



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:56 PM GMT

PDB ID : 3VI3
Title : Crystal structure of alpha5beta1 integrin headpiece (ligand-free form)
Authors : Nagae, M.; Nogi, T.; Takagi, J.
Deposited on : 2011-09-21
Resolution : 2.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

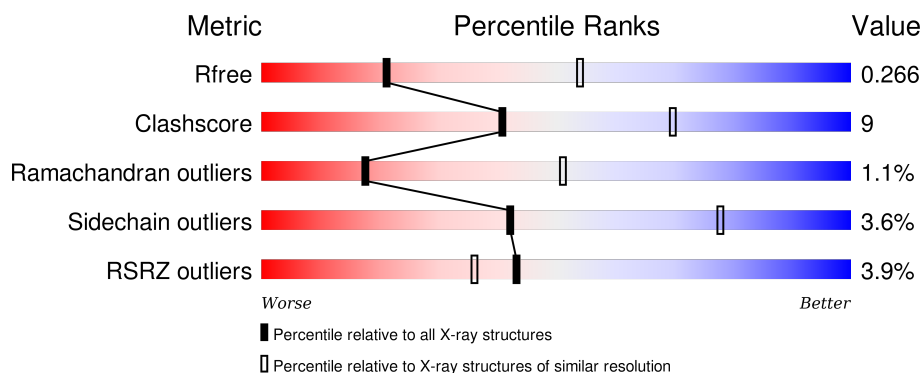
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.90 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.



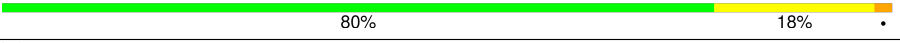


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 $\leq 5\%$. 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	632	 2% 73% 20% • 5%
1	C	632	 6% 71% 21% • 7%
2	B	454	 9% 72% 21% • 6%
2	D	454	 3% 75% 18% • 5%
3	E	219	 77% 21% •

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Mol	Chain	Length	Quality of chain
3	L	219	
4	F	218	
4	H	218	

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
8	MG	B	2003	-	-	-	X
8	MG	D	2003	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22803 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-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4567	2892	768	893	14			
1	C	589	Total	C	N	O	S	0	0	0
			4470	2832	748	876	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	GLY	-	EXPRESSION TAG	UNP P08648
A	625	GLY	-	EXPRESSION TAG	UNP P08648
A	626	LEU	-	EXPRESSION TAG	UNP P08648
A	627	GLU	-	EXPRESSION TAG	UNP P08648
A	628	ASN	-	EXPRESSION TAG	UNP P08648
A	629	LEU	-	EXPRESSION TAG	UNP P08648
A	630	TYR	-	EXPRESSION TAG	UNP P08648
A	631	PHE	-	EXPRESSION TAG	UNP P08648
A	632	GLN	-	EXPRESSION TAG	UNP P08648
C	624	GLY	-	EXPRESSION TAG	UNP P08648
C	625	GLY	-	EXPRESSION TAG	UNP P08648
C	626	LEU	-	EXPRESSION TAG	UNP P08648
C	627	GLU	-	EXPRESSION TAG	UNP P08648
C	628	ASN	-	EXPRESSION TAG	UNP P08648
C	629	LEU	-	EXPRESSION TAG	UNP P08648
C	630	TYR	-	EXPRESSION TAG	UNP P08648
C	631	PHE	-	EXPRESSION TAG	UNP P08648
C	632	GLN	-	EXPRESSION TAG	UNP P08648

