



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2017 – 10:41 AM EST

PDB ID : 5FFG
Title : Crystal structure of integrin alpha V beta 6 head
Authors : Dong, X.; Springer, T.A.
Deposited on : 2015-12-18
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

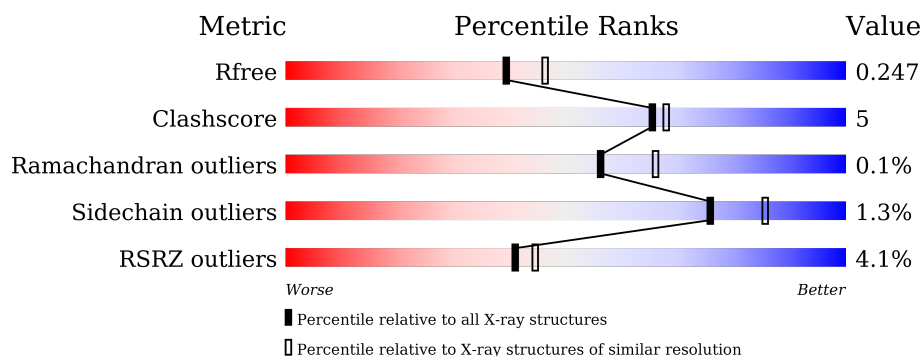
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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>4%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
2	B	257	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>

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
9	PEG	B	2004	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7099 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	591	Total	C	N	O	S	0	0	0
			4580	2904	778	877	21			

There are 6 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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1941	1240	311	379	11			

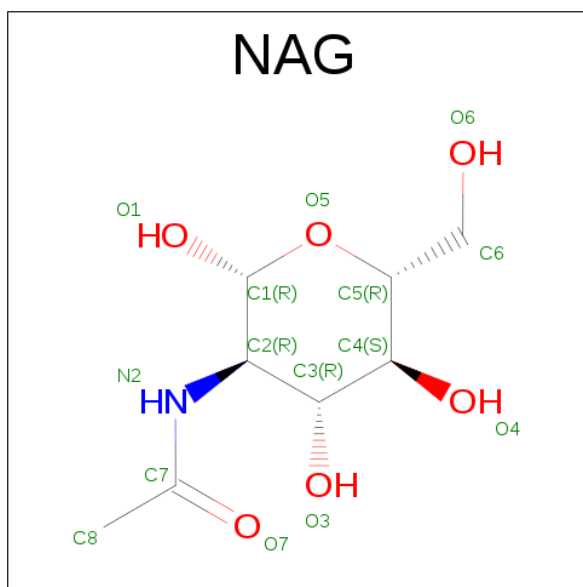
There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	4	Total	Ca	0	0
			4	4		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



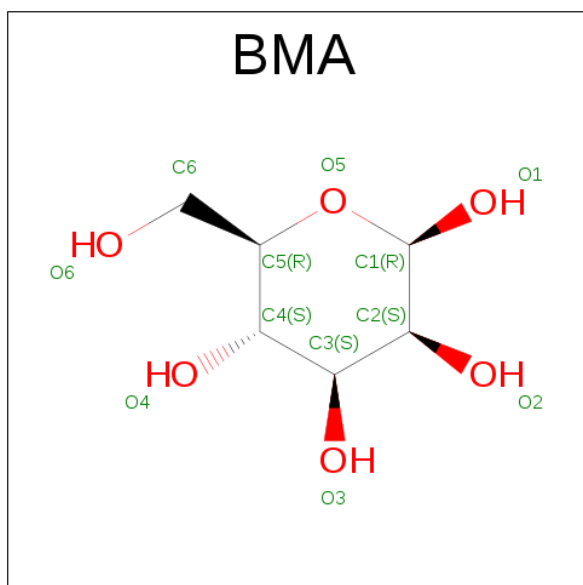
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1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

