



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID : 3K6S
Title : Structure of integrin alphaXbeta2 ectodomain
Authors : Xie, C.; Zhu, J.; Chen, X.; Mi, L.; Nishida, N.; Springer, T.A.
Deposited on : 2009-10-09
Resolution : 3.50 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

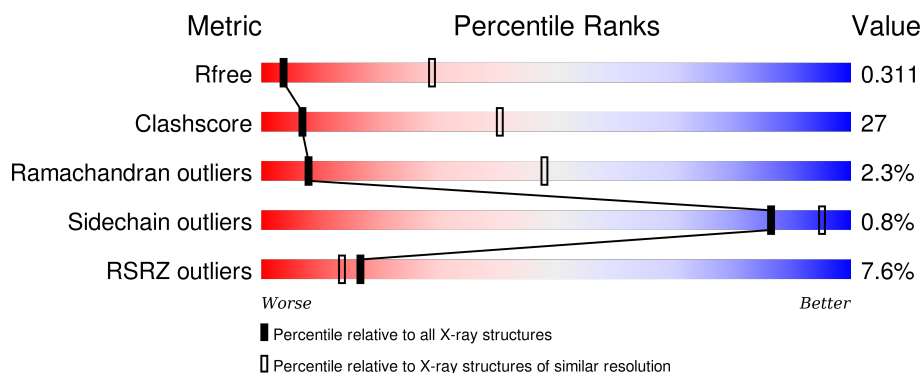
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	1095	<div> <div>2%</div> <div>56%</div> <div>40%</div> <div>..</div> </div>
1	C	1095	<div> <div>5%</div> <div>43%</div> <div>35%</div> <div>..</div> <div>19%</div> </div>
1	E	1095	<div> <div>3%</div> <div>43%</div> <div>35%</div> <div>.</div> <div>19%</div> </div>
1	G	1095	<div> <div>3%</div> <div>43%</div> <div>35%</div> <div>.</div> <div>19%</div> </div>
2	B	687	<div> <div>7%</div> <div>64%</div> <div>33%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	687	
2	F	687	
2	H	687	

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
3	NAG	C	3373	X	-	-	-
4	NAG	A	3373	X	-	-	-
4	MAN	A	3375	X	-	-	-
9	NAG	E	3373	X	-	-	-
9	MAN	E	3375	X	-	-	-
9	NAG	G	3373	X	-	-	-
9	MAN	G	3375	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 50187 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-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1082	Total	C	N	O	S	0	0	0
			8392	5304	1454	1596	38			
1	C	885	Total	C	N	O	S	0	0	0
			6825	4311	1182	1298	34			
1	E	884	Total	C	N	O	S	0	0	0
			6819	4308	1181	1296	34			
1	G	885	Total	C	N	O	S	0	0	0
			6825	4311	1182	1298	34			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	EXPRESSION TAG	UNP P20702
A	1086	CYS	-	EXPRESSION TAG	UNP P20702
A	1087	GLY	-	EXPRESSION TAG	UNP P20702
A	1088	GLY	-	EXPRESSION TAG	UNP P20702
A	1089	LEU	-	EXPRESSION TAG	UNP P20702
A	1090	GLU	-	EXPRESSION TAG	UNP P20702
A	1091	ASN	-	EXPRESSION TAG	UNP P20702
A	1092	LEU	-	EXPRESSION TAG	UNP P20702
A	1093	TYR	-	EXPRESSION TAG	UNP P20702
A	1094	PHE	-	EXPRESSION TAG	UNP P20702
A	1095	GLN	-	EXPRESSION TAG	UNP P20702
C	1085	GLY	-	EXPRESSION TAG	UNP P20702
C	1086	CYS	-	EXPRESSION TAG	UNP P20702
C	1087	GLY	-	EXPRESSION TAG	UNP P20702
C	1088	GLY	-	EXPRESSION TAG	UNP P20702
C	1089	LEU	-	EXPRESSION TAG	UNP P20702
C	1090	GLU	-	EXPRESSION TAG	UNP P20702
C	1091	ASN	-	EXPRESSION TAG	UNP P20702
C	1092	LEU	-	EXPRESSION TAG	UNP P20702
C	1093	TYR	-	EXPRESSION TAG	UNP P20702
C	1094	PHE	-	EXPRESSION TAG	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1095	GLN	-	EXPRESSION TAG	UNP P20702
E	1085	GLY	-	EXPRESSION TAG	UNP P20702
E	1086	CYS	-	EXPRESSION TAG	UNP P20702
E	1087	GLY	-	EXPRESSION TAG	UNP P20702
E	1088	GLY	-	EXPRESSION TAG	UNP P20702
E	1089	LEU	-	EXPRESSION TAG	UNP P20702
E	1090	GLU	-	EXPRESSION TAG	UNP P20702
E	1091	ASN	-	EXPRESSION TAG	UNP P20702
E	1092	LEU	-	EXPRESSION TAG	UNP P20702
E	1093	TYR	-	EXPRESSION TAG	UNP P20702
E	1094	PHE	-	EXPRESSION TAG	UNP P20702
E	1095	GLN	-	EXPRESSION TAG	UNP P20702
G	1085	GLY	-	EXPRESSION TAG	UNP P20702
G	1086	CYS	-	EXPRESSION TAG	UNP P20702
G	1087	GLY	-	EXPRESSION TAG	UNP P20702
G	1088	GLY	-	EXPRESSION TAG	UNP P20702
G	1089	LEU	-	EXPRESSION TAG	UNP P20702
G	1090	GLU	-	EXPRESSION TAG	UNP P20702
G	1091	ASN	-	EXPRESSION TAG	UNP P20702
G	1092	LEU	-	EXPRESSION TAG	UNP P20702
G	1093	TYR	-	EXPRESSION TAG	UNP P20702
G	1094	PHE	-	EXPRESSION TAG	UNP P20702
G	1095	GLN	-	EXPRESSION TAG	UNP P20702

