



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 5, 2017 – 10:56 AM EST

PDB ID : 5FFO
Title : Integrin alpha V beta 6 in complex with pro-TGF-beta
Authors : Dong, X.; Zhao, B.; Springer, T.A.
Deposited on : 2015-12-18
Resolution : 3.49 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

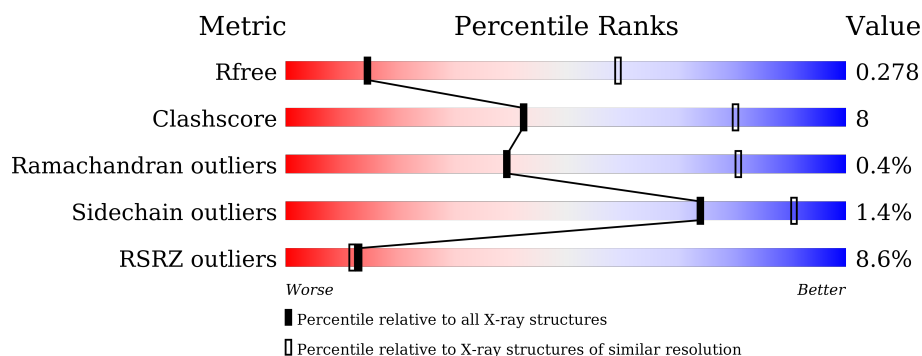
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	601	<div> <div>8%</div> <div>80%18%</div> <div>.</div> </div>
1	E	601	<div> <div>9%</div> <div>82%16%</div> <div>.</div> </div>
2	B	257	<div> <div>%</div> <div>68%26%6%</div> </div>
2	F	257	<div> <div>6%</div> <div>72%23%6%</div> </div>
3	C	363	<div> <div>10%</div> <div>62%21%16%</div> </div>
3	D	363	<div> <div>11%</div> <div>65%22%11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	363	
3	H	363	

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
7	MAN	A	2012	-	-	-	X
8	MN	B	2001	-	-	-	X
8	MN	B	2002	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23786 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-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4570	2898	776	875	21			
1	E	587	Total	C	N	O	S	0	0	0
			4547	2880	772	874	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	GLY	-	insertion	UNP P06756
A	401	CYS	MET	conflict	UNP P06756
A	597	THR	CYS	conflict	UNP P06756
A	599	GLY	-	expression tag	UNP P06756
A	600	LEU	-	expression tag	UNP P06756
A	601	GLU	-	expression tag	UNP P06756
E	400	GLY	-	insertion	UNP P06756
E	401	CYS	MET	conflict	UNP P06756
E	597	THR	CYS	conflict	UNP P06756
E	599	GLY	-	expression tag	UNP P06756
E	600	LEU	-	expression tag	UNP P06756
E	601	GLU	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1891	1210	302	368	11			
2	F	242	Total	C	N	O	S	0	0	0
			1891	1210	302	368	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	270	CYS	ILE	conflict	UNP P18564
B	362	HIS	-	expression tag	UNP P18564
B	363	HIS	-	expression tag	UNP P18564
B	364	HIS	-	expression tag	UNP P18564
B	365	HIS	-	expression tag	UNP P18564
B	366	HIS	-	expression tag	UNP P18564
B	367	HIS	-	expression tag	UNP P18564
F	270	CYS	ILE	conflict	UNP P18564
F	362	HIS	-	expression tag	UNP P18564
F	363	HIS	-	expression tag	UNP P18564
F	364	HIS	-	expression tag	UNP P18564
F	365	HIS	-	expression tag	UNP P18564
F	366	HIS	-	expression tag	UNP P18564
F	367	HIS	-	expression tag	UNP P18564

- Molecule 3 is a protein called Transforming growth factor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	305	Total	C	N	O	S	0	0	0
			2445	1555	434	439	17			
3	D	322	Total	C	N	O	S	0	0	0
			2590	1650	457	466	17			
3	G	297	Total	C	N	O	S	0	0	0
			2399	1529	425	429	16			
3	H	325	Total	C	N	O	S	0	0	0
			2612	1660	465	471	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P01137
C	0	PRO	-	expression tag	UNP P01137
C	1	LEU	-	expression tag	UNP P01137
C	2	SER	-	expression tag	UNP P01137
C	3	THR	-	expression tag	UNP P01137
C	4	SER	-	expression tag	UNP P01137
C	107	GLN	ASN	conflict	UNP P01137
C	147	GLN	ASN	conflict	UNP P01137
D	-1	GLY	-	expression tag	UNP P01137
D	0	PRO	-	expression tag	UNP P01137
D	1	LEU	-	expression tag	UNP P01137
D	2	SER	-	expression tag	UNP P01137
D	3	THR	-	expression tag	UNP P01137

