wwPDB X-ray Structure Validation Summary Report (i)

Mar 21, 2016 – 04:35 AM EDT

PDB ID	:	4Z7O
Title	:	Integrin alphaIIbbeta3 in complex with AGDV peptide
Authors	:	Lin, F.Y.; Zhu, J.; Springer, T.A.
Deposited on	:	2015-04-07
Resolution	:	2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

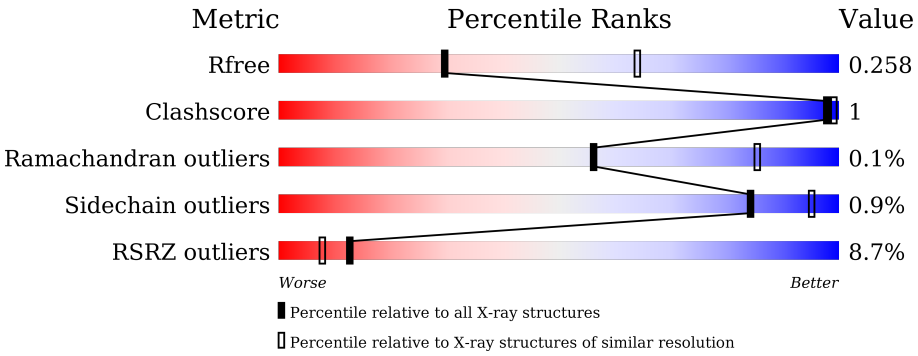
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	455	96%
1	C	455	2% 96%
2	B	469	5% 94% 5%
2	D	469	9% 97%
3	E	221	30% 95%
3	H	221	9% 94%

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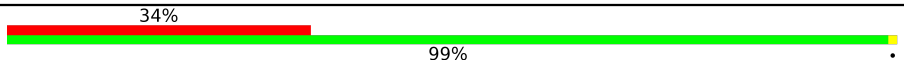
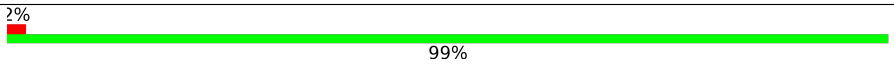
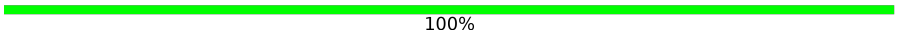
Mol	Chain	Length	Quality of chain
4	F	214	
4	L	214	
5	G	4	
5	I	4	

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	501	-	-	-	X
6	SO4	C	501	-	-	-	X
8	MN	B	2002	-	-	-	X
8	MN	D	2002	-	-	-	X
8	MN	D	2003	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 41839 atoms, of which 20230 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	0	5	0
			6886	2237	3369	607	665	8			
1	C	453	Total	C	H	N	O	S	0	1	0
			6796	2212	3315	600	661	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	0	1	0
			7066	2230	3484	612	707	33			
2	D	469	Total	C	H	N	O	S	0	0	0
			7140	2248	3528	617	713	34			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3243	1041	1601	266	329	6			

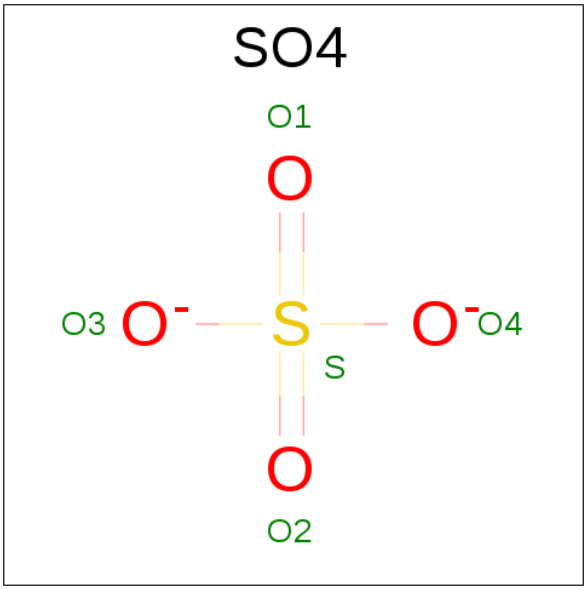
- Molecule 4 is a protein called Monoclonal antibody 10E5 Fab light chain.

