



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 07:53 PM 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 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/ValidationPDFNotes.html>

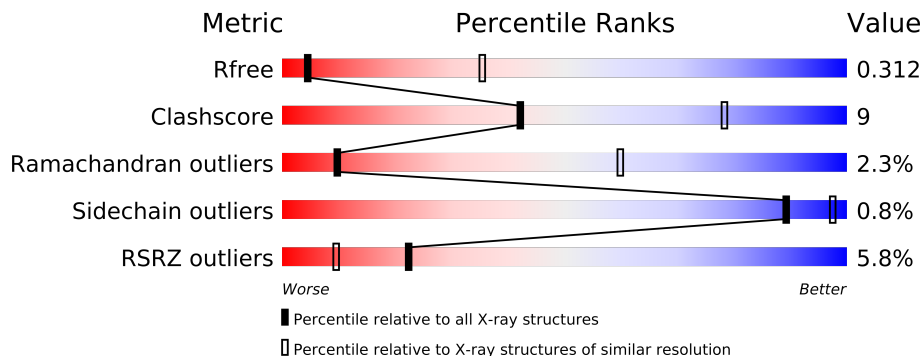
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1095	
1	C	1095	
1	E	1095	
1	G	1095	
2	B	687	
2	D	687	
2	F	687	
2	H	687	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	NAG	A	3678	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	NAG	C	3678	-	X
6	NAG	D	3094	-	X
6	NAG	G	3678	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 50187 atoms, of which 0 are hydrogen and 0 are deuterium.

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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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		

There are 99 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	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
C	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
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
E	1085	GLY	-	EXPRESSION TAG	UNP P20702
E	1086	CYS	-	EXPRESSION TAG	UNP P20702
E	1087	GLY	-	EXPRESSION TAG	UNP P20702

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 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		

There are 11 discrepancies between the modelled and reference sequences:

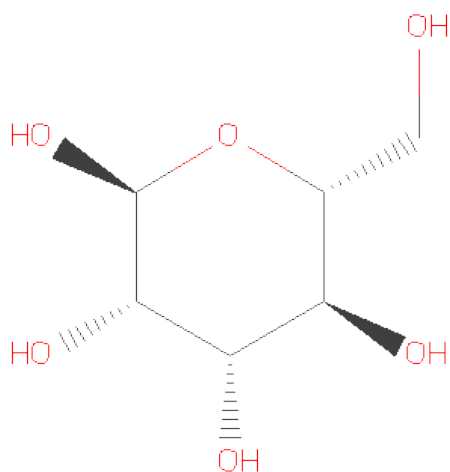
Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	EXPRESSION TAG	UNP P20702
A	1086	CYS	-	EXPRESSION TAG	UNP P20702

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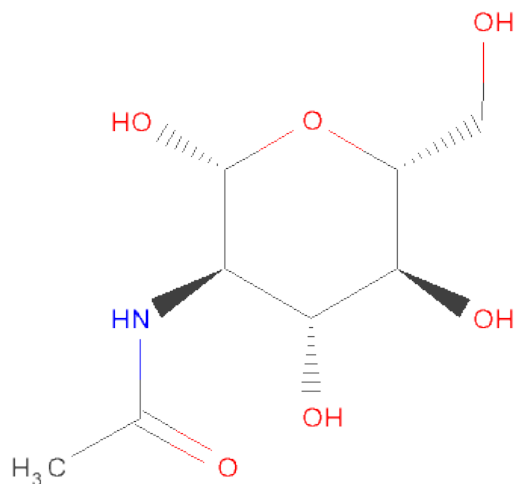
Chain	Residue	Modelled	Actual	Comment	Reference
A	1087	GLY	-	EXPRESSION TAG	UNP P20702
A	1088	GLY	-	EXPRESSION TAG	UNP P20702
A	1089	LEU	-	EXPRESSION TAG	UNP P20702
A	1090	GLU	-	EXPRESSION TAG	UNP P20702
A	1091	ASN	-	EXPRESSION TAG	UNP P20702
A	1092	LEU	-	EXPRESSION TAG	UNP P20702
A	1093	TYR	-	EXPRESSION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

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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: $C_8H_{15}NO_6$).