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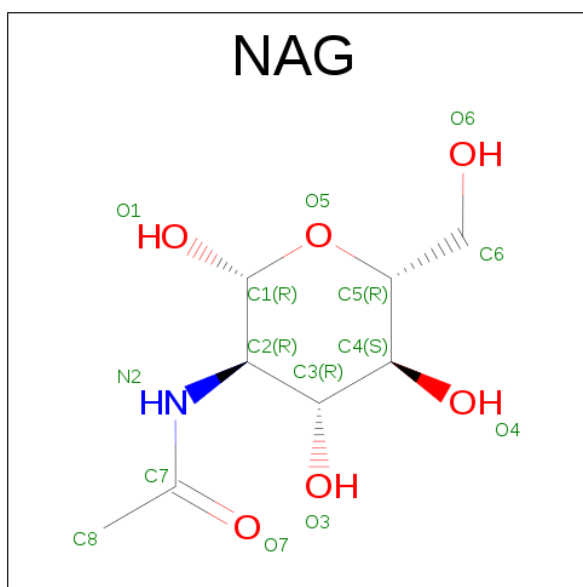
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Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	-	expression tag	UNP P01137
D	107	GLN	ASN	conflict	UNP P01137
D	147	GLN	ASN	conflict	UNP P01137
G	-1	GLY	-	expression tag	UNP P01137
G	0	PRO	-	expression tag	UNP P01137
G	1	LEU	-	expression tag	UNP P01137
G	2	SER	-	expression tag	UNP P01137
G	3	THR	-	expression tag	UNP P01137
G	4	SER	-	expression tag	UNP P01137
G	107	GLN	ASN	conflict	UNP P01137
G	147	GLN	ASN	conflict	UNP P01137
H	-1	GLY	-	expression tag	UNP P01137
H	0	PRO	-	expression tag	UNP P01137
H	1	LEU	-	expression tag	UNP P01137
H	2	SER	-	expression tag	UNP P01137
H	3	THR	-	expression tag	UNP P01137
H	4	SER	-	expression tag	UNP P01137
H	107	GLN	ASN	conflict	UNP P01137
H	147	GLN	ASN	conflict	UNP P01137

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Ca 4 4	0	0
4	E	4	Total Ca 4 4	0	0

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



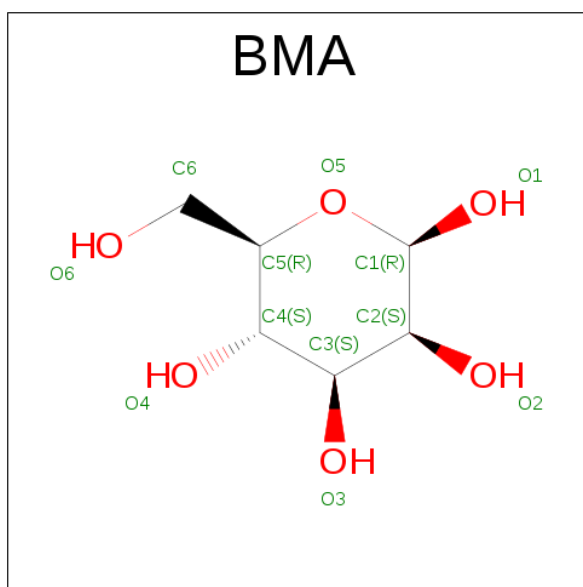
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1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

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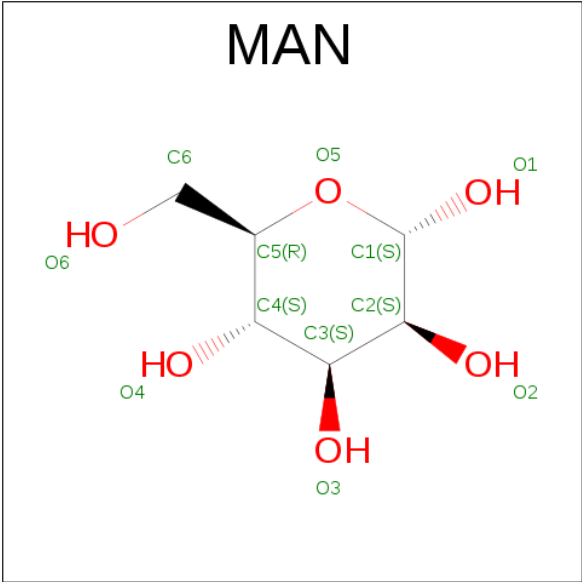
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	H	1	Total	C	O	0	0
			11	6	5		
7	H	1	Total	C	O	0	0
			11	6	5		
7	H	1	Total	C	O	0	0
			11	6	5		

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

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

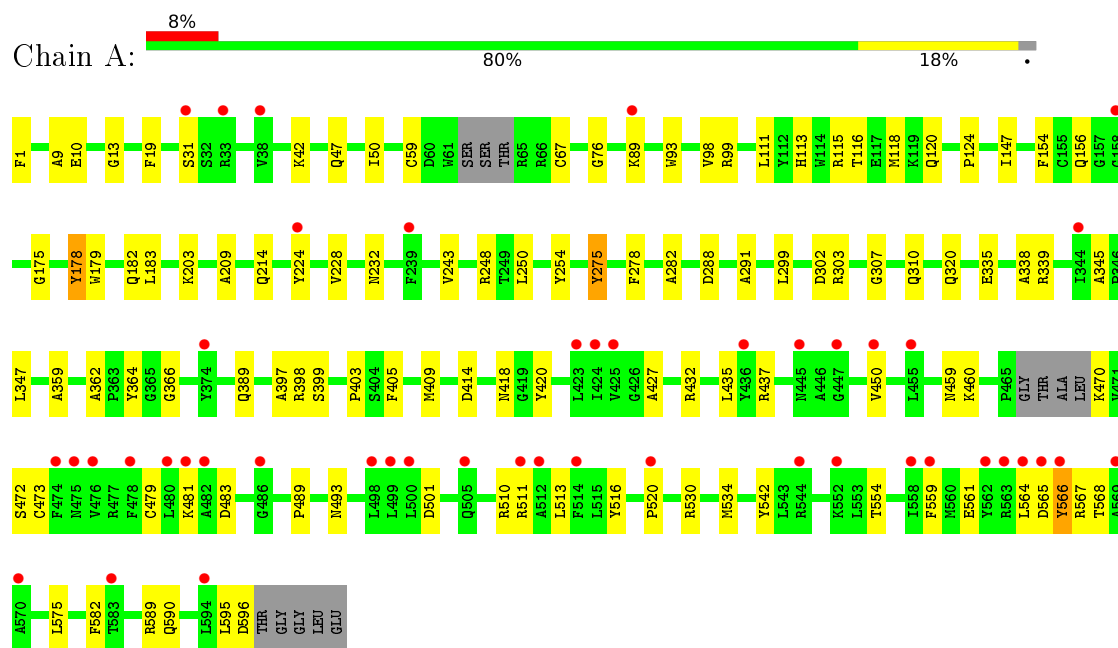
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	3	Total	O	0	0
			3	3		
9	F	2	Total	O	0	0
			2	2		

