S191 Y192 T193 C194 E195 I205 V206 K207 S208 F209 N212 E213 C214

● Molecule 4: 10E5 FAB LIGHT CHAIN

Chain L:

%
97%

D1 S43 F44 L104 L136 N137 N138 F139 Y140 P141 C214

● Molecule 5: RGD PEPTIDE

Chain I:

83%   17%

G492 R493 P497

● Molecule 5: RGD PEPTIDE

Chain J:

17%
100%

G492 P497

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	258.97Å 144.56Å 104.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 3.00 48.23 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.23-3.00) 98.2 (48.23-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.14 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.233 0.176 , 0.234	Depositor DCC
R_{free} test set	1052 reflections (1.35%)	DCC
Wilson B-factor (Å^2)	64.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 85.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.31$	Xtriage
Outliers	0 of 77953 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	41577	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: BMA, NAG, CL, CA, MN, SO4, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.23	0/3619	0.40	0/4932
1	C	0.22	0/3596	0.38	0/4900
2	B	0.22	0/3654	0.39	0/4954
2	D	0.21	0/3692	0.36	0/5005
3	E	0.21	0/1684	0.38	0/2305
3	H	0.21	0/1684	0.39	0/2305
4	F	0.21	0/1673	0.37	0/2269
4	L	0.22	0/1673	0.37	0/2269
5	I	0.19	0/41	0.33	0/52
5	J	0.18	0/41	0.34	0/52
All	All	0.22	0/21357	0.38	0/29043

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	3510	3350	3359	10	0
1	C	3490	3317	3328	14	0
2	B	3585	3498	3504	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3620	3526	3537	18	0
3	E	1642	1597	1600	6	0
3	H	1642	1597	1600	8	0
4	F	1637	1550	1553	4	0
4	L	1637	1550	1553	3	0
5	I	41	34	34	1	0
5	J	41	34	34	0	0
6	A	10	0	0	0	0
6	L	5	0	0	0	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
8	B	3	0	0	0	0
8	D	3	0	0	0	0
9	B	14	13	13	0	0
9	D	14	13	13	2	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	2	0
12	C	1	0	0	0	0
13	A	161	0	0	3	1
13	B	61	0	0	1	0
13	C	50	0	0	1	1
13	D	16	0	0	0	0
13	E	2	0	0	0	0
13	H	5	0	0	0	0
13	I	1	0	0	0	0
13	J	1	0	0	0	0
13	L	6	0	0	0	0
All	All	21362	20215	20264	84	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 84 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)
9:D:3099:NAG:HO6	11:D:3372:NAG:HO6	1.39	0.64
1:C:15:ASN:ND2	13:C:4007:HOH:O	2.33	0.62
13:A:4048:HOH:O	2:B:168:SER:O	2.17	0.58
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ASP:OD1	2:D:77:SER:N	2.39	0.56

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:4055:HOH:O	13:C:4041:HOH:O[1_554]	2.16	0.04

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	457/457 (100%)	438 (96%)	18 (4%)	1 (0%)	52	88
1	C	454/457 (99%)	423 (93%)	30 (7%)	1 (0%)	52	88
2	B	463/472 (98%)	433 (94%)	28 (6%)	2 (0%)	39	80
2	D	469/472 (99%)	433 (92%)	36 (8%)	0	100	100
3	E	212/221 (96%)	194 (92%)	17 (8%)	1 (0%)	34	76
3	H	212/221 (96%)	197 (93%)	14 (7%)	1 (0%)	34	76
4	F	212/214 (99%)	200 (94%)	10 (5%)	2 (1%)	21	64
4	L	212/214 (99%)	200 (94%)	11 (5%)	1 (0%)	34	76
5	I	4/6 (67%)	4 (100%)	0	0	100	100
5	J	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2699/2740 (98%)	2526 (94%)	164 (6%)	9 (0%)	46	84

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	341	LEU

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Mol	Chain	Res	Type
1	A	123	GLU
4	L	138	ASN
2	B	343	LEU
1	C	123	GLU

5.3.2 Protein sidechains (i)

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%)	361 (98%)	6 (2%)	70	92
1	C	364/364 (100%)	360 (99%)	4 (1%)	80	94
2	B	412/417 (99%)	405 (98%)	7 (2%)	68	91
2	D	417/417 (100%)	416 (100%)	1 (0%)	95	99
3	E	187/190 (98%)	187 (100%)	0	100	100
3	H	187/190 (98%)	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	I	4/4 (100%)	4 (100%)	0	100	100
5	J	4/4 (100%)	4 (100%)	0	100	100
All	All	2318/2326 (100%)	2299 (99%)	19 (1%)	86	96

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	132	GLN
2	B	215	ASN
1	C	270	LEU
2	B	118	MET
1	C	288	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	C	197	GLN
2	D	450	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

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	0.51	0	15,19,21	0.65	0
10	NAG	B	3321	10	14,14,15	0.55	0	15,19,21	0.67	0
10	BMA	B	3322	10	11,11,12	0.60	0	14,15,17	0.86	1 (7%)
10	MAN	B	3323	10	11,11,12	0.60	0	14,15,17	0.69	0
11	NAG	B	3371	11,2	14,14,15	0.55	0	15,19,21	0.83	0
11	NAG	B	3372	11	14,14,15	0.51	0	15,19,21	0.57	0
10	NAG	D	3320	10,2	14,14,15	0.51	0	15,19,21	0.69	0
10	NAG	D	3321	10	14,14,15	0.54	0	15,19,21	0.64	0
10	BMA	D	3322	10	11,11,12	0.63	0	14,15,17	0.89	1 (7%)
10	MAN	D	3323	10	11,11,12	0.63	0	14,15,17	0.71	0
11	NAG	D	3371	11,2	14,14,15	0.59	0	15,19,21	0.84	1 (6%)
11	NAG	D	3372	11	14,14,15	0.51	0	15,19,21	0.64	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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	3371	NAG	C4-C3-C2	2.15	114.58	111.23
10	B	3322	BMA	C1-C2-C3	2.39	112.36	109.54
10	D	3322	BMA	C1-C2-C3	2.75	112.80	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	3372	NAG	2	0