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

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 10 is water.

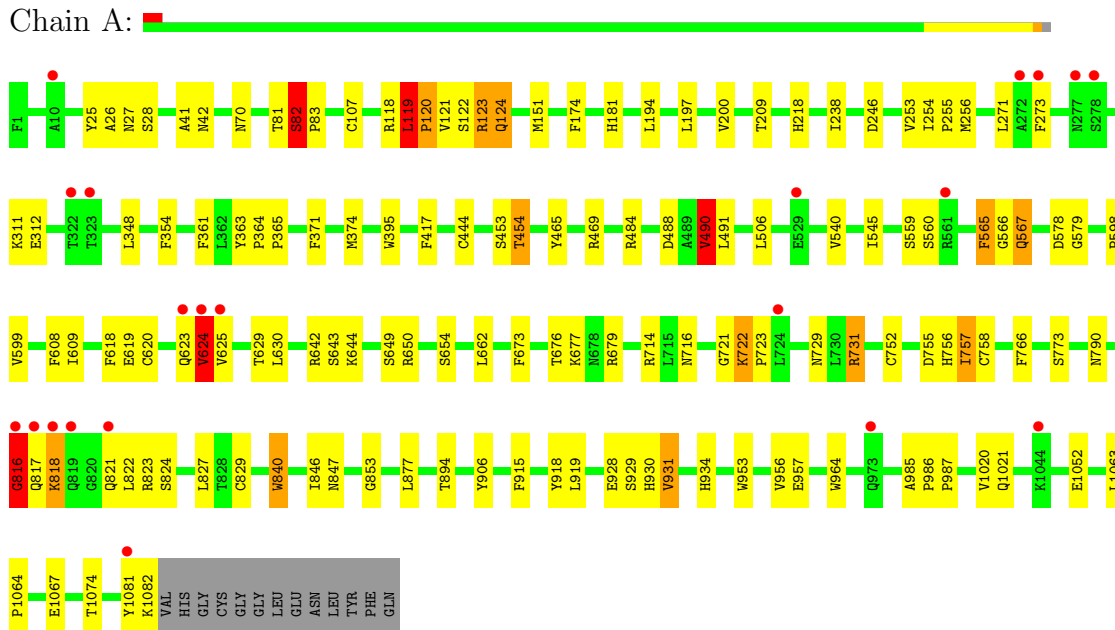
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total O 3 3	0	0

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.