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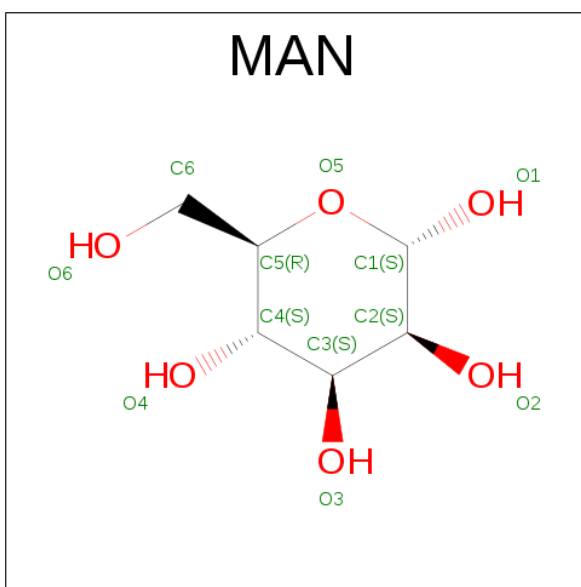
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



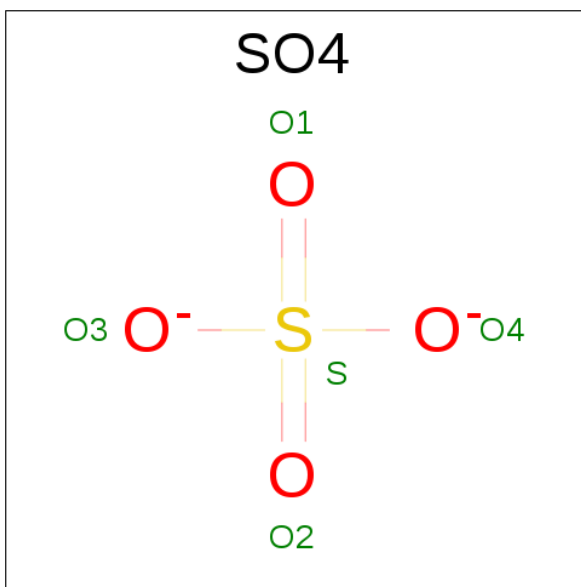
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



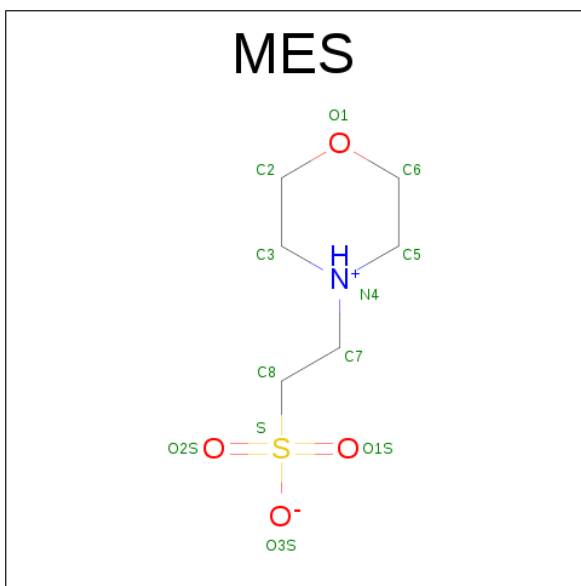
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



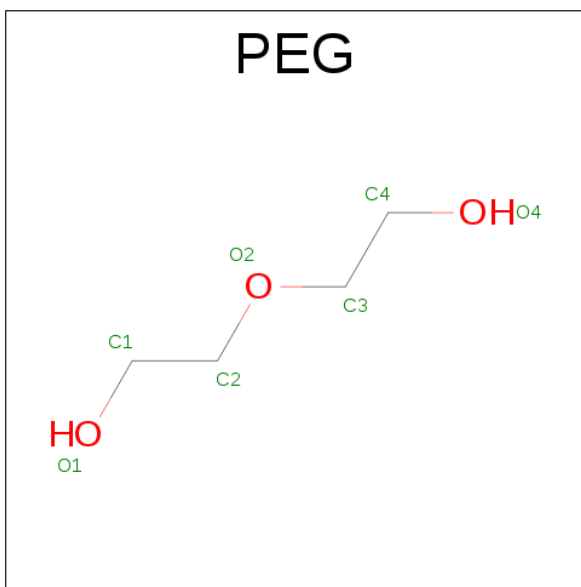
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0
			12	6	1	4	1	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		