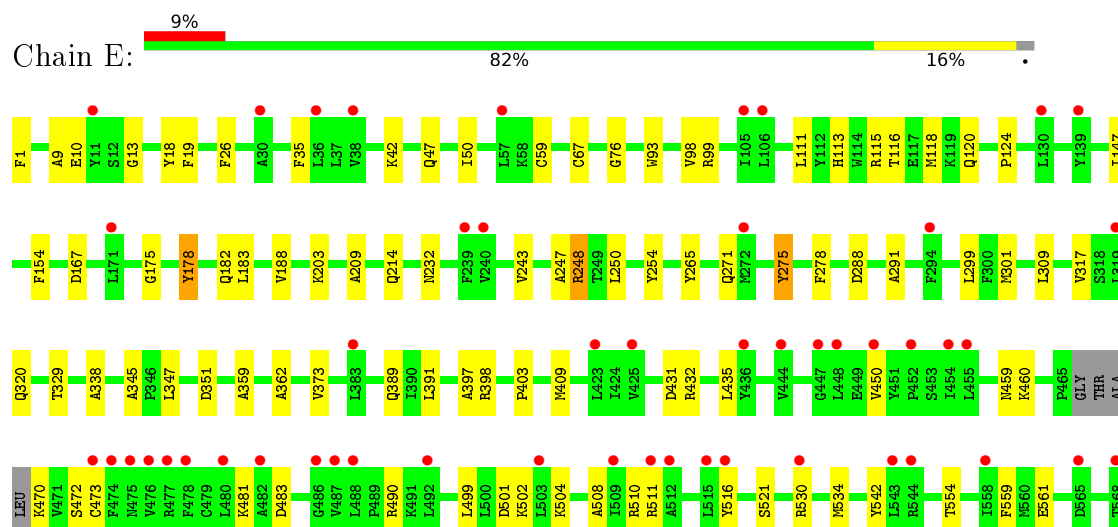
3 Residue-property plots

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.