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	D	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	F	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			
2	H	674	Total	C	N	O	S	0	0	0
			5184	3186	930	1004	64			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	EXPRESSION TAG	UNP P05107
B	679	GLY	-	EXPRESSION TAG	UNP P05107
B	680	CYS	-	EXPRESSION TAG	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	GLY	-	EXPRESSION TAG	UNP P05107
B	682	GLU	-	EXPRESSION TAG	UNP P05107
B	684	LEU	-	EXPRESSION TAG	UNP P05107
B	685	TYR	-	EXPRESSION TAG	UNP P05107
B	686	PHE	-	EXPRESSION TAG	UNP P05107
B	687	GLN	-	EXPRESSION TAG	UNP P05107
D	678	ASP	-	EXPRESSION TAG	UNP P05107
D	679	GLY	-	EXPRESSION TAG	UNP P05107
D	680	CYS	-	EXPRESSION TAG	UNP P05107
D	681	GLY	-	EXPRESSION TAG	UNP P05107
D	682	GLU	-	EXPRESSION TAG	UNP P05107
D	684	LEU	-	EXPRESSION TAG	UNP P05107
D	685	TYR	-	EXPRESSION TAG	UNP P05107
D	686	PHE	-	EXPRESSION TAG	UNP P05107
D	687	GLN	-	EXPRESSION TAG	UNP P05107
F	678	ASP	-	EXPRESSION TAG	UNP P05107
F	679	GLY	-	EXPRESSION TAG	UNP P05107
F	680	CYS	-	EXPRESSION TAG	UNP P05107
F	681	GLY	-	EXPRESSION TAG	UNP P05107
F	682	GLU	-	EXPRESSION TAG	UNP P05107
F	684	LEU	-	EXPRESSION TAG	UNP P05107
F	685	TYR	-	EXPRESSION TAG	UNP P05107
F	686	PHE	-	EXPRESSION TAG	UNP P05107
F	687	GLN	-	EXPRESSION TAG	UNP P05107
H	678	ASP	-	EXPRESSION TAG	UNP P05107
H	679	GLY	-	EXPRESSION TAG	UNP P05107
H	680	CYS	-	EXPRESSION TAG	UNP P05107
H	681	GLY	-	EXPRESSION TAG	UNP P05107
H	682	GLU	-	EXPRESSION TAG	UNP P05107
H	684	LEU	-	EXPRESSION TAG	UNP P05107
H	685	TYR	-	EXPRESSION TAG	UNP P05107
H	686	PHE	-	EXPRESSION TAG	UNP P05107
H	687	GLN	-	EXPRESSION TAG	UNP P05107

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

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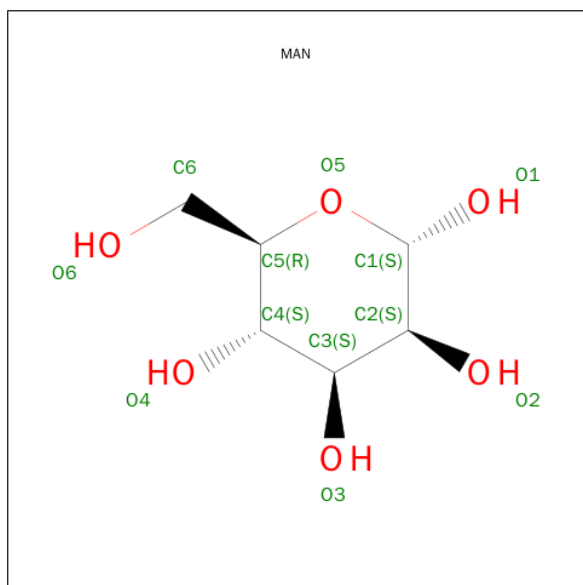
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

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

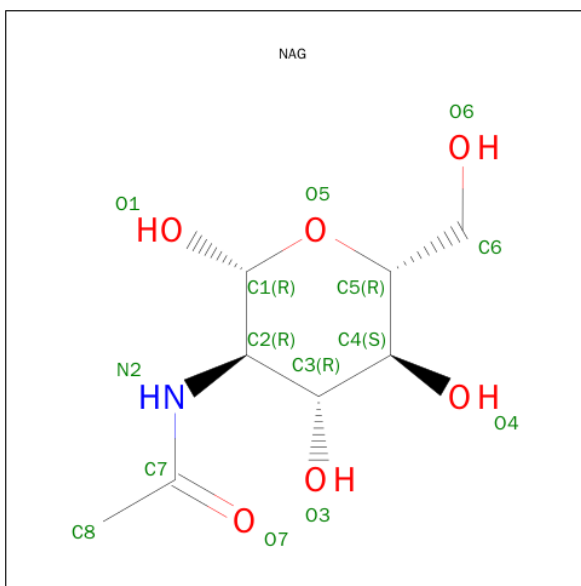
- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- 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	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	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	3	Total Ca 3 3	0	0
7	D	1	Total Ca 1 1	0	0
7	E	3	Total Ca 3 3	0	0
7	H	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	3	Total Ca 3 3	0	0
7	A	3	Total Ca 3 3	0	0
7	F	1	Total Ca 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mg 1 1	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	3	Total C N O 39 22 2 15	0	0
9	G	3	Total C N O 39 22 2 15	0	0