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
			3191	1019	1554	268	341	9			

- Molecule 5 is a protein called Tetrapeptide ALA-GLY-ASP-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	4	Total	C	H	N	O	0	0	0
			45	14	20	4	7			
5	I	4	Total	C	H	N	O	0	0	0
			45	14	20	4	7			

- 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	C	1	Total	O	S		0	0
			5	4	1			
6	L	1	Total	O	S		0	0
			5	4	1			

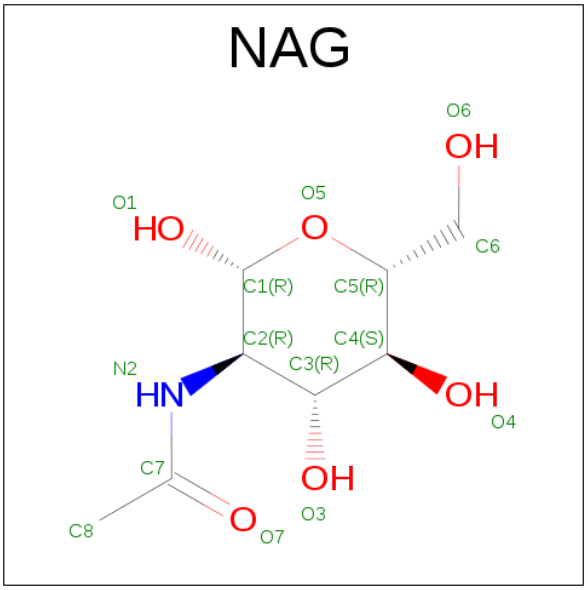
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

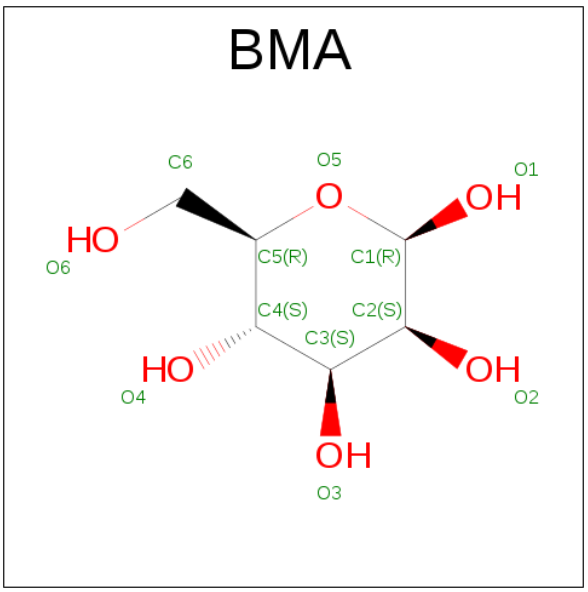
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	3	Total Mn 3 3	0	0
8	D	3	Total Mn 3 3	0	0

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



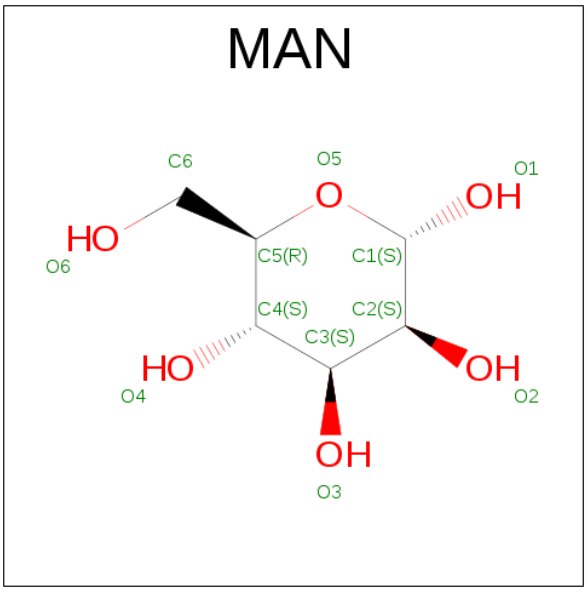
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C H N O 28 8 14 1 5	0	0
9	B	1	Total C H N O 27 8 13 1 5	0	0
9	B	1	Total C H N O 27 8 13 1 5	0	0
9	B	1	Total C H N O 27 8 13 1 5	0	0
9	B	1	Total C H N O 28 8 14 1 5	0	0
9	D	1	Total C H N O 28 8 14 1 5	0	0
9	D	1	Total C H N O 27 8 13 1 5	0	0
9	D	1	Total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