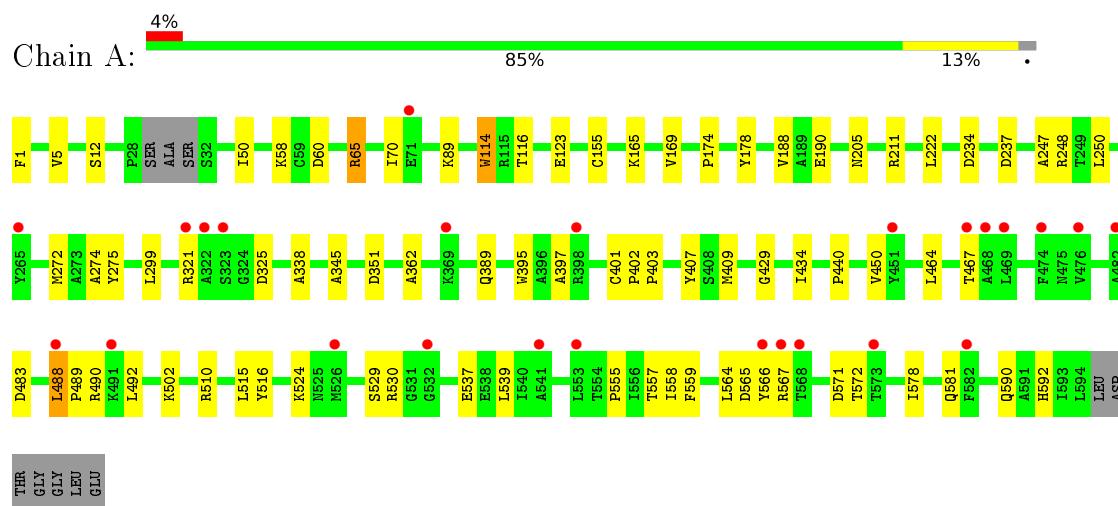
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	168	Total	O	0	0
			168	168		
10	B	73	Total	O	0	0
			73	73		

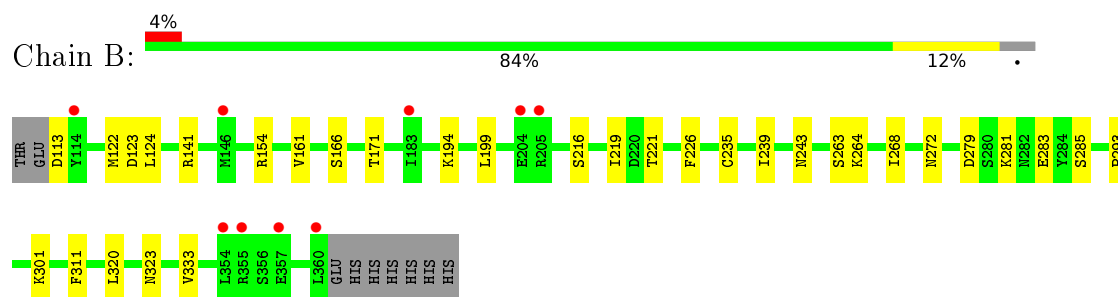
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Integrin alpha-V



• Molecule 2: Integrin beta-6



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.59Å 77.56Å 59.07Å 90.00° 101.46° 90.00°	Depositor
Resolution (Å)	46.99 – 2.25 46.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.99-2.25) 98.5 (46.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.208 , 0.246 0.207 , 0.247	Depositor DCC
R_{free} test set	905 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7099	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, SO4, MES, PEG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	1/4683 (0.0%)	0.46	0/6338
2	B	0.26	0/1980	0.45	0/2685
All	All	0.27	1/6663 (0.0%)	0.46	0/9023