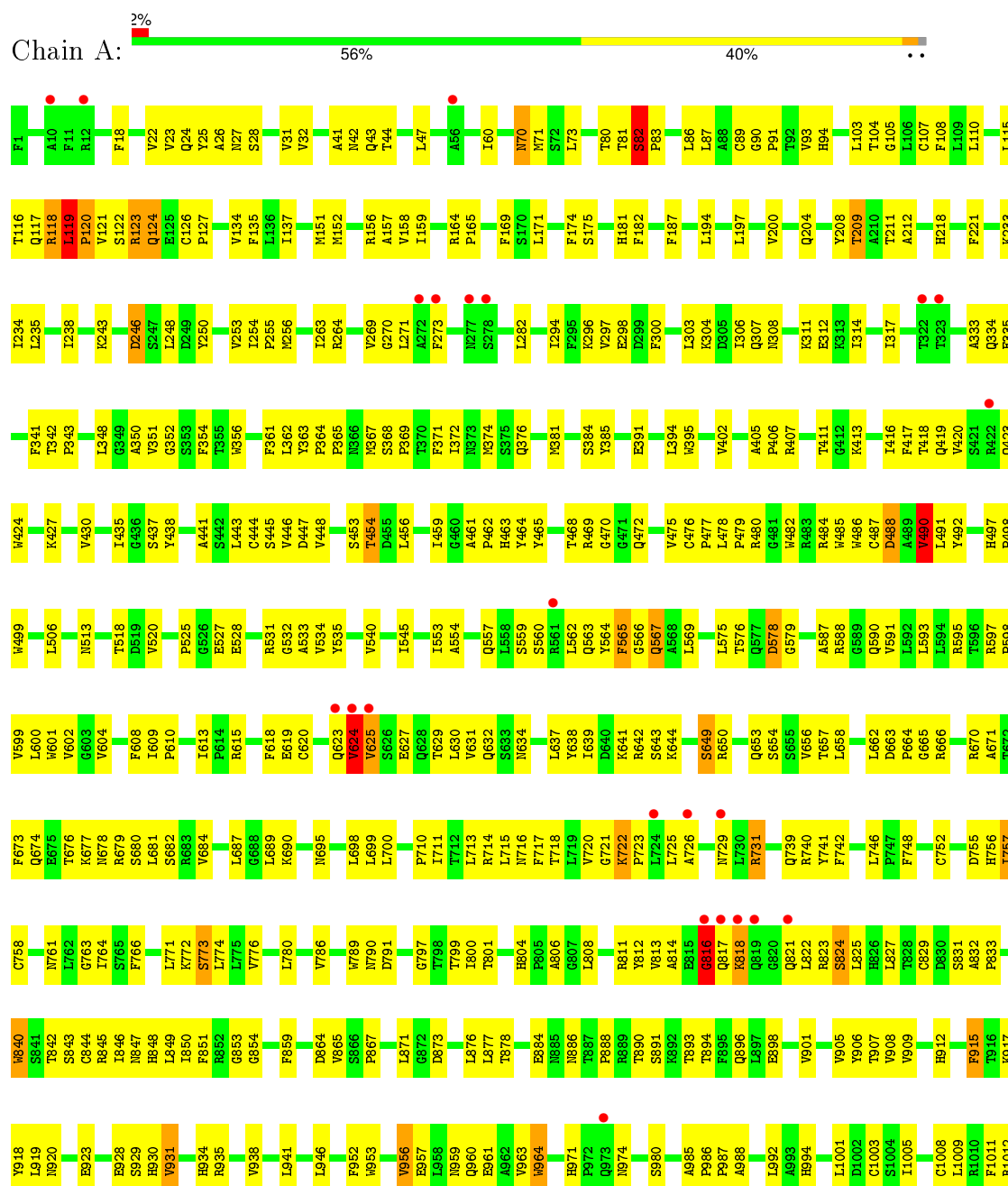
- Molecule 10 is water.

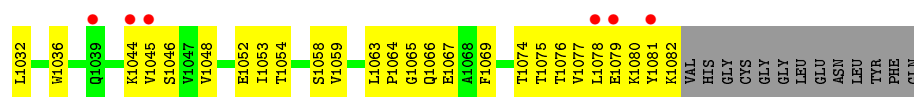
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total O 3 3	0	0

3 Residue-property plots

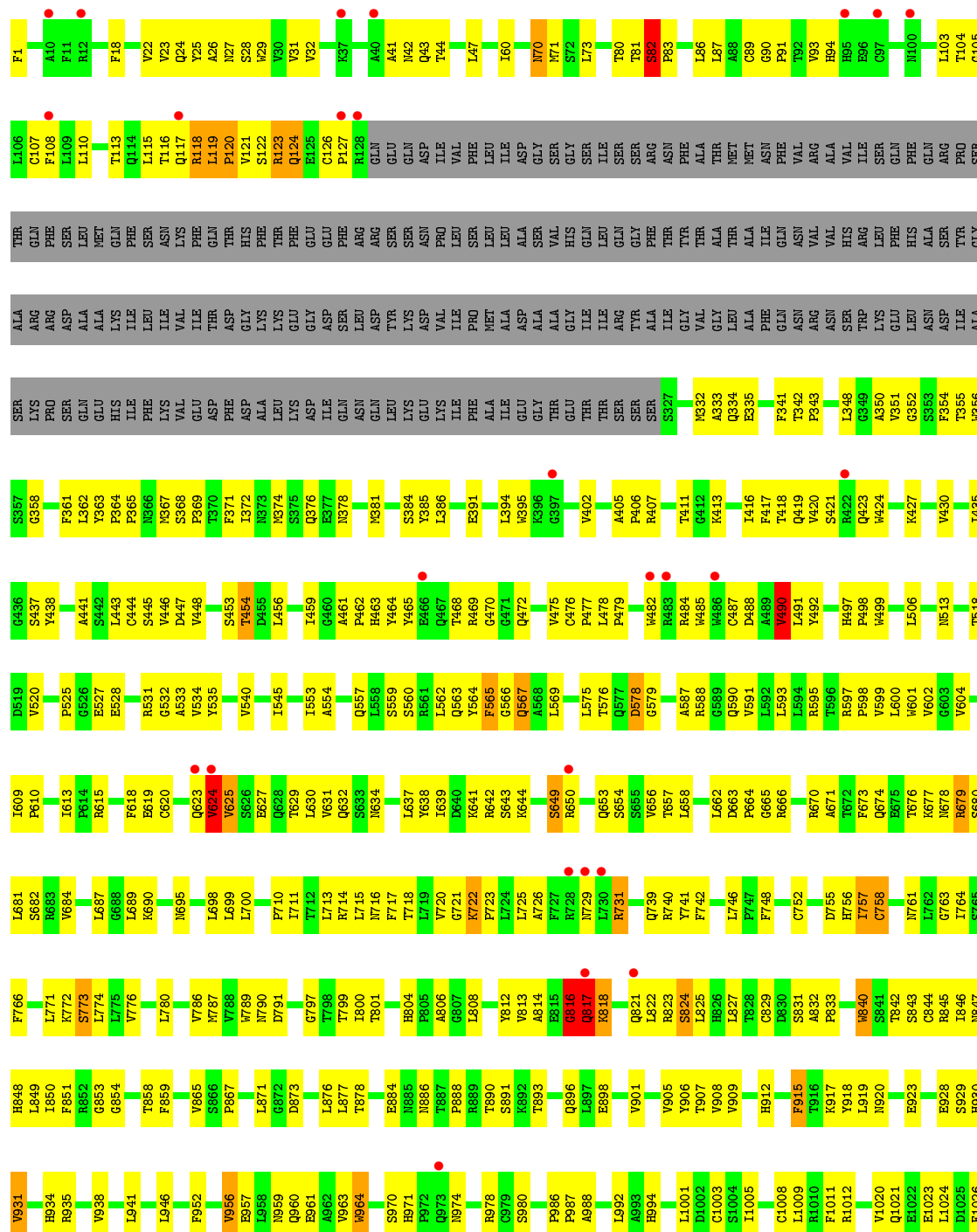
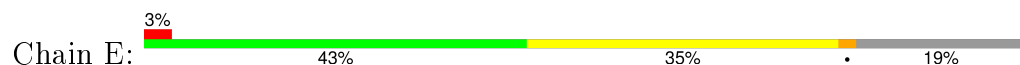
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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-X