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3327	2082	567	654	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	432	Total	C	N	O	S	0	0	0
			3367	2106	574	663	24			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	SEE REMARK 999	UNP P05556
B	195	THR	SER	SEE REMARK 999	UNP P05556
B	446	GLY	-	EXPRESSION TAG	UNP P05556
B	447	GLY	-	EXPRESSION TAG	UNP P05556
B	448	LEU	-	EXPRESSION TAG	UNP P05556
B	449	GLU	-	EXPRESSION TAG	UNP P05556
B	450	ASN	-	EXPRESSION TAG	UNP P05556
B	451	LEU	-	EXPRESSION TAG	UNP P05556
B	452	TYR	-	EXPRESSION TAG	UNP P05556
B	453	PHE	-	EXPRESSION TAG	UNP P05556
B	454	GLN	-	EXPRESSION TAG	UNP P05556
D	92	HIS	THR	SEE REMARK 999	UNP P05556
D	195	THR	SER	SEE REMARK 999	UNP P05556
D	446	GLY	-	EXPRESSION TAG	UNP P05556
D	447	GLY	-	EXPRESSION TAG	UNP P05556
D	448	LEU	-	EXPRESSION TAG	UNP P05556
D	449	GLU	-	EXPRESSION TAG	UNP P05556
D	450	ASN	-	EXPRESSION TAG	UNP P05556
D	451	LEU	-	EXPRESSION TAG	UNP P05556
D	452	TYR	-	EXPRESSION TAG	UNP P05556
D	453	PHE	-	EXPRESSION TAG	UNP P05556
D	454	GLN	-	EXPRESSION TAG	UNP P05556

- Molecule 3 is a protein called SG/19 Fab fragment (Light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1701	1066	292	335	8			
3	E	219	Total	C	N	O	S	0	0	0
			1701	1066	292	335	8			

- Molecule 4 is a protein called SG/19 Fab fragment (Heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	218	Total	C	N	O	S	0	0	0
			1651	1051	268	324	8			

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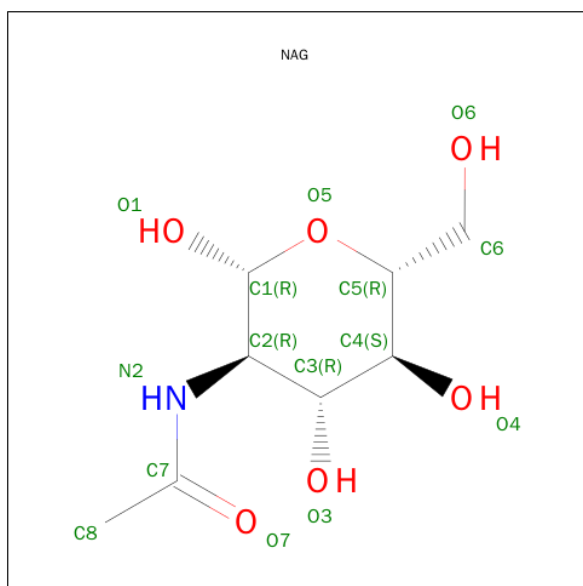
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	218	Total	C	N	O	S	0	0	0
			1651	1051	268	324	8			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	6	Total	C	N	O	0	0
			72	40	2	30		
7	C	6	Total	C	N	O	0	0
			72	40	2	30		

- 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		

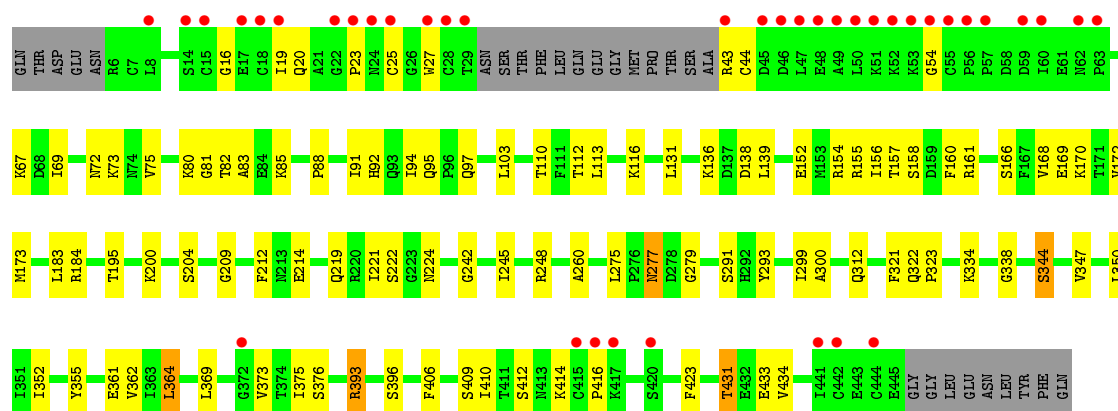
- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