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	GLU	C-N	5.22	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4580	0	4428	48	0
2	B	1941	0	1917	20	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
4	A	154	0	134	3	0
4	B	14	0	13	0	0
5	A	44	0	36	0	0
6	A	88	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	5	0	0	1	0
8	A	12	0	12	0	0
9	A	7	0	10	2	0
9	B	7	0	10	0	0
10	A	168	0	0	8	0
10	B	73	0	0	2	0
All	All	7099	0	6636	67	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 5.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ARG:NH1	10:B:2101:HOH:O	2.23	0.72
1:A:440:PRO:HB2	1:A:488:LEU:HD12	1.71	0.71
2:B:113:ASP:N	10:B:2102:HOH:O	2.27	0.68
1:A:397:ALA:HB2	1:A:403:PRO:HD3	1.76	0.67
1:A:488:LEU:HD21	1:A:492:LEU:HD21	1.78	0.66
1:A:165:LYS:NZ	1:A:237:ASP:OD1	2.29	0.63
1:A:321:ARG:HD3	1:A:325:ASP:HB2	1.81	0.63
1:A:211:ARG:NH1	10:A:2110:HOH:O	2.36	0.59
2:B:263:SER:HB2	2:B:268:ILE:HB	1.85	0.58
1:A:450:VAL:HG21	1:A:558:ILE:HD13	1.87	0.57
1:A:524:LYS:NZ	1:A:537:GLU:OE1	2.32	0.57
2:B:161:VAL:HG21	2:B:216:SER:HB3	1.87	0.57
1:A:467:THR:OG1	10:A:2101:HOH:O	2.17	0.56
1:A:248:ARG:HE	2:B:320:LEU:HB2	1.70	0.55
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.91	0.53
1:A:58:LYS:HB2	1:A:70:ILE:HD11	1.91	0.52
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.92	0.52
1:A:407:TYR:OH	2:B:264:LYS:NZ	2.32	0.51
2:B:154:ARG:HE	2:B:199:LEU:HD12	1.77	0.50
1:A:539:LEU:HD11	9:A:2030:PEG:H32	1.93	0.50
1:A:169:VAL:HG23	1:A:188:VAL:HG12	1.92	0.50
1:A:488:LEU:HG	1:A:489:PRO:HD2	1.92	0.50
2:B:279:ASP:O	2:B:281:LYS:N	2.37	0.49
2:B:279:ASP:HB3	2:B:285:SER:HB3	1.94	0.49
1:A:464:LEU:HD23	1:A:515:LEU:HD12	1.95	0.48
1:A:566:TYR:CE1	1:A:578:ILE:HA	2.48	0.48
1:A:114:TRP:CZ2	1:A:116:THR:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:LYS:HG2	2:B:283:GLU:HG2	1.96	0.48
1:A:1:PHE:CD1	1:A:581:GLN:HG2	2.49	0.48
1:A:190:GLU:OE1	1:A:205:ASN:N	2.36	0.47
1:A:345:ALA:HB2	1:A:409:MET:HG3	1.94	0.47
2:B:226:PHE:HB3	2:B:293:PRO:HG2	1.96	0.47
1:A:395:TRP:CH2	1:A:434:ILE:HG12	2.50	0.47
2:B:166:SER:HB2	2:B:171:THR:HG21	1.96	0.47
2:B:235:CYS:HB2	2:B:239:ILE:HD13	1.97	0.46
2:B:272:ASN:HD22	2:B:293:PRO:HD3	1.80	0.46
2:B:311:PHE:HB2	2:B:333:VAL:HG22	1.97	0.46
1:A:338:ALA:HB1	1:A:362:ALA:HB1	1.97	0.46
1:A:502:LYS:N	10:A:2104:HOH:O	2.48	0.46
1:A:234:ASP:CG	10:A:2102:HOH:O	2.54	0.45
1:A:272:MET:HG3	2:B:323:ASN:HB3	1.98	0.45
1:A:571:ASP:OD1	1:A:572:THR:N	2.45	0.45
1:A:488:LEU:HD23	1:A:489:PRO:O	2.16	0.45
4:A:2011:NAG:H81	10:A:2152:HOH:O	2.17	0.45
1:A:567:ARG:NH2	10:A:2114:HOH:O	2.40	0.45
1:A:557:THR:HA	1:A:590:GLN:HA	1.99	0.44
1:A:559:PHE:CE1	4:A:2027:NAG:H82	2.53	0.44
1:A:274:ALA:HA	1:A:299:LEU:HB2	2.00	0.43
2:B:219:ILE:HG22	2:B:221:THR:H	1.84	0.43
1:A:351:ASP:N	1:A:351:ASP:OD1	2.52	0.42
1:A:557:THR:HB	10:A:2104:HOH:O	2.19	0.42
1:A:247:ALA:O	1:A:250:LEU:HB2	2.19	0.42
1:A:490:ARG:O	1:A:529:SER:HA	2.19	0.42
2:B:124:LEU:HD23	2:B:124:LEU:HA	1.80	0.42
4:A:2016:NAG:H83	10:A:2247:HOH:O	2.20	0.42
1:A:174:PRO:HA	1:A:222:LEU:O	2.20	0.42
1:A:1:PHE:CE1	1:A:581:GLN:HG2	2.55	0.41
2:B:301:LYS:HD3	2:B:301:LYS:HA	1.88	0.41
2:B:122:MET:HG2	2:B:123:ASP:O	2.20	0.41
1:A:402:PRO:O	1:A:429:GLY:HA3	2.19	0.41
1:A:564:LEU:HB3	1:A:566:TYR:CE1	2.56	0.41
1:A:510:ARG:NH2	7:A:2028:SO4:O2	2.41	0.41
1:A:516:TYR:HB2	9:A:2030:PEG:H22	2.02	0.41
1:A:483:ASP:HA	1:A:530:ARG:HB2	2.03	0.41
1:A:565:ASP:C	1:A:567:ARG:H	2.24	0.41
1:A:555:PRO:HB3	1:A:592:HIS:CE1	2.56	0.40
1:A:12:SER:H	1:A:65:ARG:HE	1.70	0.40