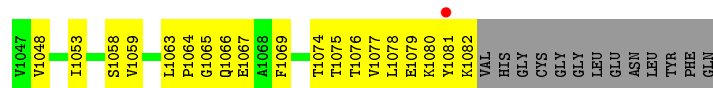




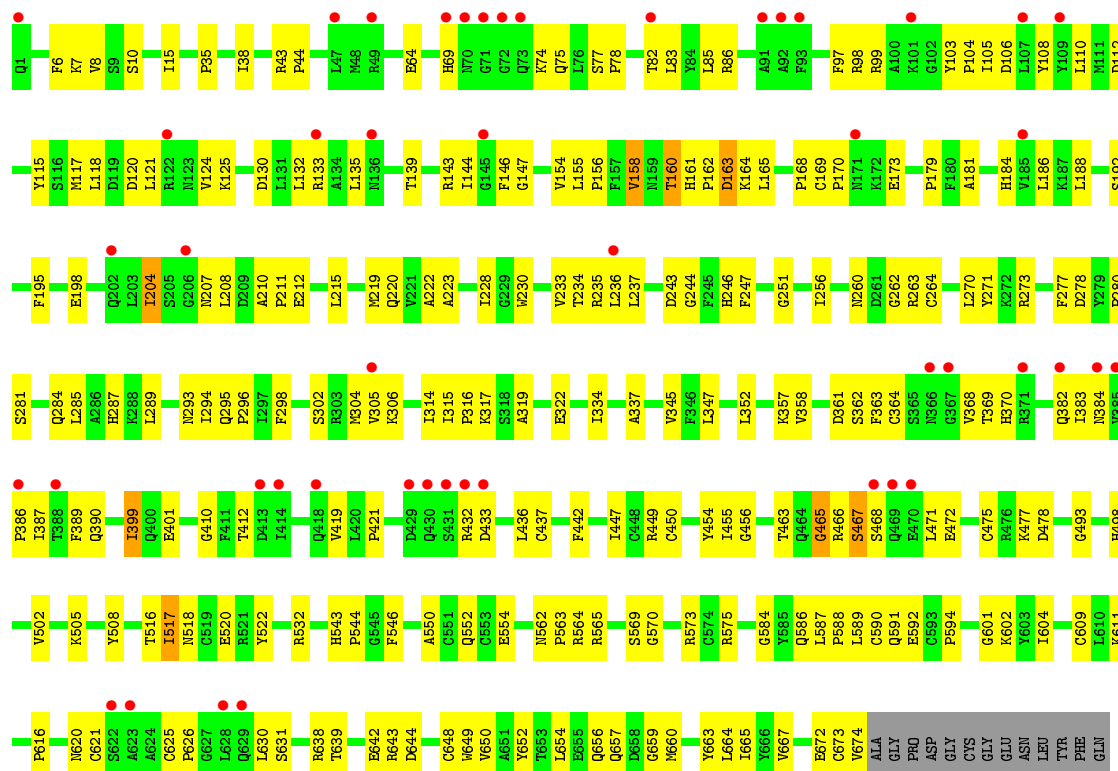
• Molecule 1: Integrin alpha-X



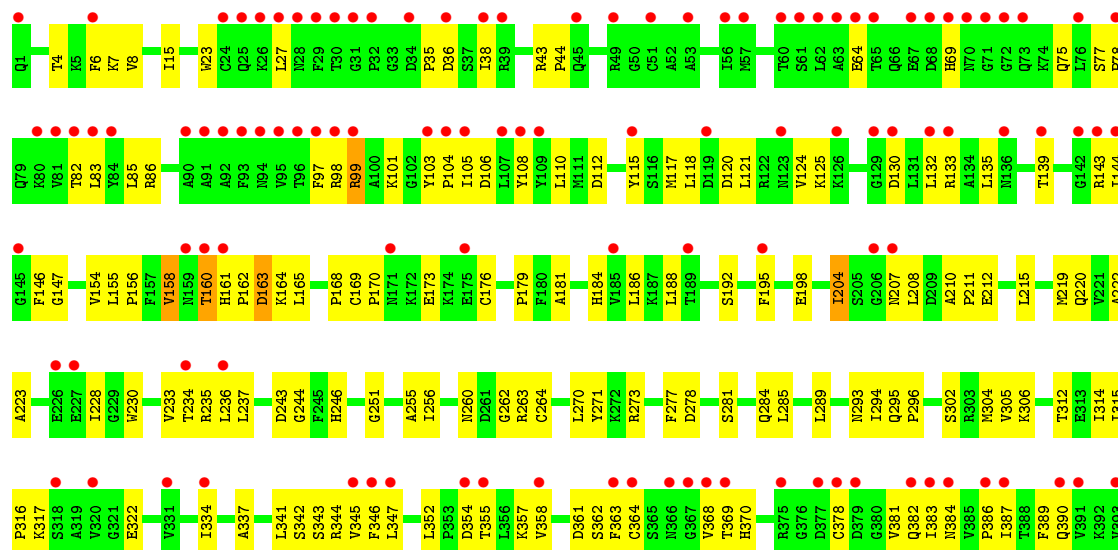


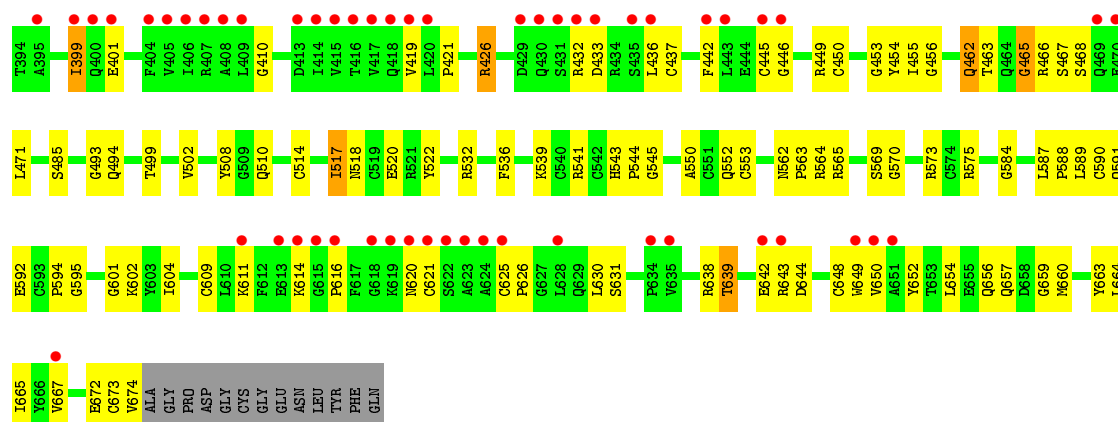


• Molecule 2: Integrin beta-2

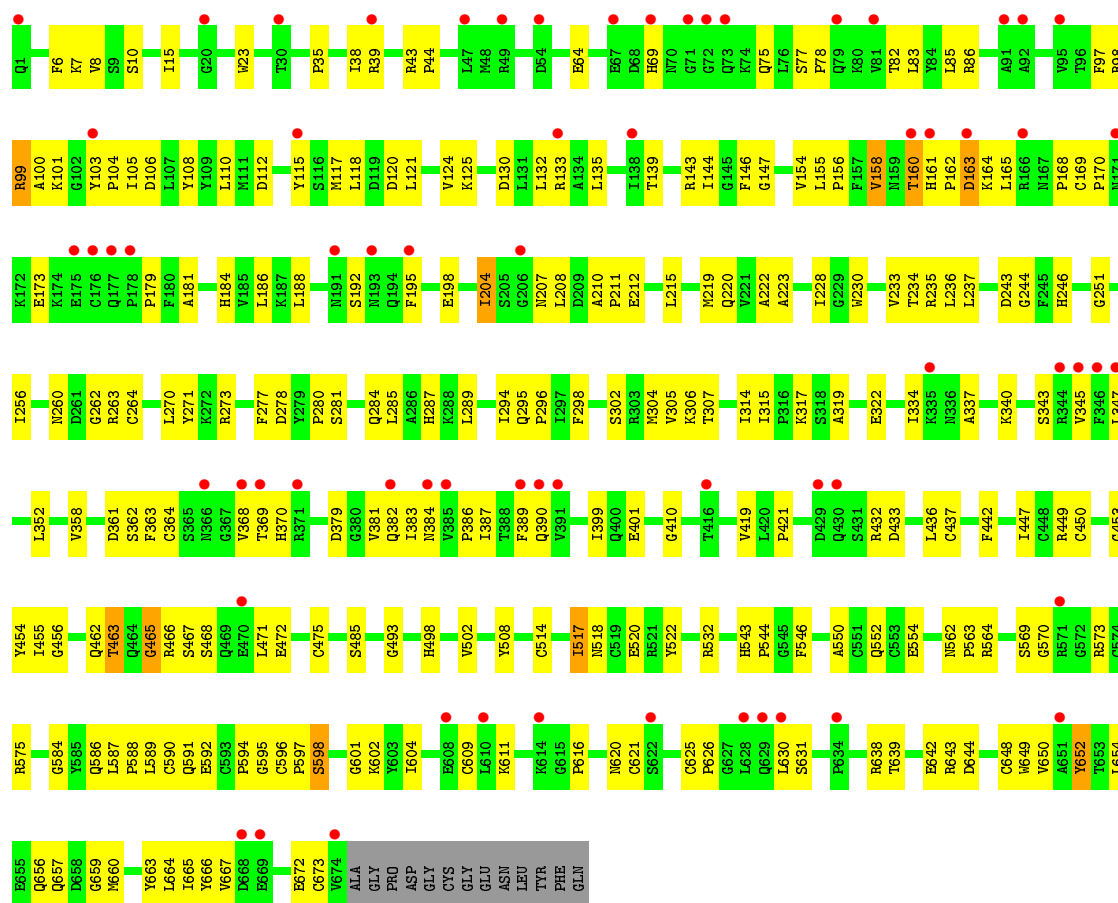


• Molecule 2: Integrin beta-2

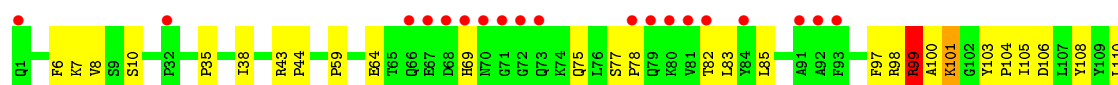




• Molecule 2: Integrin beta-2



• Molecule 2: Integrin beta-2



PRO	L589	G465	C378	F277	L186	V411
ASP	C590	R466	V381	D278	K187	D112
GLY	Q591	S467	Q382	S281	L188	Y115
CYS	S468	S468	I383	Q284	T189	S116
GLU	C593	Q469	I384	L285	S192	M117
ASN	P594	E470	V385	A286	F195	L118
LEU	S598	L471	P386	H287	E198	D119
TYR	G601	E473	I387	K288	I204	D120
PHE	K602	S474	T388	F389	E205	L121
GLN	C475	C475	F389	L289	G206	K126
	Y603	S485	Q390	L294	N207	L127
	I604		V391	Q295	L208	V124
	C609	D489	K392	P296		K125
	L610		V393			K126
	K611	Q493	I399	M304		L130
	P616	H498	Q400	V305		L131
	M620		E401	K306		L132