- Molecule 10 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C H O 20 6 9 5	0	0
10	D	1	Total C H O 21 6 10 5	0	0

- Molecule 11 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C H O 22 6 11 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C H O 22 6 11 5	0	0
11	D	1	Total C H O 22 6 11 5	0	0

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

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

- Molecule 13 is water.

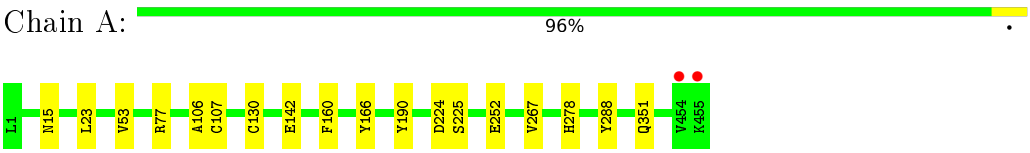
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	265	Total O 265 265	0	0
13	B	117	Total O 117 117	0	0
13	C	84	Total O 84 84	0	0
13	D	64	Total O 64 64	0	0
13	E	5	Total O 5 5	0	0
13	F	9	Total O 9 9	0	0
13	H	22	Total O 22 22	0	0
13	L	16	Total O 16 16	0	0
13	G	2	Total O 2 2	0	0

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.

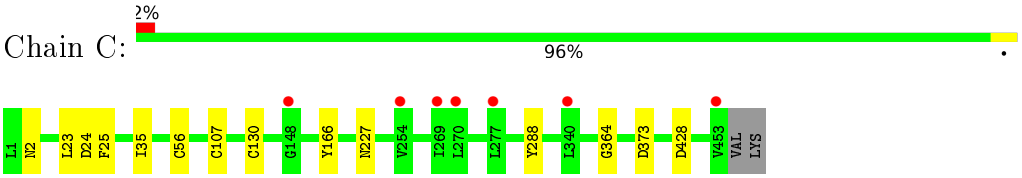
- Molecule 1: Integrin alpha-IIb

Chain A:



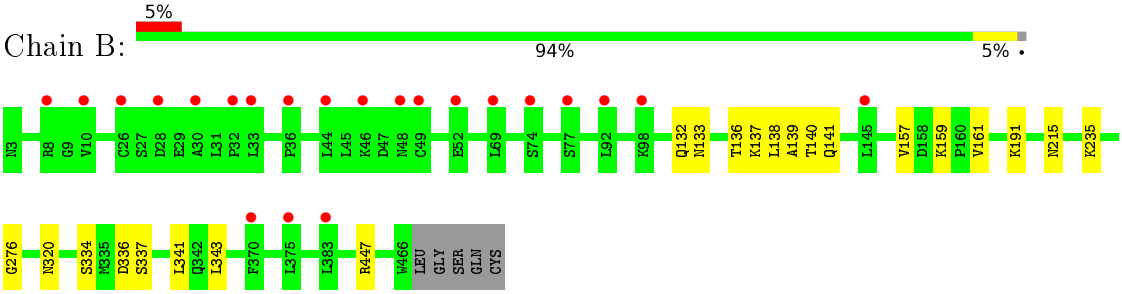
- Molecule 1: Integrin alpha-IIb

Chain C:



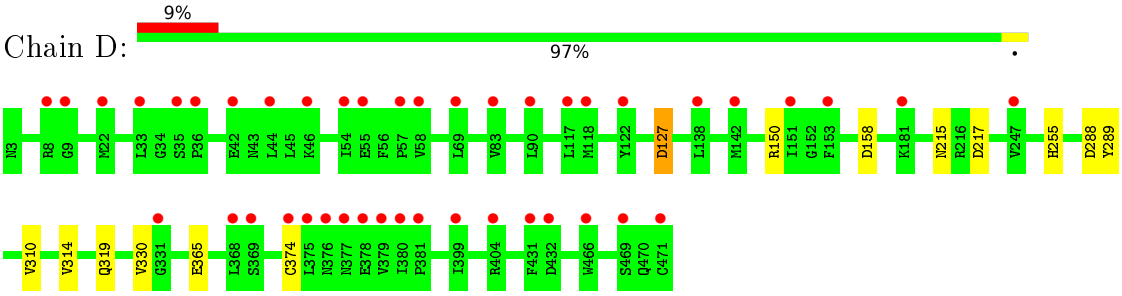
- Molecule 2: Integrin beta-3

Chain B:



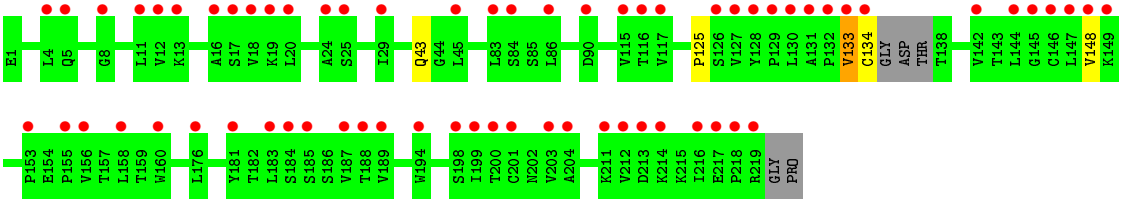
- Molecule 2: Integrin beta-3

Chain D:

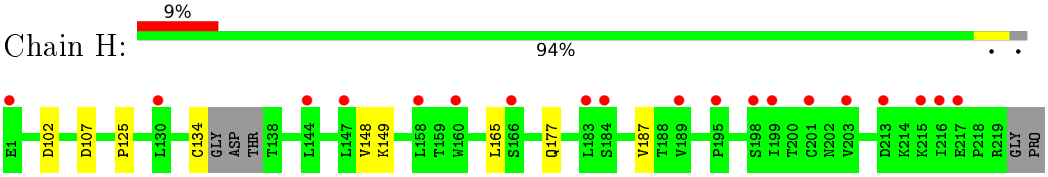


- Molecule 3: Monoclonal antibody 10E5 Fab heavy chain

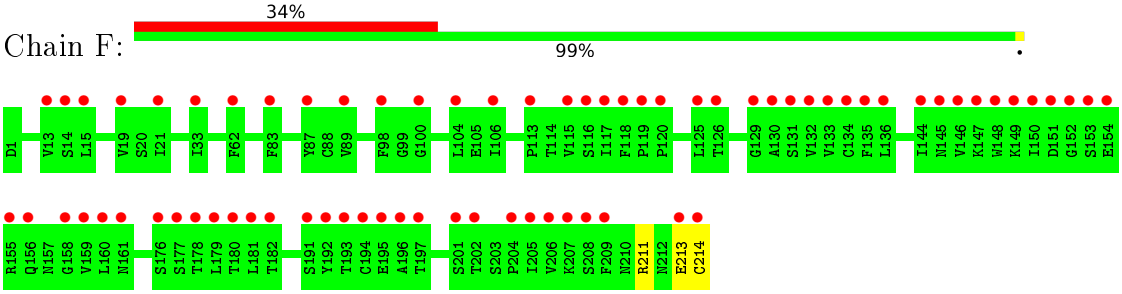
Chain E:



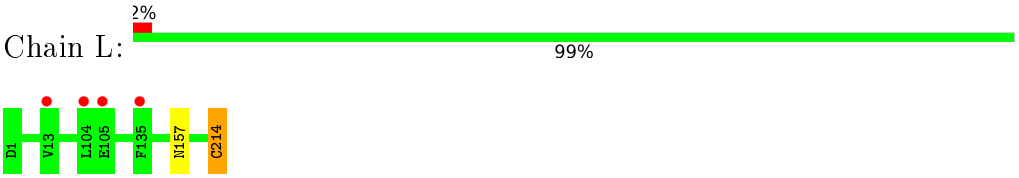
• Molecule 3: Monoclonal antibody 10E5 Fab heavy chain



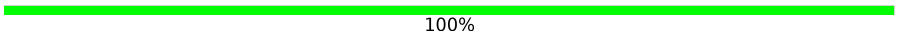
• Molecule 4: Monoclonal antibody 10E5 Fab light chain



• Molecule 4: Monoclonal antibody 10E5 Fab light chain

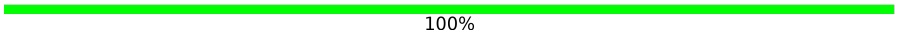


• Molecule 5: Tetrapeptide ALA-GLY-ASP-VAL



There are no outlier residues recorded for this chain.