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	587/601 (98%)	565 (96%)	21 (4%)	1 (0%)	52	61
2	B	246/257 (96%)	234 (95%)	12 (5%)	0	100	100
All	All	833/858 (97%)	799 (96%)	33 (4%)	1 (0%)	56	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/491 (99%)	476 (98%)	8 (2%)	68	79
2	B	221/230 (96%)	220 (100%)	1 (0%)	92	95
All	All	705/721 (98%)	696 (99%)	9 (1%)	76	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	60	ASP
1	A	114	TRP
1	A	155	CYS
1	A	178	TYR

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Mol	Chain	Res	Type
1	A	275	TYR
1	A	401	CYS
1	A	488	LEU
2	B	243	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 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	$\# Z > 2$
4	NAG	A	2005	1,4	14,14,15	0.53	0	15,19,21	0.41	0
4	NAG	A	2006	4	14,14,15	0.23	0	15,19,21	0.48	0
4	NAG	A	2007	1,4	14,14,15	0.21	0	15,19,21	0.43	0
4	NAG	A	2008	5,4	14,14,15	0.21	0	15,19,21	0.26	0
5	BMA	A	2009	4	11,11,12	0.60	0	15,15,17	0.80	0
4	NAG	A	2010	1,4	14,14,15	0.30	0	15,19,21	0.29	0
4	NAG	A	2011	5,4	14,14,15	0.35	0	15,19,21	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	A	2012	4,6	11,11,12	0.78	1 (9%)	15,15,17	0.87	0
6	MAN	A	2013	5	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
6	MAN	A	2014	5,6	11,11,12	1.01	1 (9%)	15,15,17	0.89	0
6	MAN	A	2015	6	11,11,12	0.75	0	15,15,17	0.98	1 (6%)
4	NAG	A	2016	1,4	14,14,15	0.31	0	15,19,21	0.35	0
4	NAG	A	2017	5,4	14,14,15	0.25	0	15,19,21	0.37	0
5	BMA	A	2018	4	11,11,12	0.60	0	15,15,17	0.87	0
4	NAG	A	2019	1,4	14,14,15	0.25	0	15,19,21	0.50	0
4	NAG	A	2020	5,4	14,14,15	0.31	0	15,19,21	0.44	0
5	BMA	A	2021	4,6	11,11,12	0.83	0	15,15,17	0.71	0
6	MAN	A	2022	5,6	11,11,12	0.85	0	15,15,17	1.06	2 (13%)
6	MAN	A	2023	6	11,11,12	0.62	0	15,15,17	1.08	2 (13%)
6	MAN	A	2024	6	11,11,12	0.75	0	15,15,17	1.07	2 (13%)
6	MAN	A	2025	5,6	11,11,12	2.10	3 (27%)	15,15,17	2.02	5 (33%)
6	MAN	A	2026	6	11,11,12	0.91	1 (9%)	15,15,17	1.60	4 (26%)
4	NAG	A	2027	1	14,14,15	0.30	0	15,19,21	0.25	0
7	SO4	A	2028	-	4,4,4	0.24	0	6,6,6	0.08	0
8	MES	A	2029	-	12,12,12	2.14	1 (8%)	15,16,16	2.40	5 (33%)
9	PEG	A	2030	-	6,6,6	0.63	0	5,5,5	0.69	0
4	NAG	B	2003	2	14,14,15	0.22	0	15,19,21	0.32	0
9	PEG	B	2004	-	6,6,6	0.64	0	5,5,5	0.69	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
4	NAG	A	2005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2006	4	-	0/6/23/26	0/1/1/1