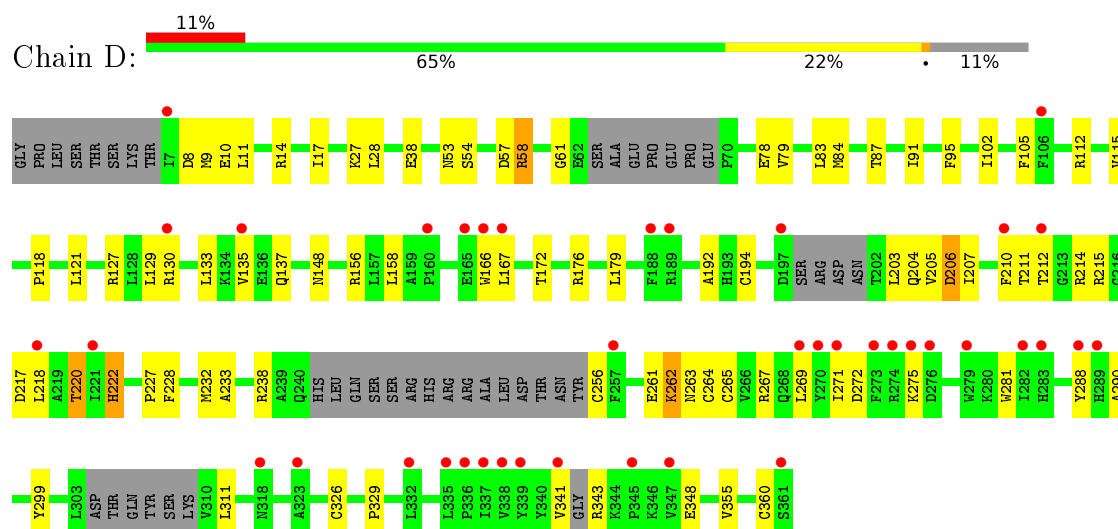
• Molecule 1: Integrin alpha-V



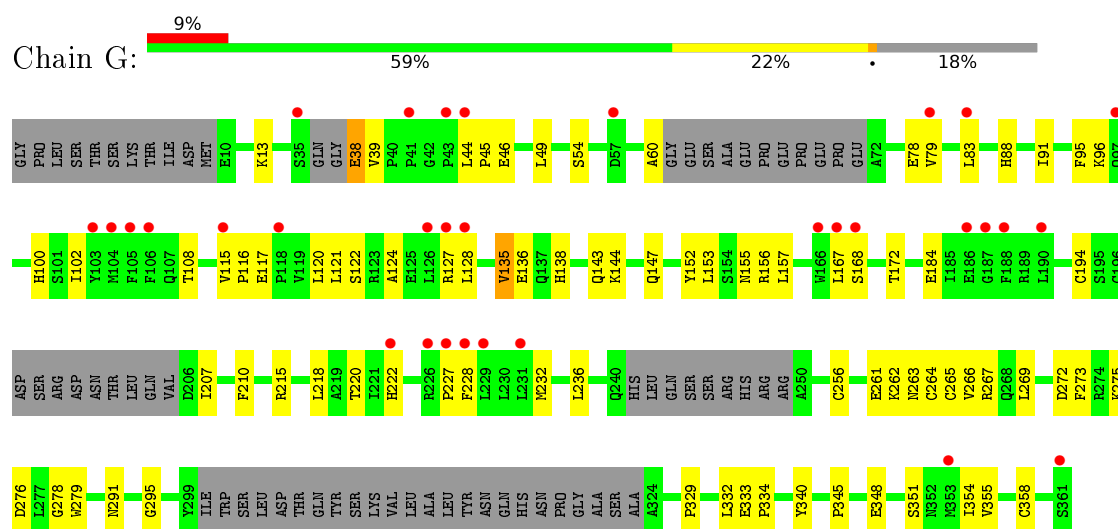
• Molecule 1: Integrin alpha-V



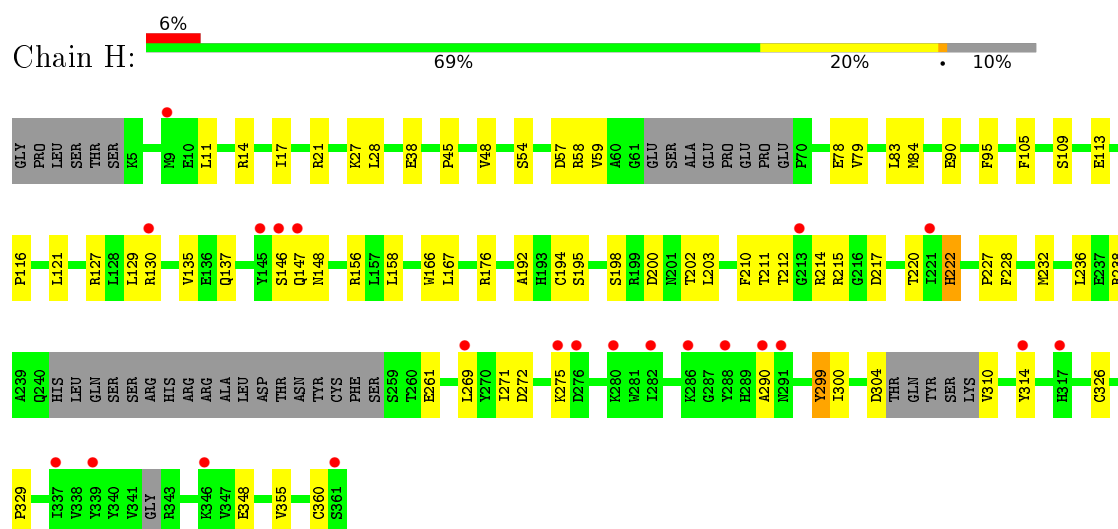
• Molecule 3: Transforming growth factor beta-1



• Molecule 3: Transforming growth factor beta-1



• Molecule 3: Transforming growth factor beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 91.44Å 131.03Å 89.98° 86.25° 89.85°	Depositor
Resolution (Å)	45.72 – 3.49 45.72 – 3.49	Depositor EDS
% Data completeness (in resolution range)	94.4 (45.72-3.49) 94.0 (45.72-3.49)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.224 , 0.277 0.224 , 0.278	Depositor DCC
R_{free} test set	1059 reflections (2.34%)	DCC
Wilson B-factor (Å ²)	124.4	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 159.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.286 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23786	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MAN, CA, BMA, NAG, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/4672	0.49	1/6321 (0.0%)
1	E	0.28	0/4649	0.48	0/6291
2	B	0.35	0/1930	0.50	0/2618
2	F	0.32	1/1930 (0.1%)	0.44	0/2618
3	C	0.35	2/2501 (0.1%)	0.47	1/3381 (0.0%)
3	D	0.45	5/2650 (0.2%)	0.51	0/3585
3	G	0.37	2/2454 (0.1%)	0.45	0/3317
3	H	0.45	4/2672 (0.1%)	0.52	0/3616
All	All	0.35	14/23458 (0.1%)	0.48	2/31747 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	38	GLU	CG-CD	8.88	1.65	1.51
3	D	38	GLU	CG-CD	8.35	1.64	1.51
3	C	38	GLU	CG-CD	8.05	1.64	1.51
3	H	148	ASN	CB-CG	7.88	1.69	1.51
3	H	38	GLU	CB-CG	7.88	1.67	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	LEU	CA-CB-CG	7.55	132.66	115.30
3	C	319	PRO	N-CA-CB	5.96	110.45	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4570	0	4414	73	0
1	E	4547	0	4388	60	0
2	B	1891	0	1866	48	0
2	F	1891	0	1866	33	0
3	C	2445	0	2435	51	0
3	D	2590	0	2580	55	0
3	G	2399	0	2394	52	0
3	H	2612	0	2608	45	0
4	A	4	0	0	0	0
4	E	4	0	0	0	0
5	A	154	0	134	3	0
5	B	14	0	13	0	0
5	C	28	0	24	1	0
5	D	28	0	24	0	0
5	E	154	0	134	6	0
5	F	14	0	13	0	0
5	G	28	0	24	0	0
5	H	28	0	24	0	0
6	A	44	0	35	2	0
6	C	11	0	9	0	0
6	D	11	0	9	0	0
6	E	44	0	35	2	0
6	G	11	0	9	0	0
6	H	11	0	8	0	0
7	A	88	0	77	1	0
7	C	11	0	10	0	0
7	D	11	0	10	0	0
7	E	88	0	77	2	0
7	G	11	0	10	0	0
7	H	33	0	29	0	0
8	B	3	0	0	0	0
8	F	3	0	0	0	0
9	B	3	0	0	0	0
9	F	2	0	0	0	0
All	All	23786	0	23259	390	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 8.