• Molecule 5: Tetrapeptide ALA-GLY-ASP-VAL



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	259.92Å 144.52Å 104.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 2.85 49.03 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.03-2.85) 84.1 (49.03-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
R, R_{free}	0.223 , 0.257 0.223 , 0.258	Depositor DCC
R_{free} test set	1699 reflections (2.18%)	DCC
Wilson B-factor (Å^2)	57.9	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 92354 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	41839	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.29	0/3629	0.44	0/4944
1	C	0.26	0/3581	0.42	0/4880
2	B	0.26	0/3651	0.43	0/4950
2	D	0.26	0/3678	0.41	0/4986
3	E	0.25	0/1684	0.42	0/2305
3	H	0.24	0/1684	0.43	0/2305
4	F	0.25	0/1673	0.41	0/2269
4	L	0.25	0/1673	0.42	0/2269
5	G	0.19	0/24	0.45	0/30
5	I	0.25	0/24	0.48	0/30
All	All	0.26	0/21301	0.42	0/28968

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	3517	3369	3370	10	0
1	C	3481	3315	3315	8	0
2	B	3582	3484	3495	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3612	3528	3526	6	0
3	E	1642	1600	1600	3	0
3	H	1642	1601	1600	6	0
4	F	1637	1553	1553	1	0
4	L	1637	1554	1553	2	0
5	G	25	20	20	0	0
5	I	25	20	20	0	0
6	A	5	0	0	0	0
6	C	5	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	70	67	62	1	0
9	D	70	67	62	0	0
10	B	11	9	8	0	0
10	D	11	10	9	0	0
11	B	22	22	20	0	0
11	D	11	11	10	0	0
12	C	1	0	0	0	0
13	A	265	0	0	5	1
13	B	117	0	0	1	0
13	C	84	0	0	4	1
13	D	64	0	0	1	0
13	E	5	0	0	0	0
13	F	9	0	0	0	0
13	G	2	0	0	0	0
13	H	22	0	0	1	0
13	L	16	0	0	1	0
All	All	21609	20230	20223	44	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 1.

The worst 5 of 44 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)
1:A:351:GLN:OE1	13:A:601:HOH:O	2.13	0.67
1:A:15[B]:ASN:OD1	13:A:602:HOH:O	2.15	0.65
4:L:157:ASN:OD1	13:L:401:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASN:ND2	9:B:2005:NAG:O7	2.37	0.56
1:A:142:GLU:OE1	13:A:603:HOH:O	2.18	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:833:HOH:O	13:C:650:HOH:O[1_554]	2.14	0.06

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	458/455 (101%)	432 (94%)	26 (6%)	0	100	100
1	C	452/455 (99%)	429 (95%)	23 (5%)	0	100	100
2	B	463/469 (99%)	435 (94%)	26 (6%)	2 (0%)	39	71
2	D	467/469 (100%)	438 (94%)	28 (6%)	1 (0%)	52	82
3	E	212/221 (96%)	198 (93%)	13 (6%)	1 (0%)	34	67
3	H	212/221 (96%)	202 (95%)	10 (5%)	0	100	100
4	F	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
5	G	2/4 (50%)	2 (100%)	0	0	100	100
5	I	2/4 (50%)	2 (100%)	0	0	100	100
All	All	2692/2726 (99%)	2545 (94%)	143 (5%)	4 (0%)	56	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	133	VAL
2	B	139	ALA
2	D	374	CYS
2	B	157	VAL