4	NAG	A	2007	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2008	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	2009	4	-	0/2/19/22	0/1/1/1
4	NAG	A	2010	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2011	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	2012	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	2013	5	-	0/2/19/22	0/1/1/1
6	MAN	A	2014	5,6	-	0/2/19/22	0/1/1/1
6	MAN	A	2015	6	-	0/2/19/22	0/1/1/1
4	NAG	A	2016	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2017	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	2018	4	-	0/2/19/22	0/1/1/1
4	NAG	A	2019	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2020	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	2021	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	2022	5,6	-	0/2/19/22	0/1/1/1
6	MAN	A	2023	6	-	0/2/19/22	0/1/1/1
6	MAN	A	2024	6	-	0/2/19/22	0/1/1/1
6	MAN	A	2025	5,6	-	0/2/19/22	0/1/1/1
6	MAN	A	2026	6	-	0/2/19/22	0/1/1/1
4	NAG	A	2027	1	-	0/6/23/26	0/1/1/1
7	SO4	A	2028	-	-	0/0/0/0	0/0/0/0
8	MES	A	2029	-	-	0/6/14/14	0/1/1/1
9	PEG	A	2030	-	-	0/4/4/4	0/0/0/0
4	NAG	B	2003	2	-	0/6/23/26	0/1/1/1
9	PEG	B	2004	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2029	MES	C8-S	-7.13	1.66	1.77
6	A	2014	MAN	O5-C1	-2.34	1.39	1.43
5	A	2012	BMA	O5-C1	-2.14	1.40	1.43
6	A	2026	MAN	C1-C2	2.19	1.57	1.52
6	A	2025	MAN	C1-C2	2.56	1.58	1.52
6	A	2025	MAN	O2-C2	3.56	1.51	1.43
6	A	2025	MAN	C2-C3	4.73	1.58	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2029	MES	C6-C5-N4	-2.74	105.92	110.11
6	A	2013	MAN	O2-C2-C3	-2.51	105.12	110.19
6	A	2023	MAN	O2-C2-C3	-2.40	105.35	110.19
6	A	2026	MAN	O2-C2-C3	-2.22	105.71	110.19
6	A	2024	MAN	O2-C2-C3	-2.21	105.73	110.19
6	A	2022	MAN	O2-C2-C3	-2.05	106.05	110.19
6	A	2015	MAN	O2-C2-C3	-2.04	106.08	110.19
6	A	2024	MAN	C1-O5-C5	2.16	115.31	112.14
6	A	2022	MAN	C1-O5-C5	2.25	115.44	112.14
6	A	2025	MAN	O3-C3-C2	2.31	114.25	110.01
6	A	2013	MAN	C1-O5-C5	2.39	115.65	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2023	MAN	C1-O5-C5	2.43	115.72	112.14
6	A	2025	MAN	O2-C2-C1	2.46	114.16	109.23
6	A	2025	MAN	C1-C2-C3	2.57	112.67	109.55
8	A	2029	MES	C7-N4-C5	2.71	117.15	111.25
6	A	2026	MAN	C1-O5-C5	2.81	116.27	112.14
6	A	2026	MAN	O5-C1-C2	2.82	115.41	110.89
6	A	2026	MAN	C1-C2-C3	3.04	113.24	109.55
6	A	2025	MAN	O5-C1-C2	3.28	116.13	110.89
8	A	2029	MES	O1S-S-C8	3.97	109.67	106.87
8	A	2029	MES	C5-N4-C3	4.23	118.34	108.87
8	A	2029	MES	O2S-S-C8	4.34	109.93	106.87