The worst 5 of 390 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:248:ARG:HE	2:B:320:LEU:HD12	1.35	0.92
1:A:460:LYS:HB3	1:A:470:LYS:HB3	1.63	0.80
1:E:502:LYS:HE2	5:E:2026:NAG:H81	1.65	0.79
3:C:100:HIS:HA	3:C:210:PHE:HB2	1.68	0.75
3:C:261:GLU:HG3	3:C:263:ASN:H	1.51	0.74

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	583/601 (97%)	548 (94%)	34 (6%)	1 (0%)	52	88
1	E	583/601 (97%)	552 (95%)	31 (5%)	0	100	100
2	B	240/257 (93%)	217 (90%)	23 (10%)	0	100	100
2	F	240/257 (93%)	218 (91%)	22 (9%)	0	100	100
3	C	295/363 (81%)	263 (89%)	30 (10%)	2 (1%)	26	72
3	D	310/363 (85%)	272 (88%)	35 (11%)	3 (1%)	19	66
3	G	285/363 (78%)	254 (89%)	28 (10%)	3 (1%)	17	63
3	H	315/363 (87%)	273 (87%)	39 (12%)	3 (1%)	19	66
All	All	2851/3168 (90%)	2597 (91%)	242 (8%)	12 (0%)	39	81

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	135	VAL
3	G	135	VAL

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Mol	Chain	Res	Type
1	A	566	TYR
3	H	135	VAL
3	H	202	THR

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	483/491 (98%)	478 (99%)	5 (1%)	82	93
1	E	481/491 (98%)	475 (99%)	6 (1%)	78	92
2	B	215/230 (94%)	213 (99%)	2 (1%)	84	94
2	F	215/230 (94%)	213 (99%)	2 (1%)	84	94
3	C	268/323 (83%)	265 (99%)	3 (1%)	80	92
3	D	286/323 (88%)	278 (97%)	8 (3%)	51	82
3	G	265/323 (82%)	262 (99%)	3 (1%)	80	92
3	H	288/323 (89%)	281 (98%)	7 (2%)	57	85
All	All	2501/2734 (92%)	2465 (99%)	36 (1%)	74	91