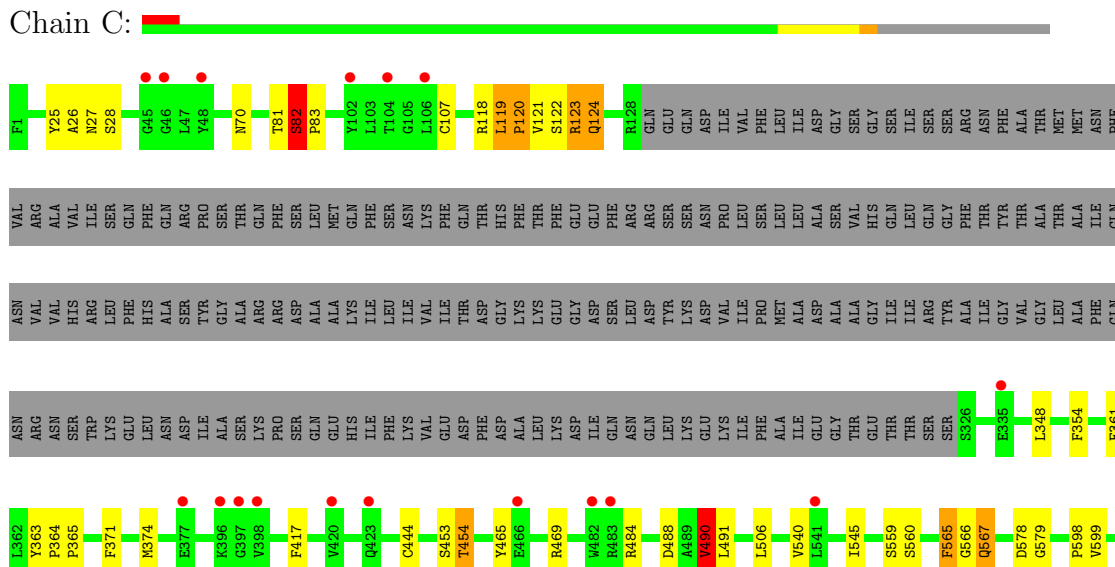
• Molecule 1: Integrin alpha-X

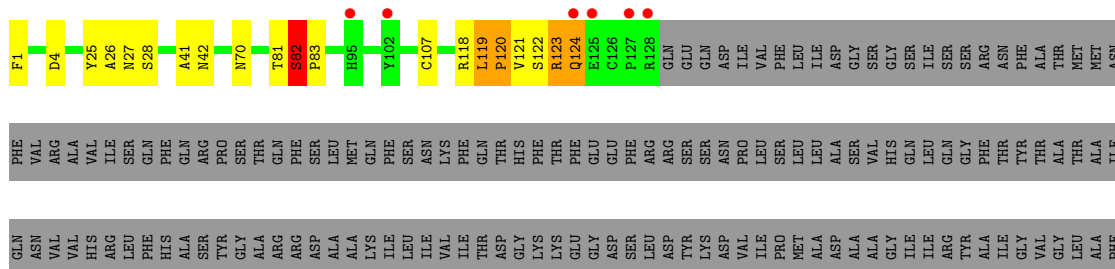
Chain A:

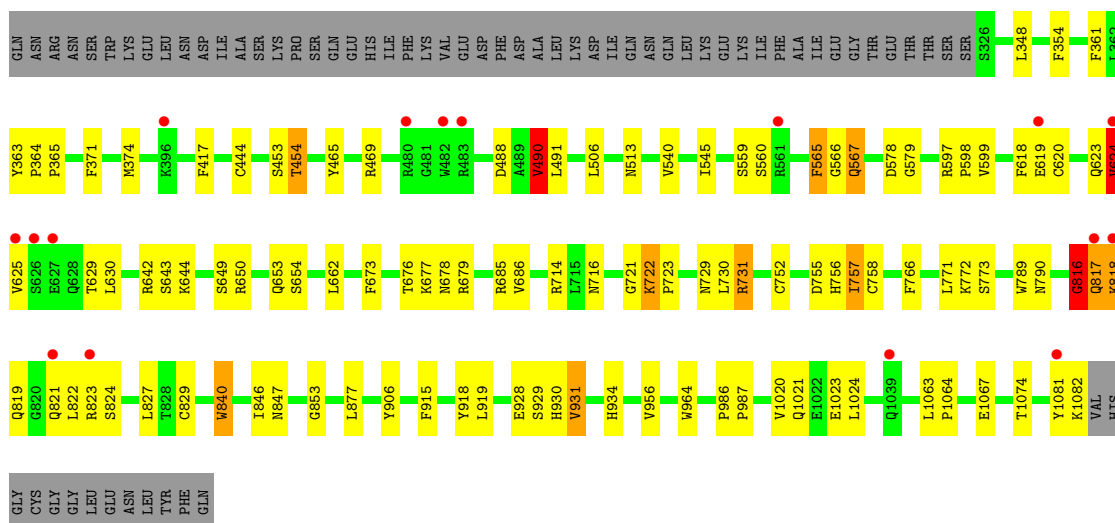


• Molecule 1: Integrin alpha-X

Chain C:

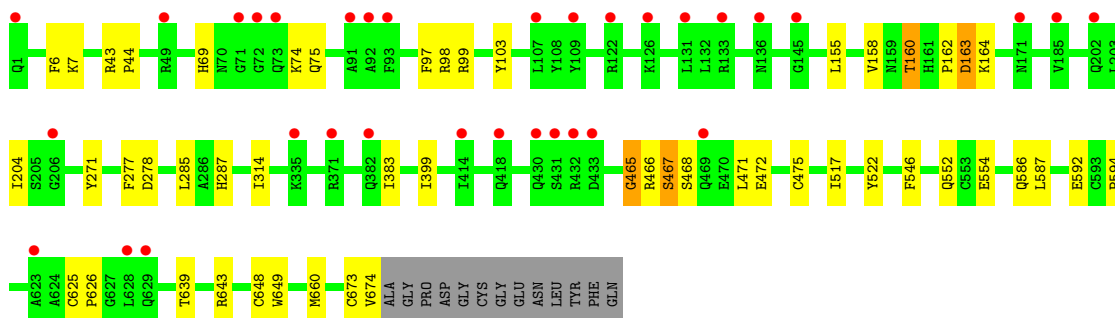






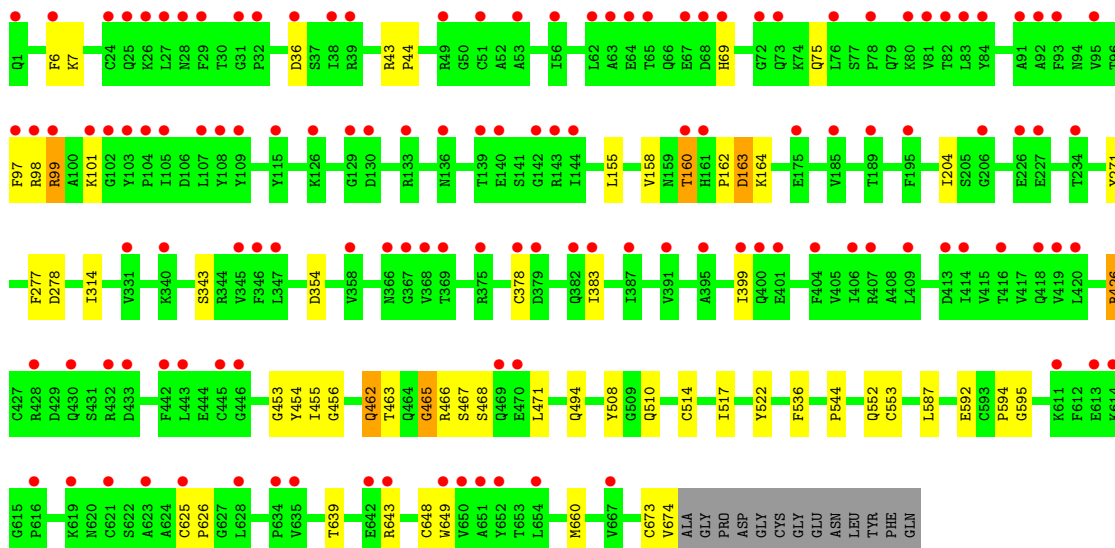
• Molecule 2: Integrin beta-2

Chain B:



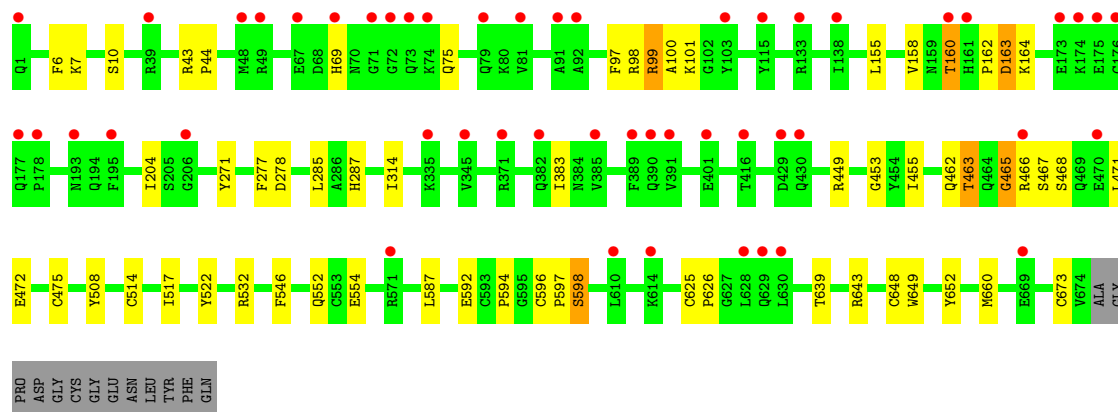
• Molecule 2: Integrin beta-2

Chain D:



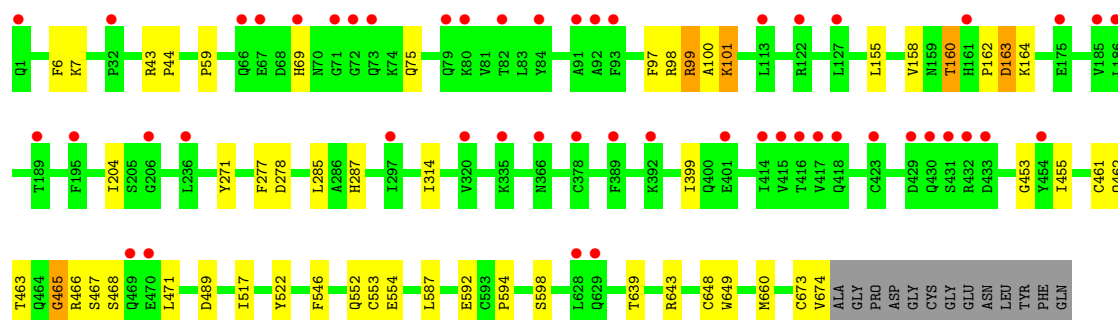
• Molecule 2: Integrin beta-2

Chain F:



- Molecule 2: Integrin beta-2

Chain H:



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 , 0.312	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 , 135.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	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.

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8392	0	180	89	0
1	C	6825	0	134	81	0
1	E	6819	0	129	78	0
1	G	6825	0	134	86	0
2	B	5184	0	174	33	0
2	D	5184	0	174	40	0
2	F	5184	0	174	40	0
2	H	5184	0	174	33	0
3	A	56	0	50	0	0
3	C	84	0	75	3	0
3	E	56	0	50	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	56	0	50	1	0
4	A	61	0	52	9	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	5	0
9	G	39	0	34	6	0
10	A	3	0	0	0	0
All	All	50187	0	1779	470	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 470 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:455:ILE:CG2	2:D:494:GLN:NE2	2.36	0.89
4:A:3377:MAN:H4	5:A:3378:MAN:C1	2.02	0.88
1:G:816:GLY:O	1:G:818:LYS:N	2.13	0.82
1:A:985:ALA:CB	1:C:621:ARG:CD	2.57	0.82
9:G:3374:NAG:O3	9:G:3375:MAN:H2	1.79	0.82

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%)	9	59
1	C	881/1095 (80%)	663 (75%)	194 (22%)	24 (3%)	8	56
1	E	880/1095 (80%)	665 (76%)	190 (22%)	25 (3%)	8	55
1	G	881/1095 (80%)	666 (76%)	191 (22%)	24 (3%)	8	56
2	B	672/687 (98%)	514 (76%)	147 (22%)	11 (2%)	14	68
2	D	672/687 (98%)	515 (77%)	145 (22%)	12 (2%)	13	65
2	F	672/687 (98%)	514 (76%)	145 (22%)	13 (2%)	12	64
2	H	672/687 (98%)	512 (76%)	146 (22%)	14 (2%)	11	62
All	All	6410/7128 (90%)	4888 (76%)	1373 (21%)	149 (2%)	10	60

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%)	84	96
1	C	754/934 (81%)	742 (98%)	12 (2%)	75	95
1	E	753/934 (81%)	743 (99%)	10 (1%)	80	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	754/934 (81%)	744 (99%)	10 (1%)	80	96
2	B	583/592 (98%)	583 (100%)	0	100	100
2	D	583/592 (98%)	582 (100%)	1 (0%)	96	99
2	F	583/592 (98%)	582 (100%)	1 (0%)	96	99
2	H	583/592 (98%)	581 (100%)	2 (0%)	96	99
All	All	5517/6104 (90%)	5471 (99%)	46 (1%)	89	97