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	368/363 (101%)	362 (98%)	6 (2%)	70 90
1	C	362/363 (100%)	359 (99%)	3 (1%)	86 96
2	B	411/415 (99%)	405 (98%)	6 (2%)	72 91
2	D	415/415 (100%)	411 (99%)	4 (1%)	82 94
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%)	187 (100%)	1 (0%)	92 97
4	L	188/188 (100%)	187 (100%)	1 (0%)	92 97
5	G	2/2 (100%)	2 (100%)	0	100 100
5	I	2/2 (100%)	2 (100%)	0	100 100
All	All	2310/2316 (100%)	2289 (99%)	21 (1%)	84 95

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	337	SER
2	B	447	ARG
2	D	215	ASN
2	B	215	ASN
2	D	365	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	132	GLN
2	D	280	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 33 ligands modelled in this entry, 15 are monoatomic - leaving 18 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	501	-	4,4,4	0.27	0	6,6,6	0.07	0
9	NAG	B	2004	2	14,14,15	0.55	0	15,19,21	0.70	1 (6%)
9	NAG	B	2005	9,2	14,14,15	0.38	0	15,19,21	0.57	0
9	NAG	B	2006	9,10	14,14,15	0.23	0	15,19,21	0.40	0
10	BMA	B	2007	9,11	11,11,12	0.61	0	15,15,17	1.06	0
11	MAN	B	2008	10	11,11,12	0.48	0	15,15,17	0.90	1 (6%)
11	MAN	B	2009	10	11,11,12	0.62	0	15,15,17	1.25	2 (13%)
9	NAG	B	2010	9,2	14,14,15	0.48	0	15,19,21	0.37	0
9	NAG	B	2011	9	14,14,15	0.16	0	15,19,21	0.37	0
6	SO4	C	501	-	4,4,4	0.25	0	6,6,6	0.07	0
9	NAG	D	2004	2	14,14,15	0.36	0	15,19,21	0.50	0
9	NAG	D	2005	9,2	14,14,15	0.57	0	15,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	D	2006	9,10	14,14,15	0.34	0	15,19,21	0.45	0
10	BMA	D	2007	9,11	11,11,12	0.68	0	15,15,17	0.82	0
11	MAN	D	2008	10	11,11,12	0.51	0	15,15,17	1.03	2 (13%)
9	NAG	D	2009	9,2	14,14,15	0.41	0	15,19,21	0.47	0
9	NAG	D	2010	9	14,14,15	0.28	0	15,19,21	0.37	0
6	SO4	L	301	-	4,4,4	0.26	0	6,6,6	0.06	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	501	-	-	0/0/0/0	0/0/0/0
9	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
9	NAG	B	2005	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	2006	9,10	-	0/6/23/26	0/1/1/1
10	BMA	B	2007	9,11	-	0/2/19/22	0/1/1/1
11	MAN	B	2008	10	-	0/2/19/22	0/1/1/1
11	MAN	B	2009	10	-	0/2/19/22	0/1/1/1
9	NAG	B	2010	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	2011	9	-	0/6/23/26	0/1/1/1
6	SO4	C	501	-	-	0/0/0/0	0/0/0/0
9	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
9	NAG	D	2005	9,2	-	0/6/23/26	0/1/1/1
9	NAG	D	2006	9,10	-	0/6/23/26	0/1/1/1
10	BMA	D	2007	9,11	-	0/2/19/22	0/1/1/1
11	MAN	D	2008	10	-	0/2/19/22	0/1/1/1
9	NAG	D	2009	9,2	-	0/6/23/26	0/1/1/1
9	NAG	D	2010	9	-	0/6/23/26	0/1/1/1
6	SO4	L	301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	2009	MAN	O2-C2-C3	-2.26	105.63	110.19
11	D	2008	MAN	O2-C2-C3	-2.18	105.79	110.19
11	B	2008	MAN	O2-C2-C3	-2.06	106.03	110.19
9	B	2004	NAG	C1-O5-C5	2.36	115.60	112.14
11	D	2008	MAN	C1-O5-C5	2.66	116.05	112.14