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	299	TYR
1	E	275	TYR
3	H	222	HIS
1	E	178	TYR
1	E	490	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	342	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 80 ligands modelled in this entry, 14 are monoatomic - leaving 66 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	NAG	A	2005	1,5	14,14,15	0.45	0	15,19,21	0.37	0
5	NAG	A	2006	5,6	14,14,15	0.28	0	15,19,21	0.40	0
6	BMA	A	2007	5	11,11,12	0.52	0	15,15,17	0.92	0
5	NAG	A	2008	1,5	14,14,15	0.28	0	15,19,21	0.30	0
5	NAG	A	2009	5,6	14,14,15	0.43	0	15,19,21	0.38	0
6	BMA	A	2010	5,7	11,11,12	1.00	1 (9%)	15,15,17	1.17	2 (13%)
7	MAN	A	2011	7,6	11,11,12	0.77	0	15,15,17	1.36	4 (26%)
7	MAN	A	2012	7	11,11,12	0.84	1 (9%)	15,15,17	1.19	2 (13%)
7	MAN	A	2013	6	11,11,12	1.01	1 (9%)	15,15,17	1.13	1 (6%)
5	NAG	A	2014	1,5	14,14,15	0.58	1 (7%)	15,19,21	0.43	0
5	NAG	A	2015	5,6	14,14,15	0.34	0	15,19,21	0.35	0
6	BMA	A	2016	5,7	11,11,12	0.75	0	15,15,17	1.14	1 (6%)
7	MAN	A	2017	6	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
7	MAN	A	2018	7,6	11,11,12	1.19	2 (18%)	15,15,17	2.14	4 (26%)
7	MAN	A	2019	7	11,11,12	0.77	0	15,15,17	1.07	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	A	2020	7	11,11,12	0.77	0	15,15,17	0.85	1 (6%)
5	NAG	A	2021	1,5	14,14,15	0.20	0	15,19,21	0.27	0
5	NAG	A	2022	5,6	14,14,15	0.28	0	15,19,21	0.35	0
6	BMA	A	2023	5,7	11,11,12	0.71	0	15,15,17	1.29	4 (26%)
7	MAN	A	2024	6	11,11,12	0.69	0	15,15,17	1.28	2 (13%)
5	NAG	A	2025	1	14,14,15	0.57	0	15,19,21	0.27	0
5	NAG	A	2026	1,5	14,14,15	0.43	0	15,19,21	0.35	0
5	NAG	A	2027	5	14,14,15	0.36	0	15,19,21	0.36	0
5	NAG	B	2004	2	14,14,15	0.32	0	15,19,21	0.26	0
5	NAG	C	401	3,5	14,14,15	0.40	0	15,19,21	0.32	0
5	NAG	C	402	5,6	14,14,15	0.35	0	15,19,21	0.53	0
6	BMA	C	403	5,7	11,11,12	0.58	0	15,15,17	0.86	0
7	MAN	C	404	6	11,11,12	0.85	0	15,15,17	1.12	1 (6%)
5	NAG	D	401	3,5	14,14,15	0.38	0	15,19,21	0.49	0
5	NAG	D	402	5,6	14,14,15	0.35	0	15,19,21	0.22	0
6	BMA	D	403	5,7	11,11,12	0.53	0	15,15,17	0.86	0
7	MAN	D	404	6	11,11,12	0.57	0	15,15,17	1.10	2 (13%)
5	NAG	E	2005	1,5	14,14,15	0.34	0	15,19,21	0.36	0
5	NAG	E	2006	5,6	14,14,15	0.51	0	15,19,21	0.52	0
6	BMA	E	2007	5	11,11,12	0.62	0	15,15,17	1.04	2 (13%)
5	NAG	E	2008	1,5	14,14,15	0.32	0	15,19,21	0.33	0
5	NAG	E	2009	5,6	14,14,15	0.44	0	15,19,21	0.40	0
6	BMA	E	2010	5,7	11,11,12	1.01	1 (9%)	15,15,17	1.15	2 (13%)
7	MAN	E	2011	7,6	11,11,12	0.80	0	15,15,17	1.32	2 (13%)
7	MAN	E	2012	7	11,11,12	0.76	0	15,15,17	1.15	1 (6%)
7	MAN	E	2013	6	11,11,12	1.04	1 (9%)	15,15,17	1.13	1 (6%)
5	NAG	E	2014	1,5	14,14,15	0.64	1 (7%)	15,19,21	0.47	0
5	NAG	E	2015	5,6	14,14,15	0.30	0	15,19,21	0.30	0
6	BMA	E	2016	5,7	11,11,12	0.67	0	15,15,17	1.12	1 (6%)
7	MAN	E	2017	6	11,11,12	0.65	0	15,15,17	1.03	1 (6%)
7	MAN	E	2018	7,6	11,11,12	1.25	2 (18%)	15,15,17	2.16	4 (26%)
7	MAN	E	2019	7	11,11,12	0.90	0	15,15,17	1.12	2 (13%)
7	MAN	E	2020	7	11,11,12	0.84	1 (9%)	15,15,17	0.86	1 (6%)
5	NAG	E	2021	1,5	14,14,15	0.23	0	15,19,21	0.26	0
5	NAG	E	2022	5,6	14,14,15	0.22	0	15,19,21	0.35	0
6	BMA	E	2023	5,7	11,11,12	0.83	0	15,15,17	1.38	3 (20%)
7	MAN	E	2024	6	11,11,12	0.71	0	15,15,17	1.41	3 (20%)
5	NAG	E	2025	1	14,14,15	0.65	1 (7%)	15,19,21	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	2026	1,5	14,14,15	0.57	0	15,19,21	0.23	0
5	NAG	E	2027	5	14,14,15	0.32	0	15,19,21	0.33	0
5	NAG	F	2004	2	14,14,15	0.20	0	15,19,21	0.21	0
5	NAG	G	401	3,5	14,14,15	0.48	0	15,19,21	0.57	0
5	NAG	G	402	5,6	14,14,15	0.33	0	15,19,21	0.58	0
6	BMA	G	403	5,7	11,11,12	1.19	1 (9%)	15,15,17	1.23	1 (6%)
7	MAN	G	404	6	11,11,12	1.11	1 (9%)	15,15,17	1.72	4 (26%)
5	NAG	H	401	3,5	14,14,15	0.33	0	15,19,21	0.59	0
5	NAG	H	402	5,6	14,14,15	0.39	0	15,19,21	0.32	0
6	BMA	H	403	5,7	11,11,12	1.33	1 (9%)	15,15,17	1.33	2 (13%)
7	MAN	H	404	7,6	11,11,12	1.64	2 (18%)	15,15,17	1.53	2 (13%)
7	MAN	H	405	6	11,11,12	0.88	1 (9%)	15,15,17	1.23	2 (13%)
7	MAN	H	406	7	11,11,12	0.69	0	15,15,17	0.99	2 (13%)