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

PRO
ASP
LEU
GLN
LEU
GLU
VAL
PHE
GLY
GLN
ASN
GLY
GLY
LEU
LEU
ASN
LEU
TYR
PHE
GLN

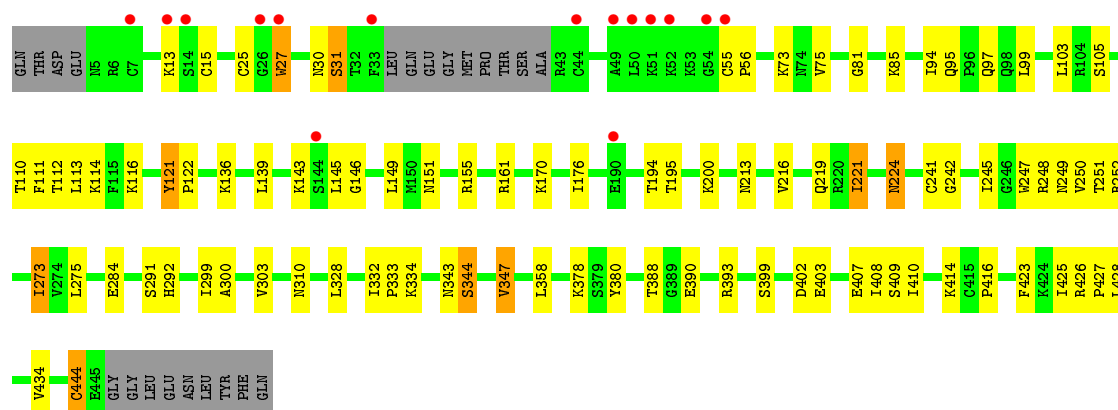
• Molecule 2: Integrin beta-1

Chain B: 9% 72% 21% 6%



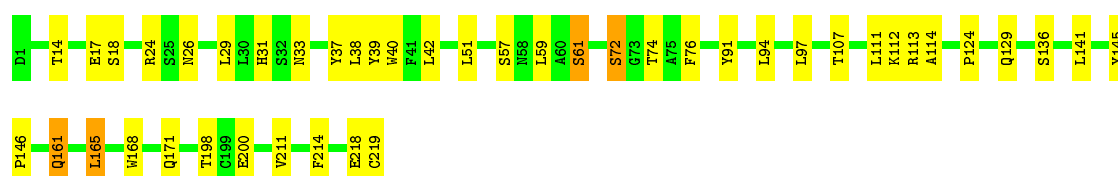
• Molecule 2: Integrin beta-1

Chain D: 3% 75% 18% 5%



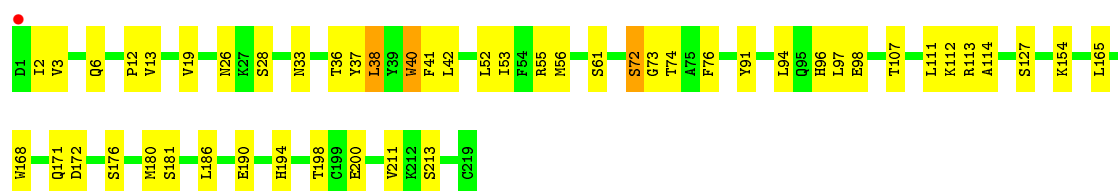
• Molecule 3: SG/19 Fab fragment (Light chain)