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
9	B	2005	NAG	1	0

5.7 Other polymers

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^{th} 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	455/455 (100%)	0.29	2 (0%) 93 92	47, 67, 100, 194	0
1	C	453/455 (99%)	0.41	7 (1%) 76 73	60, 95, 134, 174	0
2	B	464/469 (98%)	0.38	22 (4%) 35 29	52, 103, 182, 241	0
2	D	469/469 (100%)	0.64	43 (9%) 11 7	73, 128, 183, 256	0
3	E	216/221 (97%)	1.51	66 (30%) 1 0	113, 178, 252, 271	0
3	H	216/221 (97%)	0.40	19 (8%) 12 7	74, 130, 191, 221	0
4	F	214/214 (100%)	1.55	72 (33%) 0 0	115, 171, 252, 305	0
4	L	214/214 (100%)	0.17	4 (1%) 70 66	79, 118, 150, 227	0
5	G	4/4 (100%)	0.58	0 100 100	60, 84, 89, 93	0
5	I	4/4 (100%)	0.64	0 100 100	91, 100, 111, 123	0
All	All	2709/2726 (99%)	0.58	235 (8%) 13 8	47, 112, 207, 305	0

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	193	THR	16.9
4	F	181	LEU	12.2
4	F	180	THR	9.1
1	A	455	LYS	9.0
3	E	144	LEU	8.9

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 (i)

There are no carbohydrates in this entry.

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, 95^{th} 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
8	MN	D	2002	1/1	0.62	0.57	5.16	431,431,431,431	0
8	MN	D	2003	1/1	0.65	0.36	4.36	216,216,216,216	0
6	SO4	C	501	5/5	0.78	0.38	3.68	184,193,196,198	0
8	MN	B	2002	1/1	0.49	0.33	3.46	361,361,361,361	0
6	SO4	A	501	5/5	0.95	0.31	3.24	118,124,133,142	0
7	CA	C	506	1/1	0.92	0.20	1.17	108,108,108,108	0
8	MN	B	2003	1/1	0.95	0.25	0.64	90,90,90,90	0
8	MN	B	2001	1/1	0.97	0.24	0.61	57,57,57,57	0
7	CA	A	503	1/1	0.97	0.18	0.31	80,80,80,80	0
7	CA	C	503	1/1	0.76	0.22	0.25	197,197,197,197	0
7	CA	C	505	1/1	0.79	0.16	0.06	99,99,99,99	0
12	CL	C	502	1/1	0.82	0.25	0.03	85,85,85,85	0
9	NAG	B	2010	14/15	0.82	0.23	-0.08	106,133,156,160	0
7	CA	A	502	1/1	0.95	0.14	-0.23	77,77,77,77	0
8	MN	D	2001	1/1	0.81	0.20	-0.36	121,121,121,121	0
7	CA	A	505	1/1	0.96	0.21	-0.37	66,66,66,66	0
6	SO4	L	301	5/5	0.90	0.13	-0.44	151,154,159,161	0
7	CA	A	504	1/1	0.91	0.19	-0.52	57,57,57,57	0
7	CA	C	504	1/1	0.72	0.15	-0.74	168,168,168,168	0
9	NAG	D	2009	14/15	0.88	0.23	-0.87	120,141,169,170	0
9	NAG	D	2005	14/15	0.90	0.14	-1.44	94,125,155,157	0
11	MAN	B	2009	11/12	0.78	0.18	-	103,138,164,166	0
9	NAG	D	2006	14/15	0.83	0.20	-	127,139,163,173	0
10	BMA	B	2007	11/12	0.84	0.14	-	98,134,169,169	0
11	MAN	D	2008	11/12	0.89	0.28	-	129,155,171,179	0
9	NAG	B	2006	14/15	0.92	0.20	-	87,116,134,159	0
11	MAN	B	2008	11/12	0.92	0.13	-	115,133,147,159	0
9	NAG	B	2005	14/15	0.93	0.18	-	69,90,110,110	0
9	NAG	B	2004	14/15	0.89	0.27	-	118,139,166,167	0
9	NAG	B	2011	14/15	0.88	0.25	-	135,155,178,186	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	NAG	D	2004	14/15	0.83	0.23	-	114,142,170,175	0
10	BMA	D	2007	11/12	0.78	0.18	-	118,147,176,179	0
9	NAG	D	2010	14/15	0.84	0.24	-	119,154,187,187	0

6.5 Other polymers (i)

There are no such residues in this entry.