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	NAG	A	2005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2006	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	2007	5	-	0/2/19/22	0/1/1/1
5	NAG	A	2008	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2009	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	2010	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	2011	7,6	-	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	6	-	0/2/19/22	0/1/1/1
5	NAG	A	2014	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2015	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	2016	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	2017	6	-	0/2/19/22	0/1/1/1
7	MAN	A	2018	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	2019	7	-	0/2/19/22	0/1/1/1
7	MAN	A	2020	7	-	0/2/19/22	0/1/1/1
5	NAG	A	2021	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2022	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	2023	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	2024	6	-	0/2/19/22	1/1/1/1
5	NAG	A	2025	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	2026	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2027	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
5	NAG	C	401	3,5	-	0/6/23/26	0/1/1/1
5	NAG	C	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	404	6	-	0/2/19/22	0/1/1/1
5	NAG	D	401	3,5	-	0/6/23/26	0/1/1/1
5	NAG	D	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	D	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	D	404	6	-	0/2/19/22	0/1/1/1
5	NAG	E	2005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2006	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	2007	5	-	0/2/19/22	0/1/1/1
5	NAG	E	2008	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2009	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	2010	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	2011	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	2012	7	-	0/2/19/22	0/1/1/1
7	MAN	E	2013	6	-	0/2/19/22	0/1/1/1
5	NAG	E	2014	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2015	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	2016	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	2017	6	-	0/2/19/22	0/1/1/1
7	MAN	E	2018	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	2019	7	-	0/2/19/22	0/1/1/1
7	MAN	E	2020	7	-	0/2/19/22	0/1/1/1
5	NAG	E	2021	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2022	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	2023	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	2024	6	-	0/2/19/22	0/1/1/1
5	NAG	E	2025	1	-	0/6/23/26	0/1/1/1
5	NAG	E	2026	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2027	5	-	0/6/23/26	0/1/1/1
5	NAG	F	2004	2	-	0/6/23/26	0/1/1/1
5	NAG	G	401	3,5	-	0/6/23/26	0/1/1/1
5	NAG	G	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	404	6	-	0/2/19/22	0/1/1/1
5	NAG	H	401	3,5	-	0/6/23/26	0/1/1/1
5	NAG	H	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	H	403	5,7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	H	404	7,6	-	0/2/19/22	0/1/1/1
7	MAN	H	405	6	-	0/2/19/22	0/1/1/1
7	MAN	H	406	7	-	0/2/19/22	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	2020	MAN	O5-C1	-2.29	1.40	1.43
5	E	2014	NAG	O5-C1	-2.18	1.40	1.43
5	A	2014	NAG	O5-C1	-2.02	1.40	1.43
5	E	2025	NAG	O5-C1	-2.01	1.40	1.43
6	A	2010	BMA	O3-C3	2.01	1.47	1.43

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	405	MAN	O2-C2-C3	-2.82	104.50	110.19
7	E	2019	MAN	O2-C2-C3	-2.67	104.80	110.19
7	G	404	MAN	O2-C2-C3	-2.55	105.06	110.19
7	A	2024	MAN	O2-C2-C3	-2.44	105.26	110.19
7	A	2011	MAN	O2-C2-C3	-2.43	105.28	110.19

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2024	MAN	C1-C2-C3-C4-C5-O5

17 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2008	NAG	1	0
5	A	2009	NAG	3	0
6	A	2010	BMA	1	0
7	A	2011	MAN	1	0
7	A	2012	MAN	1	0
6	A	2016	BMA	1	0
5	C	401	NAG	1	0
5	E	2008	NAG	1	0
5	E	2009	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	2010	BMA	1	0
7	E	2012	MAN	1	0
6	E	2016	BMA	1	0
7	E	2018	MAN	1	0
7	E	2019	MAN	1	0
5	E	2021	NAG	2	0
5	E	2022	NAG	2	0
5	E	2026	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(Å ²)	Q<0.9
1	A	589/601 (98%)	0.37	46 (7%) 16 13	133, 206, 281, 311	0
1	E	587/601 (97%)	0.44	53 (9%) 12 10	139, 222, 286, 333	0
2	B	242/257 (94%)	0.17	3 (1%) 81 72	63, 146, 259, 309	0
2	F	242/257 (94%)	0.38	16 (6%) 22 16	171, 224, 261, 287	0
3	C	305/363 (84%)	0.59	38 (12%) 5 6	159, 243, 294, 338	0
3	D	322/363 (88%)	0.50	40 (12%) 5 6	158, 225, 274, 300	0
3	G	297/363 (81%)	0.46	32 (10%) 8 7	127, 227, 284, 315	0
3	H	325/363 (89%)	0.35	22 (6%) 20 16	133, 202, 256, 273	0
All	All	2909/3168 (91%)	0.41	250 (8%) 13 12	63, 219, 280, 338	0

The worst 5 of 250 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	455	LEU	11.9
1	A	482	ALA	10.4
3	G	35	SER	9.0
1	E	487	VAL	8.9
1	A	455	LEU	8.6

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 ⓘ

There are no carbohydrates in this entry.