	C621	V502	D413	T312		R133
	L628	Q510	I414	E313		A134
	Q629	I517	V415	I314		N136
	L630	N518	T416	I315		T139
	S631	N519	V417	P316		
	R638	E520	Q418	K317		R143
	T639	E521	V419	A222		G145
		Y522	L420	A223		I144
	B642		Q422	I228		F146
	R643	R532	C423	G229		G147
	D644	H543	D429	W230		V154
	C648	P544	Q430	V233		L155
	W649	G545	S431	T234		P156
	W650	F546	R432	R235		F157
	A651	A550	D433	L236		V158
	C551	C551	R434	L237		N159
	T653	Q552	S435	D243		T160
	L654	C553	L436	G244		H161
	E655	C553	C437	F245		P162
	Q656	E554	F442	H246		D163
	Q657	N562	G446	G251		K164
	D658	P563	I447			L165
	G659	H564	C448	I256		P168
	M660	H564	R449	L257		C169
	Y663	S569	C450	V358		P170
	L664	G570	D451	D361		N171
	I665	R573	T452	S362		K172
	Y666	C574	G453	F363		E173
	V667	H575	Y454	C364		K174
			I455	R263		E175
	B672	G584	G456	S365		
	C673	H588	N366	N367		P179
	W674	Q586	G367	L270		F180
ALA	ALA	L587	V368	Y271		A181
GLY	GLY	P588	T463	R272		H184
			Q464	R273		V185