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 15 are monoatomic - leaving 5 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	1456	-	4,4,4	0.22	0	6,6,6	0.08	0
6	SO4	A	1457	-	4,4,4	0.23	0	6,6,6	0.08	0
9	NAG	B	3099	2	14,14,15	0.50	0	15,19,21	0.66	0
9	NAG	D	3099	2	14,14,15	0.49	0	15,19,21	0.58	0
6	SO4	L	1215	-	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	1456	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1457	-	-	0/0/0/0	0/0/0/0
9	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
9	NAG	D	3099	2	-	0/6/23/26	0/1/1/1
6	SO4	L	1215	-	-	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	3099	NAG	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	455/457 (99%)	-0.02	1 (0%)	95	87	29, 51, 91, 147	1 (0%)
1	C	453/457 (99%)	0.02	1 (0%)	95	87	45, 84, 129, 195	0
2	B	464/472 (98%)	0.33	21 (4%)	37	15	32, 90, 183, 217	2 (0%)
2	D	469/472 (99%)	0.50	34 (7%)	18	7	57, 125, 192, 221	1 (0%)
3	E	216/221 (97%)	0.77	29 (13%)	4	1	86, 151, 204, 230	0
3	H	216/221 (97%)	0.12	10 (4%)	36	14	58, 118, 184, 219	0
4	F	214/214 (100%)	1.09	47 (21%)	1	1	89, 153, 226, 284	0
4	L	214/214 (100%)	0.09	2 (0%)	85	64	65, 106, 147, 242	0
5	I	6/6 (100%)	0.27	0	100	100	48, 57, 97, 118	0
5	J	6/6 (100%)	0.91	1 (16%)	2	1	108, 121, 149, 165	2 (33%)
All	All	2713/2740 (99%)	0.31	146 (5%)	29	11	29, 103, 190, 284	6 (0%)

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	181	LEU	8.4
4	F	193	THR	8.1
2	B	36	PRO	7.8
3	E	194	TRP	5.9
4	F	214	CYS	5.4

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	NAG	D	3371	14/15	0.81	0.39	0.57	137,170,200,210	0
11	NAG	B	3371	14/15	0.90	0.24	-0.03	116,142,165,172	0
10	NAG	D	3320	14/15	0.95	0.16	-1.24	74,107,135,142	0
10	NAG	B	3320	14/15	0.97	0.18	-1.57	19,59,87,104	0
11	NAG	D	3372	14/15	0.87	0.43	-	163,190,227,228	0
10	MAN	B	3323	11/12	0.88	0.30	-	143,163,188,191	0
10	MAN	D	3323	11/12	0.85	0.31	-	205,211,252,253	0
10	BMA	B	3322	11/12	0.87	0.14	-	143,167,200,201	0
11	NAG	B	3372	14/15	0.89	0.34	-	138,171,206,212	0
10	NAG	D	3321	14/15	0.90	0.20	-	108,146,181,185	0
10	NAG	B	3321	14/15	0.94	0.16	-	88,112,146,150	0
10	BMA	D	3322	11/12	0.76	0.28	-	176,197,235,237	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	SO4	A	1457	5/5	0.93	0.33	5.12	109,126,139,157	0
12	CL	C	2001	1/1	0.91	0.27	1.82	81,81,81,81	0
9	NAG	D	3099	14/15	0.67	0.44	1.65	144,168,198,202	0
9	NAG	B	3099	14/15	0.87	0.40	0.91	123,153,182,187	0
8	MN	B	2001	1/1	1.00	0.27	0.83	48,48,48,48	0
8	MN	D	2001	1/1	0.98	0.24	0.15	119,119,119,119	0
8	MN	B	2003	1/1	0.99	0.26	-0.17	61,61,61,61	0
7	CA	A	2007	1/1	0.99	0.19	-0.29	49,49,49,49	0
6	SO4	L	1215	5/5	0.86	0.20	-0.33	152,153,156,164	0
7	CA	C	2007	1/1	0.95	0.14	-0.41	71,71,71,71	0
7	CA	A	2006	1/1	1.00	0.18	-0.51	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
8	MN	B	2002	1/1	0.99	0.19	-0.61	63,63,63,63	0
7	CA	C	2006	1/1	0.97	0.12	-0.70	78,78,78,78	0
7	CA	A	2005	1/1	0.99	0.16	-0.82	41,41,41,41	0
8	MN	D	2002	1/1	0.91	0.14	-0.99	174,174,174,174	0
7	CA	A	2004	1/1	0.99	0.12	-1.22	47,47,47,47	0
8	MN	D	2003	1/1	0.97	0.18	-1.45	120,120,120,120	0
7	CA	C	2004	1/1	0.95	0.09	-1.70	113,113,113,113	0
7	CA	C	2005	1/1	0.97	0.07	-1.90	107,107,107,107	0
6	SO4	A	1456	5/5	0.91	0.23	-	83,99,114,131	0

6.5 Other polymers (i)

There are no such residues in this entry.