Chain L: 80% 18%

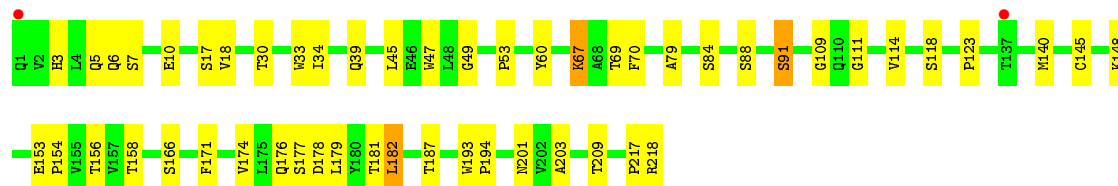
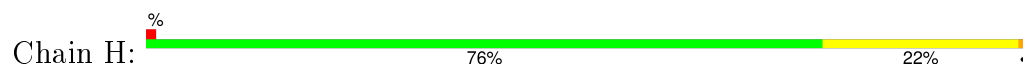


• Molecule 3: SG/19 Fab fragment (Light chain)

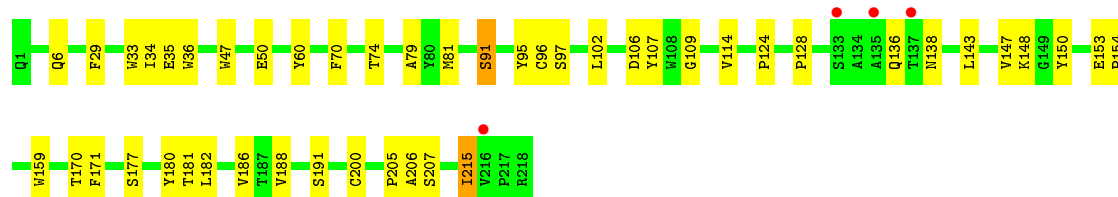
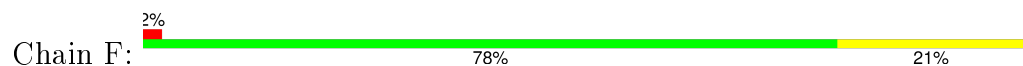
Chain E: 77% 21%



- Molecule 4: SG/19 Fab fragment (Heavy chain)



- Molecule 4: SG/19 Fab fragment (Heavy chain)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.96Å 102.81Å 125.08Å 76.10° 70.19° 71.28°	Depositor
Resolution (Å)	100.00 – 2.90 46.03 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.9 (100.00-2.90) 93.6 (46.03-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.267 0.206 , 0.266	Depositor DCC
R_{free} test set	4473 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 90984 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22803	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, MG, BMA, CA, NAG

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	0.46	4/4684 (0.1%)	0.61	0/6374
1	C	0.47	4/4584 (0.1%)	0.63	0/6240
2	B	0.41	1/3384 (0.0%)	0.58	0/4565
2	D	0.43	1/3425 (0.0%)	0.61	0/4621
3	E	0.49	2/1741 (0.1%)	0.63	0/2364
3	L	0.50	2/1741 (0.1%)	0.63	1/2364 (0.0%)
4	F	0.55	0/1698	0.62	0/2323
4	H	0.55	0/1698	0.64	0/2323
All	All	0.47	14/22955 (0.1%)	0.61	1/31174 (0.0%)

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
1	C	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	168	TRP	CD2-CE2	5.50	1.48	1.41
1	A	100	TRP	CD2-CE2	5.42	1.47	1.41
1	C	509	TRP	CD2-CE2	5.34	1.47	1.41
1	C	157	TRP	CD2-CE2	5.28	1.47	1.41
3	L	168	TRP	CD2-CE2	5.24	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	94	LEU	CA-CB-CG	6.05	129.23	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	155	PHE	Peptide

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	4567	0	4363	73	0
1	C	4470	0	4259	81	0
2	B	3327	0	3283	69	0
2	D	3367	0	3317	65	0
3	E	1701	0	1649	38	0
3	L	1701	0	1649	28	0
4	F	1651	0	1610	27	0
4	H	1651	0	1610	28	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	70	0	65	3	0
6	B	14	0	13	0	0
6	C	56	0	52	0	0
6	D	14	0	13	0	0
7	A	72	0	61	0	0
7	C	72	0	61	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	28	0	25	0	0
9	C	28	0	25	0	0
All	All	22803	0	22055	387	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 9.