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.09Å 163.56Å 536.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.50 48.61 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.61-3.50) 100.0 (48.61-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.297 , 0.335 0.280 , 0.311	Depositor DCC
R_{free} test set	1531 reflections (1.04%)	DCC
Wilson B-factor (Å ²)	80.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 177.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 147305 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	50187	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MAN, 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	0.23	0/8579	0.44	1/11652 (0.0%)
1	C	0.24	0/6980	0.46	0/9494
1	E	0.23	0/6974	0.45	0/9486
1	G	0.24	0/6980	0.45	0/9494
2	B	0.22	0/5280	0.41	0/7129
2	D	0.24	0/5280	0.43	0/7129
2	F	0.23	0/5280	0.42	0/7129
2	H	0.23	0/5280	0.42	0/7129
All	All	0.23	0/50633	0.44	1/68642 (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	A	0	10
1	C	0	11
1	E	0	10
1	G	0	11
2	B	0	2
2	D	0	3
2	F	0	2
2	H	0	3
3	C	1	0
4	A	2	0
9	E	2	0
9	G	2	0
All	All	7	52

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	119	LEU	C-N-CD	-5.77	107.90	120.60

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3373	NAG	C1
4	A	3375	MAN	C1
3	C	3373	NAG	C1
9	E	3373	NAG	C1
9	E	3375	MAN	C1

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Peptide
1	A	119	LEU	Peptide
1	A	488	ASP	Peptide
1	A	490	VAL	Peptide
1	A	82	SER	Peptide

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	8392	0	8227	495	0
1	C	6825	0	6685	457	0
1	E	6819	0	6680	428	0
1	G	6825	0	6685	438	0
2	B	5184	0	4975	218	0
2	D	5184	0	4975	255	0
2	F	5184	0	4975	228	0
2	H	5184	0	4975	216	0
3	A	56	0	50	0	0
3	C	84	0	75	4	0
3	E	56	0	50	1	0
3	G	56	0	50	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	61	0	52	10	0
5	A	11	0	10	4	0
6	A	28	0	25	0	0
6	B	14	0	13	0	0
6	C	28	0	25	1	0
6	D	14	0	13	0	0
6	E	28	0	25	0	0
6	F	14	0	13	0	0
6	G	28	0	24	1	0
6	H	14	0	13	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
7	E	3	0	0	0	0
7	F	1	0	0	0	0
7	G	3	0	0	0	0
7	H	1	0	0	0	0
8	A	1	0	0	0	0
9	E	39	0	34	6	0
9	G	39	0	34	7	0
10	A	3	0	0	0	0
All	All	50187	0	48683	2634	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 27.

The worst 5 of 2634 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:985:ALA:CB	1:C:621:ARG:HB2	1.81	1.11
1:A:985:ALA:HB2	1:C:621:ARG:CB	1.90	1.01
1:A:985:ALA:HB2	1:C:621:ARG:CD	1.91	1.00
1:C:484:ARG:NH2	1:C:1021:GLN:HA	1.81	0.95
1:A:985:ALA:HB2	1:C:621:ARG:HB2	1.42	0.94

There are no symmetry-related clashes.

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	1080/1095 (99%)	839 (78%)	215 (20%)	26 (2%)	7	47
1	C	881/1095 (80%)	663 (75%)	194 (22%)	24 (3%)	6	44
1	E	880/1095 (80%)	665 (76%)	190 (22%)	25 (3%)	6	43
1	G	881/1095 (80%)	666 (76%)	191 (22%)	24 (3%)	6	44
2	B	672/687 (98%)	514 (76%)	147 (22%)	11 (2%)	12	55
2	D	672/687 (98%)	515 (77%)	145 (22%)	12 (2%)	11	53
2	F	672/687 (98%)	514 (76%)	145 (22%)	13 (2%)	10	51
2	H	672/687 (98%)	512 (76%)	146 (22%)	14 (2%)	9	50
All	All	6410/7128 (90%)	4888 (76%)	1373 (21%)	149 (2%)	8	48

5 of 149 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	120	PRO
1	A	757	ILE
1	C	82	SER
1	C	757	ILE

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	924/934 (99%)	914 (99%)	10 (1%)	80	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	754/934 (81%)	742 (98%)	12 (2%)	70	89
1	E	753/934 (81%)	743 (99%)	10 (1%)	76	91
1	G	754/934 (81%)	744 (99%)	10 (1%)	76	91
2	B	583/592 (98%)	583 (100%)	0	100	100
2	D	583/592 (98%)	582 (100%)	1 (0%)	95	99
2	F	583/592 (98%)	582 (100%)	1 (0%)	95	99
2	H	583/592 (98%)	581 (100%)	2 (0%)	94	99
All	All	5517/6104 (90%)	5471 (99%)	46 (1%)	86	95

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	915	PHE
1	E	567	GLN
1	G	915	PHE
1	C	964	TRP
1	E	119	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	295	GLN
1	E	124	GLN
1	G	886	ASN
2	D	462	GLN
1	E	334	GLN