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. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	462	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	12,14,15	0.68	1 (8%)	15,19,21	0.84	1 (6%)
3	NAG	A	3043	3	12,14,15	0.66	0	15,19,21	1.06	1 (6%)
4	NAG	A	3373	1,4	12,14,15	0.67	1 (8%)	15,19,21	1.25	2 (13%)
4	NAG	A	3374	4	12,14,15	0.70	1 (8%)	15,19,21	1.39	2 (13%)
4	MAN	A	3375	4	10,11,12	0.65	0	11,15,17	2.31	4 (36%)
4	MAN	A	3376	4	10,11,12	0.81	1 (10%)	11,15,17	1.21	1 (9%)
4	MAN	A	3377	4	10,11,12	0.89	1 (10%)	11,15,17	1.65	3 (27%)
3	NAG	A	3716	1,3	12,14,15	0.72	1 (8%)	15,19,21	0.97	1 (6%)
3	NAG	A	3717	3	12,14,15	0.67	1 (8%)	15,19,21	0.79	0
3	NAG	C	3042	1,3	12,14,15	0.70	1 (8%)	15,19,21	0.86	1 (6%)
3	NAG	C	3043	3	12,14,15	0.70	1 (8%)	15,19,21	1.01	1 (6%)
3	NAG	C	3373	1,3	12,14,15	0.64	0	15,19,21	1.28	2 (13%)
3	NAG	C	3374	3	12,14,15	0.67	0	15,19,21	0.98	0
3	NAG	C	3716	1,3	12,14,15	0.63	0	15,19,21	1.02	1 (6%)
3	NAG	C	3717	3	12,14,15	0.67	1 (8%)	15,19,21	0.81	0
3	NAG	E	3042	1,3	12,14,15	0.70	1 (8%)	15,19,21	0.88	1 (6%)
3	NAG	E	3043	3	12,14,15	0.69	1 (8%)	15,19,21	1.09	1 (6%)
9	NAG	E	3373	1,9	12,14,15	0.65	0	15,19,21	1.23	2 (13%)
9	NAG	E	3374	9	12,14,15	0.70	1 (8%)	15,19,21	1.34	2 (13%)
9	MAN	E	3375	9	10,11,12	0.69	0	11,15,17	2.01	2 (18%)
3	NAG	E	3716	1,3	12,14,15	0.66	0	15,19,21	1.10	1 (6%)
3	NAG	E	3717	3	12,14,15	0.70	1 (8%)	15,19,21	0.77	0
3	NAG	G	3042	1,3	12,14,15	0.68	1 (8%)	15,19,21	0.90	1 (6%)
3	NAG	G	3043	3	12,14,15	0.68	1 (8%)	15,19,21	1.02	1 (6%)
9	NAG	G	3373	1,9	12,14,15	0.65	0	15,19,21	1.26	2 (13%)
9	NAG	G	3374	9	12,14,15	0.69	1 (8%)	15,19,21	1.36	1 (6%)
9	MAN	G	3375	9	10,11,12	0.71	0	11,15,17	2.00	2 (18%)
3	NAG	G	3716	1,3	12,14,15	0.68	0	15,19,21	1.23	1 (6%)
3	NAG	G	3717	3	12,14,15	0.69	1 (8%)	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
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

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3716	NAG	O5-C5	-2.19	1.41	1.45
9	E	3374	NAG	O5-C5	-2.17	1.41	1.45
9	G	3374	NAG	O5-C5	-2.16	1.41	1.45
4	A	3377	MAN	O5-C5	-2.15	1.41	1.45
4	A	3374	NAG	O5-C5	-2.15	1.41	1.45

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	3375	MAN	O5-C5-C6	5.25	112.49	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	3375	MAN	O5-C5-C6	5.10	112.33	106.98
4	A	3375	MAN	O5-C5-C6	4.11	111.29	106.98
4	A	3375	MAN	C4-C3-C2	-3.98	105.16	110.50
4	A	3375	MAN	O3-C3-C2	3.81	116.91	109.94

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.