The worst 5 of 387 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ILE:HD11	2:B:113:LEU:HD21	1.52	0.91
2:D:110:THR:HG22	2:D:409:SER:CB	2.04	0.88
2:D:73:LYS:H	2:D:97:GLN:HE22	1.22	0.86
1:A:123:THR:HG22	1:A:126:GLU:O	1.76	0.84
1:C:99:GLN:HG3	1:C:116:ALA:HB1	1.59	0.84

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	599/632 (95%)	538 (90%)	53 (9%)	8 (1%)	15	46
1	C	583/632 (92%)	515 (88%)	59 (10%)	9 (2%)	13	42
2	B	423/454 (93%)	380 (90%)	39 (9%)	4 (1%)	21	57
2	D	428/454 (94%)	381 (89%)	42 (10%)	5 (1%)	16	48
3	E	217/219 (99%)	210 (97%)	6 (3%)	1 (0%)	34	71
3	L	217/219 (99%)	204 (94%)	11 (5%)	2 (1%)	21	57
4	F	216/218 (99%)	192 (89%)	23 (11%)	1 (0%)	34	71
4	H	216/218 (99%)	198 (92%)	16 (7%)	2 (1%)	21	57
All	All	2899/3046 (95%)	2618 (90%)	249 (9%)	32 (1%)	17	51

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	SER
2	B	416	PRO
1	C	256	ASN

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Mol	Chain	Res	Type
1	C	285	PHE
1	C	575	ALA

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	486/513 (95%)	464 (96%)	22 (4%)	34	70
1	C	476/513 (93%)	465 (98%)	11 (2%)	58	87
2	B	379/402 (94%)	367 (97%)	12 (3%)	46	81
2	D	384/402 (96%)	368 (96%)	16 (4%)	36	73
3	E	194/194 (100%)	187 (96%)	7 (4%)	42	78
3	L	194/194 (100%)	187 (96%)	7 (4%)	42	78
4	F	186/186 (100%)	180 (97%)	6 (3%)	46	81
4	H	186/186 (100%)	177 (95%)	9 (5%)	31	67
All	All	2485/2590 (96%)	2395 (96%)	90 (4%)	42	78

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	284	TYR
2	D	139	LEU
3	E	186	LEU
1	C	432	ASP
2	D	25	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	489	ASN
2	D	92	HIS
3	E	171	GLN

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Mol	Chain	Res	Type
1	C	512	GLN
1	C	580	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 ⓘ

16 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	$\# Z > 2$
7	NAG	A	2009	1,7	14,14,15	0.76	0	15,19,21	0.95	0
7	NAG	A	2010	7	14,14,15	0.59	0	15,19,21	2.85	5 (33%)
7	BMA	A	2011	7	11,11,12	0.41	0	14,15,17	0.61	0
7	MAN	A	2012	7	11,11,12	0.61	0	14,15,17	0.76	0
7	MAN	A	2013	7	11,11,12	0.60	0	14,15,17	1.12	2 (14%)
7	MAN	A	2014	7	11,11,12	0.64	0	14,15,17	1.11	1 (7%)
9	NAG	B	2005	9,2	14,14,15	0.54	0	15,19,21	0.65	0
9	NAG	B	2006	9	14,14,15	0.50	0	15,19,21	0.81	0
9	NAG	C	2005	1,9	14,14,15	0.57	0	15,19,21	1.09	1 (6%)
9	NAG	C	2006	9	14,14,15	0.50	0	15,19,21	1.01	1 (6%)
7	NAG	C	2010	1,7	14,14,15	0.61	0	15,19,21	1.35	2 (13%)
7	NAG	C	2011	7	14,14,15	0.51	0	15,19,21	3.40	6 (40%)
7	BMA	C	2012	7	11,11,12	0.43	0	14,15,17	1.21	2 (14%)
7	MAN	C	2013	7	11,11,12	0.69	0	14,15,17	1.29	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	C	2014	7	11,11,12	0.69	0	14,15,17	1.63	3 (21%)
7	MAN	C	2015	7	11,11,12	0.56	0	14,15,17	1.25	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	2009	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	2010	7	-	0/6/23/26	0/1/1/1
7	BMA	A	2011	7	-	0/2/19/22	0/1/1/1
7	MAN	A	2012	7	-	0/2/19/22	0/1/1/1
7	MAN	A	2013	7	-	0/2/19/22	0/1/1/1
7	MAN	A	2014	7	-	0/2/19/22	0/1/1/1
9	NAG	B	2005	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	2006	9	-	0/6/23/26	0/1/1/1
9	NAG	C	2005	1,9	-	0/6/23/26	0/1/1/1
9	NAG	C	2006	9	-	0/6/23/26	0/1/1/1
7	NAG	C	2010	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	2011	7	-	0/6/23/26	0/1/1/1
7	BMA	C	2012	7	-	0/2/19/22	0/1/1/1
7	MAN	C	2013	7	-	0/2/19/22	0/1/1/1
7	MAN	C	2014	7	-	0/2/19/22	0/1/1/1
7	MAN	C	2015	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	2011	NAG	C4-C3-C2	-5.68	102.39	111.23
7	A	2010	NAG	C4-C3-C2	-5.62	102.50	111.23
7	C	2012	BMA	C1-C2-C3	-2.60	106.47	109.54
7	C	2012	BMA	O5-C1-C2	-2.34	107.07	110.86
7	A	2013	MAN	O5-C5-C6	2.00	111.68	107.35