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 ⓘ

29 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$
3	NAG	A	3042	1,3	14,14,15	0.52	0	15,19,21	0.63	0
3	NAG	A	3043	3	14,14,15	0.54	0	15,19,21	1.07	1 (6%)
4	NAG	A	3373	1,4	14,14,15	0.48	0	15,19,21	1.01	1 (6%)
4	NAG	A	3374	4	14,14,15	0.54	0	15,19,21	1.88	3 (20%)
4	MAN	A	3375	4	11,11,12	0.43	0	14,15,17	2.04	6 (42%)
4	MAN	A	3376	4	11,11,12	0.74	0	14,15,17	1.19	1 (7%)
4	MAN	A	3377	4	11,11,12	0.60	0	14,15,17	1.58	2 (14%)
3	NAG	A	3716	1,3	14,14,15	0.58	0	15,19,21	1.80	1 (6%)
3	NAG	A	3717	3	14,14,15	0.52	0	15,19,21	1.70	1 (6%)
3	NAG	C	3042	1,3	14,14,15	0.52	0	15,19,21	0.61	0
3	NAG	C	3043	3	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
3	NAG	C	3373	1,3	14,14,15	0.46	0	15,19,21	1.01	1 (6%)
3	NAG	C	3374	3	14,14,15	0.50	0	15,19,21	1.66	1 (6%)
3	NAG	C	3716	1,3	14,14,15	0.52	0	15,19,21	2.01	1 (6%)
3	NAG	C	3717	3	14,14,15	0.56	0	15,19,21	1.64	1 (6%)
3	NAG	E	3042	1,3	14,14,15	0.53	0	15,19,21	0.60	0
3	NAG	E	3043	3	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
9	NAG	E	3373	1,9	14,14,15	0.47	0	15,19,21	1.03	1 (6%)
9	NAG	E	3374	9	14,14,15	0.54	0	15,19,21	1.84	2 (13%)
9	MAN	E	3375	9	11,11,12	0.48	0	14,15,17	1.49	3 (21%)
3	NAG	E	3716	1,3	14,14,15	0.52	0	15,19,21	1.93	1 (6%)
3	NAG	E	3717	3	14,14,15	0.54	0	15,19,21	1.53	1 (6%)
3	NAG	G	3042	1,3	14,14,15	0.51	0	15,19,21	0.63	0
3	NAG	G	3043	3	14,14,15	0.56	0	15,19,21	1.08	1 (6%)
9	NAG	G	3373	1,9	14,14,15	0.45	0	15,19,21	0.99	1 (6%)
9	NAG	G	3374	9	14,14,15	0.53	0	15,19,21	1.90	2 (13%)
9	MAN	G	3375	9	11,11,12	0.50	0	14,15,17	1.51	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	3716	1,3	14,14,15	0.54	0	15,19,21	1.99	1 (6%)
3	NAG	G	3717	3	14,14,15	0.55	0	15,19,21	1.57	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
3	NAG	A	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3043	3	-	0/6/23/26	0/1/1/1
4	NAG	A	3373	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	3374	4	-	0/6/23/26	0/1/1/1
4	MAN	A	3375	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	3376	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3377	4	-	0/2/19/22	0/1/1/1
3	NAG	A	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3717	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3043	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3373	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	3374	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3717	3	-	0/6/23/26	0/1/1/1
3	NAG	E	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	3043	3	-	0/6/23/26	0/1/1/1
9	NAG	E	3373	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	E	3374	9	-	0/6/23/26	0/1/1/1
9	MAN	E	3375	9	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	E	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	3717	3	-	0/6/23/26	0/1/1/1
3	NAG	G	3042	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	3043	3	-	0/6/23/26	0/1/1/1
9	NAG	G	3373	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	G	3374	9	-	0/6/23/26	0/1/1/1
9	MAN	G	3375	9	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	G	3716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	3717	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3375	MAN	C2-C3-C4	-3.46	105.16	111.04
9	G	3375	MAN	C2-C3-C4	-3.15	105.70	111.04
9	E	3375	MAN	C2-C3-C4	-3.02	105.91	111.04
4	A	3376	MAN	C1-O5-C5	-2.92	108.54	112.25
4	A	3377	MAN	C6-C5-C4	-2.75	106.24	113.02

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	E	3375	MAN	C1
9	E	3373	NAG	C1
9	G	3375	MAN	C1
3	C	3373	NAG	C1
4	A	3373	NAG	C1

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3373	NAG	4	0
4	A	3374	NAG	3	0
4	A	3375	MAN	2	0
4	A	3377	MAN	4	0
3	C	3373	NAG	4	0
3	C	3374	NAG	1	0
9	E	3373	NAG	4	0
9	E	3374	NAG	3	0
9	E	3375	MAN	2	0
3	E	3716	NAG	1	0
3	E	3717	NAG	1	0
9	G	3373	NAG	4	0
9	G	3374	NAG	4	0
9	G	3375	MAN	3	0
3	G	3716	NAG	1	0
3	G	3717	NAG	1	0

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 17 are monoatomic - leaving 13 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	$\# Z > 2$
5	MAN	A	3378	-	11,11,12	1.03	0	14,15,17	6.14	6 (42%)
6	NAG	A	3678	1	14,14,15	0.49	0	15,19,21	0.95	1 (6%)
6	NAG	A	3880	1	14,14,15	0.41	0	15,19,21	1.25	1 (6%)
6	NAG	B	3094	2	14,14,15	0.47	0	15,19,21	0.74	0
6	NAG	C	3678	1	14,14,15	0.48	0	15,19,21	0.91	1 (6%)
6	NAG	C	3880	1	14,14,15	0.41	0	15,19,21	1.16	1 (6%)
6	NAG	D	3094	2	14,14,15	0.50	0	15,19,21	0.71	0
6	NAG	E	3678	1	14,14,15	0.50	0	15,19,21	0.97	1 (6%)
6	NAG	E	3880	1	14,14,15	0.40	0	15,19,21	1.25	1 (6%)
6	NAG	F	3094	2	14,14,15	0.47	0	15,19,21	0.74	0
6	NAG	G	3678	1	14,14,15	0.49	0	15,19,21	0.94	1 (6%)
6	NAG	G	3880	1	14,14,15	0.42	0	15,19,21	1.12	1 (6%)
6	NAG	H	3094	2	14,14,15	0.48	0	15,19,21	0.73	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
5	MAN	A	3378	-	-	0/2/19/22	0/1/1/1
6	NAG	A	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	A	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	C	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	C	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	D	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	E	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	E	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	F	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	G	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	G	3880	1	-	0/6/23/26	0/1/1/1
6	NAG	H	3094	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3378	MAN	C1-C2-C3	-18.07	88.17	109.54
5	A	3378	MAN	C1-O5-C5	-12.31	96.63	112.25
5	A	3378	MAN	O2-C2-C1	-2.28	104.64	109.21
5	A	3378	MAN	O3-C3-C2	2.31	114.18	110.00
5	A	3378	MAN	O5-C1-C2	2.51	114.93	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3378	MAN	4	0
6	C	3678	NAG	1	0
6	G	3678	NAG	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, 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(Å²)	Q<0.9	
1	A	1082/1095 (98%)	-0.07	25 (2%)	64	54	61, 153, 256, 362	0
1	C	885/1095 (80%)	0.21	52 (5%)	26	20	67, 172, 280, 410	0
1	E	884/1095 (80%)	-0.02	31 (3%)	48	38	65, 157, 266, 337	0
1	G	885/1095 (80%)	-0.06	28 (3%)	51	42	74, 150, 266, 342	0
2	B	674/687 (98%)	0.35	48 (7%)	19	15	100, 205, 286, 421	2 (0%)
2	D	674/687 (98%)	1.09	166 (24%)	1	1	107, 229, 313, 416	2 (0%)
2	F	674/687 (98%)	0.48	66 (9%)	10	9	98, 207, 289, 374	2 (0%)
2	H	674/687 (98%)	0.50	71 (10%)	8	8	100, 210, 293, 390	2 (0%)
All	All	6432/7128 (90%)	0.26	487 (7%)	17	14	61, 185, 283, 421	8 (0%)