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	-	10,11,12	1.08	1 (10%)	11,15,17	1.92	2 (18%)
6	NAG	A	3678	1	12,14,15	0.65	0	15,19,21	0.77	0
6	NAG	A	3880	1	12,14,15	0.56	0	15,19,21	0.82	0
6	NAG	B	3094	2	12,14,15	0.64	0	15,19,21	0.88	1 (6%)
6	NAG	C	3678	1	12,14,15	0.63	0	15,19,21	0.75	1 (6%)
6	NAG	C	3880	1	12,14,15	0.56	0	15,19,21	0.79	0
6	NAG	D	3094	2	12,14,15	0.68	0	15,19,21	0.86	1 (6%)
6	NAG	E	3678	1	12,14,15	0.65	0	15,19,21	0.73	0
6	NAG	E	3880	1	12,14,15	0.56	0	15,19,21	0.80	0
6	NAG	F	3094	2	12,14,15	0.66	0	15,19,21	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	G	3678	1	12,14,15	0.66	0	15,19,21	0.77	1 (6%)
6	NAG	G	3880	1	12,14,15	0.57	0	15,19,21	0.79	0
6	NAG	H	3094	2	12,14,15	0.66	0	15,19,21	0.88	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
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3378	MAN	O5-C5	-2.58	1.40	1.45

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3378	MAN	C3-C4-C5	4.79	118.76	110.20
6	F	3094	NAG	O5-C5-C6	2.95	110.07	106.98
6	B	3094	NAG	O5-C5-C6	2.62	109.73	106.98
6	H	3094	NAG	O5-C5-C6	2.58	109.69	106.98
6	D	3094	NAG	O5-C5-C6	2.47	109.58	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	1082/1095 (98%)	0.14	21 (1%) 64 32	61, 153, 256, 362	0
1	C	885/1095 (80%)	0.34	44 (4%) 28 12	67, 172, 280, 410	0
1	E	884/1095 (80%)	0.16	23 (2%) 53 24	65, 157, 266, 337	0
1	G	885/1095 (80%)	0.13	22 (2%) 54 25	74, 150, 266, 342	0
2	B	674/687 (98%)	0.41	33 (4%) 28 12	100, 205, 286, 421	2 (0%)
2	D	674/687 (98%)	0.96	129 (19%) 2 2	107, 229, 313, 416	2 (0%)
2	F	674/687 (98%)	0.50	50 (7%) 14 7	98, 207, 289, 374	2 (0%)
2	H	674/687 (98%)	0.51	50 (7%) 14 7	100, 210, 293, 390	2 (0%)
All	All	6432/7128 (90%)	0.36	372 (5%) 22 9	61, 185, 283, 421	8 (0%)

The worst 5 of 372 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	GLN	10.3
2	B	72	GLY	8.6
2	H	72	GLY	8.3
2	D	92	ALA	8.2
2	B	92	ALA	8.0