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 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 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	NAG	A	2005	1	14,14,15	0.54	0	15,19,21	0.90	0
6	NAG	A	2006	1	14,14,15	0.47	0	15,19,21	1.02	1 (6%)
6	NAG	A	2007	1	14,14,15	0.45	0	15,19,21	1.00	0
6	NAG	A	2008	1	14,14,15	0.36	0	15,19,21	1.98	2 (13%)
6	NAG	A	2015	1	14,14,15	0.42	0	15,19,21	1.92	1 (6%)
6	NAG	B	2004	2	14,14,15	0.52	0	15,19,21	1.28	1 (6%)
6	NAG	C	2007	1	14,14,15	0.49	0	15,19,21	1.13	1 (6%)
6	NAG	C	2008	1	14,14,15	0.51	0	15,19,21	1.28	1 (6%)
6	NAG	C	2009	1	14,14,15	0.58	0	15,19,21	0.93	0
6	NAG	C	2016	1	14,14,15	0.42	0	15,19,21	1.38	1 (6%)
6	NAG	D	2004	2	14,14,15	0.47	0	15,19,21	1.26	1 (6%)

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	NAG	A	2005	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2006	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2007	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2015	1	-	0/6/23/26	0/1/1/1
6	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
6	NAG	C	2007	1	-	0/6/23/26	0/1/1/1
6	NAG	C	2008	1	-	0/6/23/26	0/1/1/1
6	NAG	C	2009	1	-	0/6/23/26	0/1/1/1
6	NAG	C	2016	1	-	0/6/23/26	0/1/1/1
6	NAG	D	2004	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	A	2008	NAG	C6-C5-C4	-2.08	107.88	113.02
6	A	2006	NAG	C1-O5-C5	2.17	115.00	112.25
6	C	2007	NAG	C1-O5-C5	3.40	116.56	112.25
6	D	2004	NAG	C1-O5-C5	3.92	117.23	112.25
6	B	2004	NAG	C1-O5-C5	4.04	117.38	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2008	NAG	3	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, 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	601/632 (95%)	-0.10	15 (2%) 61 55	44, 68, 119, 155	0
1	C	589/632 (93%)	0.11	39 (6%) 22 16	40, 67, 140, 189	0
2	B	427/454 (94%)	0.13	39 (9%) 11 7	43, 66, 161, 185	0
2	D	432/454 (95%)	-0.14	15 (3%) 48 40	40, 59, 136, 158	0
3	E	219/219 (100%)	-0.39	1 (0%) 91 90	47, 64, 84, 97	0
3	L	219/219 (100%)	-0.45	0 100 100	40, 57, 77, 91	0
4	F	218/218 (100%)	-0.37	4 (1%) 71 68	44, 67, 101, 117	0
4	H	218/218 (100%)	-0.45	2 (0%) 85 84	38, 60, 99, 117	0
All	All	2923/3046 (95%)	-0.12	115 (3%) 43 36	38, 64, 127, 189	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	28	CYS	11.5
1	C	465	PHE	7.0
2	B	60	ILE	6.9
1	C	509	TRP	6.9
2	B	54	GLY	6.8