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	MN	B	2002	1/1	0.99	0.26	2.48	110,110,110,110	0
8	MN	B	2001	1/1	0.99	0.25	2.35	181,181,181,181	0
7	MAN	A	2012	11/12	0.74	0.40	1.81	210,237,246,247	0
5	NAG	E	2008	14/15	0.90	0.24	1.40	210,229,277,283	0
8	MN	F	2001	1/1	0.98	0.26	0.96	217,217,217,217	0
4	CA	A	2004	1/1	0.99	0.27	0.92	155,155,155,155	0
8	MN	F	2002	1/1	0.95	0.20	0.78	233,233,233,233	0
5	NAG	A	2005	14/15	0.88	0.25	0.72	155,202,243,244	0
5	NAG	D	401	14/15	0.90	0.23	0.12	193,229,252,259	0
7	MAN	E	2012	11/12	0.81	0.21	0.05	170,229,254,263	0
5	NAG	E	2014	14/15	0.94	0.26	-0.03	157,187,255,258	0
5	NAG	A	2008	14/15	0.86	0.21	-0.03	188,238,257,265	0
5	NAG	A	2021	14/15	0.78	0.37	-0.21	239,291,308,308	0
4	CA	E	2004	1/1	0.98	0.14	-0.36	225,225,225,225	0
8	MN	F	2003	1/1	0.99	0.16	-0.38	213,213,213,213	0
5	NAG	E	2015	14/15	0.97	0.21	-0.40	156,199,262,266	0
5	NAG	E	2005	14/15	0.93	0.19	-0.50	157,203,222,230	0
5	NAG	A	2014	14/15	0.93	0.21	-0.72	157,208,243,252	0
8	MN	B	2003	1/1	0.99	0.18	-0.81	144,144,144,144	0
5	NAG	A	2015	14/15	0.96	0.19	-0.83	165,185,197,203	0
5	NAG	H	401	14/15	0.94	0.16	-0.83	178,216,248,264	0
4	CA	A	2001	1/1	0.99	0.15	-0.84	189,189,189,189	0
4	CA	E	2001	1/1	0.95	0.14	-0.91	218,218,218,218	0
4	CA	A	2002	1/1	0.94	0.10	-0.95	222,222,222,222	0
4	CA	E	2002	1/1	0.96	0.12	-1.03	256,256,256,256	0
4	CA	A	2003	1/1	0.99	0.16	-1.07	199,199,199,199	0
4	CA	E	2003	1/1	0.91	0.10	-1.10	219,219,219,219	0
5	NAG	E	2021	14/15	0.84	0.19	-1.52	255,303,326,328	0
6	BMA	D	403	11/12	0.90	0.16	-	193,230,238,242	0
7	MAN	A	2013	11/12	0.79	0.21	-	144,256,279,288	0
5	NAG	C	401	14/15	0.79	0.19	-	181,240,272,278	0
6	BMA	C	403	11/12	0.88	0.14	-	246,266,287,288	0
7	MAN	H	404	11/12	0.91	0.20	-	241,259,269,273	0
7	MAN	A	2019	11/12	0.87	0.20	-	210,220,237,246	0
7	MAN	G	404	11/12	0.65	0.26	-	210,251,267,270	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	E	2022	14/15	0.87	0.14	-	251,293,309,313	0
5	NAG	C	402	14/15	0.84	0.30	-	257,291,310,311	0
6	BMA	G	403	11/12	0.90	0.12	-	207,247,255,268	0
7	MAN	H	405	11/12	0.91	0.24	-	227,249,268,271	0
7	MAN	E	2017	11/12	0.95	0.13	-	208,229,241,241	0
7	MAN	E	2018	11/12	0.86	0.12	-	205,229,252,264	0
5	NAG	E	2025	14/15	0.80	0.32	-	223,252,285,293	0
5	NAG	A	2026	14/15	0.78	0.22	-	170,256,290,295	0
6	BMA	E	2023	11/12	0.70	0.21	-	268,283,319,345	0
5	NAG	A	2006	14/15	0.87	0.22	-	194,225,238,255	0
6	BMA	A	2023	11/12	0.77	0.17	-	279,294,313,321	0
7	MAN	E	2020	11/12	0.81	0.32	-	216,259,290,308	0
6	BMA	H	403	11/12	0.82	0.15	-	204,259,281,282	0
7	MAN	A	2020	11/12	0.85	0.32	-	257,283,289,293	0
5	NAG	E	2027	14/15	0.56	0.44	-	251,324,342,342	0
6	BMA	E	2016	11/12	0.94	0.13	-	190,205,228,232	0
5	NAG	E	2026	14/15	0.81	0.22	-	256,296,331,332	0
5	NAG	A	2009	14/15	0.73	0.26	-	251,285,298,299	0
6	BMA	E	2010	11/12	0.86	0.08	-	260,279,289,294	0
5	NAG	B	2004	14/15	0.91	0.19	-	234,258,269,269	0
7	MAN	H	406	11/12	0.78	0.21	-	182,265,283,288	0
5	NAG	H	402	14/15	0.85	0.16	-	215,238,266,275	0
5	NAG	A	2025	14/15	0.76	0.60	-	280,323,340,345	0
7	MAN	A	2018	11/12	0.89	0.17	-	187,214,265,277	0
5	NAG	G	402	14/15	0.85	0.19	-	202,251,281,284	0
7	MAN	E	2024	11/12	0.76	0.31	-	260,296,321,322	0
5	NAG	E	2006	14/15	0.92	0.17	-	181,186,204,214	0
6	BMA	A	2016	11/12	0.91	0.15	-	117,192,216,216	0
7	MAN	E	2019	11/12	0.90	0.20	-	236,241,265,267	0
5	NAG	A	2027	14/15	0.72	0.27	-	189,242,281,286	0
5	NAG	D	402	14/15	0.83	0.18	-	188,213,241,242	0
7	MAN	A	2011	11/12	0.61	0.18	-	238,258,280,291	0
5	NAG	G	401	14/15	0.90	0.17	-	231,270,278,279	0
5	NAG	E	2009	14/15	0.84	0.20	-	223,250,271,275	0
7	MAN	E	2013	11/12	0.85	0.17	-	228,253,286,286	0
7	MAN	C	404	11/12	0.82	0.20	-	206,239,263,266	0
7	MAN	D	404	11/12	0.91	0.18	-	156,208,226,234	0
6	BMA	A	2010	11/12	0.77	0.12	-	242,283,305,308	0
6	BMA	A	2007	11/12	0.73	0.34	-	181,242,253,260	0
6	BMA	E	2007	11/12	0.89	0.19	-	195,223,230,231	0
7	MAN	A	2017	11/12	0.94	0.20	-	167,197,224,249	0
5	NAG	F	2004	14/15	0.85	0.21	-	258,270,279,284	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MAN	E	2011	11/12	0.87	0.15	-	224,281,298,305	0
7	MAN	A	2024	11/12	0.82	0.30	-	223,243,287,291	0
5	NAG	A	2022	14/15	0.86	0.14	-	253,281,301,303	0

6.5 Other polymers [i](#)

There are no such residues in this entry.