The worst 5 of 487 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	72	GLY	16.2
2	B	72	GLY	12.5
2	H	73	GLN	11.2
2	B	92	ALA	9.9
2	D	91	ALA	9.6

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
3	NAG	G	3716	14/15	0.90	0.22	0.47	77,188,300,303	0
3	NAG	C	3716	14/15	0.91	0.18	0.31	60,167,211,249	0
3	NAG	E	3716	14/15	0.92	0.22	0.31	49,184,277,297	0
3	NAG	A	3716	14/15	0.96	0.17	-1.01	28,156,272,274	0
3	NAG	G	3042	14/15	0.75	0.27	-	193,244,274,279	0
4	MAN	A	3377	11/12	0.70	0.20	-	99,256,308,331	0
3	NAG	C	3374	14/15	0.62	0.63	-	136,238,359,434	0
4	NAG	A	3374	14/15	0.71	0.32	-	91,240,362,435	0
3	NAG	E	3043	14/15	0.62	0.46	-	183,310,366,378	0
3	NAG	G	3043	14/15	0.63	0.26	-	176,248,297,317	0
9	NAG	E	3373	14/15	0.81	0.44	-	146,324,390,464	0
9	MAN	G	3375	11/12	0.65	0.29	-	173,208,309,351	0
3	NAG	C	3043	14/15	0.69	0.42	-	179,305,351,363	0
3	NAG	C	3373	14/15	0.68	0.42	-	198,292,381,425	0
4	NAG	A	3373	14/15	0.85	0.32	-	136,261,376,443	0
3	NAG	A	3043	14/15	0.81	0.26	-	80,233,327,333	0
3	NAG	E	3717	14/15	0.87	0.22	-	117,240,280,337	0
3	NAG	A	3717	14/15	0.88	0.32	-	185,218,319,381	0
3	NAG	C	3717	14/15	0.61	0.76	-	224,297,342,395	0
3	NAG	C	3042	14/15	0.78	0.28	-	150,232,327,335	0
9	NAG	E	3374	14/15	0.78	0.37	-	201,279,352,410	0
9	MAN	E	3375	11/12	0.36	0.30	-	171,251,305,311	0
4	MAN	A	3376	11/12	0.66	0.22	-	114,259,296,316	0
9	NAG	G	3373	14/15	0.83	0.35	-	106,265,384,401	0
9	NAG	G	3374	14/15	0.69	0.47	-	136,261,326,367	0
3	NAG	G	3717	14/15	0.84	0.30	-	192,216,305,376	0
3	NAG	E	3042	14/15	0.82	0.47	-	198,249,285,287	0
4	MAN	A	3375	11/12	0.80	0.16	-	140,207,283,324	0
3	NAG	A	3042	14/15	0.85	0.18	-	133,175,235,244	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(\AA^2)	Q<0.9
6	NAG	G	3880	14/15	0.90	0.29	1.43	84,176,236,252	0
5	MAN	A	3378	11/12	0.62	0.29	0.35	171,186,272,293	0
6	NAG	C	3880	14/15	0.92	0.23	0.12	60,171,245,293	0
7	CA	C	2006	1/1	0.85	0.16	-0.39	125,125,125,125	0
6	NAG	E	3880	14/15	0.90	0.18	-0.82	80,160,189,194	0
6	NAG	A	3880	14/15	0.91	0.18	-1.16	105,143,196,220	0
7	CA	C	2005	1/1	0.76	0.06	-1.29	200,200,200,200	0
8	MG	A	2009	1/1	0.96	0.10	-1.34	367,367,367,367	0
7	CA	D	2002	1/1	0.62	0.17	-1.34	547,547,547,547	0
7	CA	E	2006	1/1	0.90	0.13	-1.41	137,137,137,137	0
7	CA	C	2007	1/1	0.78	0.07	-1.47	206,206,206,206	0
7	CA	A	2005	1/1	0.70	0.10	-1.49	145,145,145,145	0
7	CA	H	2002	1/1	0.60	0.13	-1.53	510,510,510,510	0
7	CA	A	2007	1/1	0.92	0.08	-1.53	181,181,181,181	0
7	CA	F	2002	1/1	0.93	0.10	-1.59	578,578,578,578	0
7	CA	E	2005	1/1	0.86	0.08	-1.60	176,176,176,176	0
7	CA	E	2007	1/1	0.91	0.13	-1.69	188,188,188,188	0
7	CA	B	2002	1/1	0.80	0.09	-1.74	535,535,535,535	0
7	CA	G	2005	1/1	0.93	0.04	-2.18	139,139,139,139	0
7	CA	A	2006	1/1	0.81	0.11	-2.33	107,107,107,107	0
7	CA	G	2007	1/1	0.63	0.06	-2.91	150,150,150,150	0
7	CA	G	2006	1/1	0.86	0.06	-3.45	95,95,95,95	0
6	NAG	C	3678	14/15	0.72	0.48	-	125,245,317,319	0
6	NAG	B	3094	14/15	0.78	0.28	-	107,197,277,325	0
6	NAG	A	3678	14/15	0.82	0.41	-	117,269,324,327	0
6	NAG	D	3094	14/15	0.44	0.82	-	189,258,296,299	0
6	NAG	G	3678	14/15	0.84	0.52	-	132,218,244,251	0
6	NAG	H	3094	14/15	0.80	0.40	-	148,232,292,297	0
6	NAG	E	3678	14/15	0.85	0.24	-	104,227,276,317	0
6	NAG	F	3094	14/15	0.84	0.27	-	124,217,266,291	0

6.5 Other polymers

There are no such residues in this entry.