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, 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
9	NAG	C	2005	14/15	0.90	0.16	0.24	74,82,90,100	0
7	NAG	A	2009	14/15	0.95	0.13	-0.82	53,56,65,66	0
7	NAG	C	2010	14/15	0.98	0.09	-2.84	50,54,59,59	0
7	BMA	C	2012	11/12	0.94	0.10	-	66,73,76,77	0
7	BMA	A	2011	11/12	0.94	0.09	-	75,83,90,92	0
7	MAN	C	2013	11/12	0.79	0.14	-	69,84,89,90	0
7	MAN	A	2012	11/12	0.84	0.16	-	88,100,105,105	0
7	MAN	C	2015	11/12	0.89	0.16	-	77,85,95,96	0
7	MAN	A	2013	11/12	0.84	0.18	-	98,101,108,108	0
9	NAG	C	2006	14/15	0.81	0.31	-	108,116,118,121	0
7	MAN	A	2014	11/12	0.91	0.09	-	78,85,91,92	0
9	NAG	B	2006	14/15	0.84	0.27	-	97,105,111,113	0
7	MAN	C	2014	11/12	0.84	0.14	-	80,85,91,94	0
7	NAG	C	2011	14/15	0.96	0.12	-	55,59,64,71	0
9	NAG	B	2005	14/15	0.94	0.13	-	74,81,87,92	0
7	NAG	A	2010	14/15	0.92	0.15	-	58,63,70,71	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, 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
8	MG	D	2003	1/1	0.96	0.34	8.47	57,57,57,57	0
8	MG	B	2003	1/1	0.87	0.27	4.15	62,62,62,62	0
6	NAG	A	2008	14/15	0.92	0.21	1.38	62,68,71,72	0
6	NAG	C	2009	14/15	0.93	0.17	1.12	64,70,74,75	0
6	NAG	A	2015	14/15	0.86	0.22	0.29	82,93,103,112	0
6	NAG	A	2005	14/15	0.88	0.16	-0.05	73,78,86,86	0
5	CA	A	2001	1/1	0.95	0.12	-0.21	69,69,69,69	0
6	NAG	C	2016	14/15	0.89	0.19	-0.76	100,110,118,124	0
5	CA	C	2004	1/1	0.96	0.11	-0.83	81,81,81,81	0
5	CA	C	2001	1/1	0.96	0.12	-0.83	63,63,63,63	0
5	CA	C	2003	1/1	0.96	0.09	-0.88	84,84,84,84	0
5	CA	A	2004	1/1	0.83	0.11	-1.08	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	C	2002	1/1	0.97	0.11	-1.44	75,75,75,75	0
5	CA	A	2003	1/1	0.98	0.09	-1.50	78,78,78,78	0
5	CA	A	2002	1/1	0.89	0.07	-1.73	84,84,84,84	0
5	CA	D	2002	1/1	0.98	0.10	-1.98	54,54,54,54	0
5	CA	B	2001	1/1	0.91	0.06	-2.73	69,69,69,69	0
5	CA	D	2001	1/1	0.93	0.08	-2.79	65,65,65,65	0
5	CA	B	2002	1/1	0.98	0.07	-4.16	62,62,62,62	0
6	NAG	A	2006	14/15	0.84	0.12	-	92,104,108,108	0
6	NAG	D	2004	14/15	0.92	0.10	-	68,71,73,73	0
6	NAG	C	2008	14/15	0.84	0.17	-	97,101,105,105	0
6	NAG	A	2007	14/15	0.87	0.19	-	92,99,101,104	0
6	NAG	B	2004	14/15	0.95	0.15	-	66,71,77,78	0
6	NAG	C	2007	14/15	0.80	0.17	-	87,102,110,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.