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	C	3374	14/15	0.63	20.14	136,238,359,434	0
4	NAG	A	3373	14/15	0.32	1.41	136,261,376,443	0
4	NAG	A	3374	14/15	0.31	1.22	91,240,362,435	0
3	NAG	C	3373	14/15	0.47	1.02	198,292,381,425	0
3	NAG	G	3716	14/15	0.24	0.93	77,188,300,303	0
9	NAG	E	3373	14/15	0.42	0.90	146,324,390,464	0
3	NAG	C	3716	14/15	0.18	0.69	60,167,211,249	0
9	NAG	G	3373	14/15	0.34	0.54	106,265,384,401	0
9	NAG	G	3374	14/15	0.44	0.45	136,261,326,367	0
9	NAG	E	3374	14/15	0.33	0.44	201,279,352,410	0
4	MAN	A	3377	11/12	0.23	0.38	99,256,308,331	0
3	NAG	E	3716	14/15	0.21	0.06	49,184,277,297	0
3	NAG	E	3042	14/15	0.41	-0.36	198,249,285,287	0
3	NAG	G	3042	14/15	0.26	-0.39	193,244,274,279	0
3	NAG	C	3042	14/15	0.23	-0.47	150,232,327,335	0
3	NAG	A	3716	14/15	0.18	-0.93	28,156,272,274	0
3	NAG	A	3042	14/15	0.17	-1.07	133,175,235,244	0
4	MAN	A	3375	11/12	0.16	-2.86	140,207,283,324	0
3	NAG	C	3717	14/15	0.76	-	224,297,342,395	0
3	NAG	C	3043	14/15	0.31	-	179,305,351,363	0
9	MAN	G	3375	11/12	0.31	-	173,208,309,351	0
9	MAN	E	3375	11/12	0.25	-	171,251,305,311	0
4	MAN	A	3376	11/12	0.22	-	114,259,296,316	0
3	NAG	E	3043	14/15	0.55	-	183,310,366,378	0
3	NAG	G	3043	14/15	0.26	-	176,248,297,317	0
3	NAG	G	3717	14/15	0.31	-	192,216,305,376	0
3	NAG	A	3043	14/15	0.23	-	80,233,327,333	0
3	NAG	E	3717	14/15	0.21	-	117,240,280,337	0
3	NAG	A	3717	14/15	0.30	-	185,218,319,381	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	G	3678	14/15	0.50	6.99	132,218,244,251	0
6	NAG	C	3678	14/15	0.39	5.10	125,245,317,319	0
6	NAG	A	3678	14/15	0.49	4.52	117,269,324,327	0
6	NAG	G	3880	14/15	0.28	1.48	84,176,236,252	0
5	MAN	A	3378	11/12	0.31	0.35	171,186,272,293	0
6	NAG	C	3880	14/15	0.24	0.33	60,171,245,293	0
6	NAG	E	3678	14/15	0.21	-0.28	104,227,276,317	0
6	NAG	D	3094	14/15	0.69	-0.39	189,258,296,299	0
6	NAG	E	3880	14/15	0.18	-0.58	80,160,189,194	0
6	NAG	H	3094	14/15	0.41	-0.60	148,232,292,297	0
6	NAG	F	3094	14/15	0.29	-0.71	124,217,266,291	0
6	NAG	B	3094	14/15	0.31	-0.81	107,197,277,325	0
7	CA	C	2007	1/1	0.11	-1.05	206,206,206,206	0
6	NAG	A	3880	14/15	0.19	-1.06	105,143,196,220	0
7	CA	C	2006	1/1	0.13	-1.14	125,125,125,125	0
7	CA	C	2005	1/1	0.05	-1.26	200,200,200,200	0
7	CA	A	2005	1/1	0.10	-1.41	145,145,145,145	0
7	CA	F	2002	1/1	0.10	-1.44	578,578,578,578	0
7	CA	D	2002	1/1	0.14	-1.52	547,547,547,547	0
8	MG	A	2009	1/1	0.10	-1.53	367,367,367,367	0
7	CA	E	2005	1/1	0.09	-1.53	176,176,176,176	0
7	CA	B	2002	1/1	0.09	-1.64	535,535,535,535	0
7	CA	E	2006	1/1	0.10	-1.67	137,137,137,137	0
7	CA	H	2002	1/1	0.09	-1.69	510,510,510,510	0
7	CA	A	2007	1/1	0.05	-1.70	181,181,181,181	0
7	CA	G	2005	1/1	0.07	-1.93	139,139,139,139	0
7	CA	E	2007	1/1	0.13	-2.13	188,188,188,188	0
7	CA	A	2006	1/1	0.11	-2.32	107,107,107,107	0
7	CA	G	2007	1/1	0.08	-2.55	150,150,150,150	0
7	CA	G	2006	1/1	0.07	-2.76	95,95,95,95	0

6.5 Other polymers ⓘ

There are no such residues in this entry.