6	A	2025	MAN	C1-O5-C5	5.06	119.58	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2011	NAG	1	0
4	A	2016	NAG	1	0
4	A	2027	NAG	1	0
7	A	2028	SO4	1	0
9	A	2030	PEG	2	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	591/601 (98%)	0.44	25 (4%) 40 44	32, 68, 100, 158	0
2	B	248/257 (96%)	0.29	9 (3%) 46 50	29, 51, 89, 138	0
All	All	839/858 (97%)	0.40	34 (4%) 41 44	29, 63, 100, 158	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	TYR	8.4
1	A	488	LEU	6.7
1	A	582	PHE	6.2
1	A	469	LEU	5.8
1	A	553	LEU	4.9
1	A	568	THR	4.6
1	A	567	ARG	4.5
1	A	451	TYR	4.1
1	A	468	ALA	3.5
1	A	398	ARG	3.3
2	B	114	TYR	3.0
1	A	491	LYS	3.0
1	A	265	TYR	2.9
2	B	360	LEU	2.7
1	A	541	ALA	2.7
1	A	482	ALA	2.6
2	B	183	ILE	2.6
1	A	321	ARG	2.5
1	A	467	THR	2.5
1	A	532	GLY	2.5
1	A	476	VAL	2.4
1	A	322	ALA	2.4
2	B	354	LEU	2.2
2	B	205	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	369	LYS	2.2
1	A	71	GLU	2.2
1	A	474	PHE	2.2
1	A	526	MET	2.1
2	B	204	GLU	2.1
1	A	323	SER	2.1
1	A	573	THR	2.0
2	B	357	GLU	2.0
2	B	146	MET	2.0
2	B	355	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	PEG	B	2004	7/7	0.86	0.27	4.45	82,84,88,89	0
4	NAG	A	2027	14/15	0.83	0.20	1.51	73,92,96,100	0
8	MES	A	2029	12/12	0.94	0.22	1.24	51,79,98,98	0
6	MAN	A	2023	11/12	0.92	0.22	0.67	74,83,96,101	0
4	NAG	A	2016	14/15	0.91	0.17	-0.02	51,67,97,101	0
4	NAG	A	2007	14/15	0.92	0.16	-0.14	62,80,91,92	0
4	NAG	A	2011	14/15	0.97	0.12	-0.24	30,43,48,54	0
4	NAG	A	2010	14/15	0.94	0.14	-0.43	35,48,59,62	0
4	NAG	A	2005	14/15	0.93	0.15	-0.67	39,61,73,75	0
4	NAG	A	2017	14/15	0.92	0.19	-0.80	76,87,100,102	0
3	CA	A	2004	1/1	0.92	0.10	-1.05	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	B	2001	1/1	0.99	0.08	-1.26	39,39,39,39	0
3	CA	A	2002	1/1	0.88	0.09	-1.87	58,58,58,58	0
3	CA	A	2001	1/1	0.94	0.06	-2.10	49,49,49,49	0
3	CA	B	2002	1/1	0.97	0.07	-2.33	53,53,53,53	1
3	CA	A	2003	1/1	0.86	0.06	-2.70	55,55,55,55	0
4	NAG	A	2006	14/15	0.85	0.18	-	86,98,101,106	0
6	MAN	A	2015	11/12	0.73	0.30	-	108,112,122,123	0
5	BMA	A	2021	11/12	0.88	0.21	-	100,107,118,130	0
4	NAG	A	2020	14/15	0.92	0.22	-	88,96,99,100	0
4	NAG	A	2019	14/15	0.89	0.20	-	57,75,90,96	0
5	BMA	A	2018	11/12	0.72	0.20	-	96,105,109,110	0
5	BMA	A	2012	11/12	0.94	0.12	-	47,57,76,90	0
6	MAN	A	2026	11/12	0.31	0.34	-	116,127,139,142	0
4	NAG	B	2003	14/15	0.77	0.26	-	78,94,99,103	0
6	MAN	A	2022	11/12	0.82	0.14	-	80,92,96,104	0
9	PEG	A	2030	7/7	0.69	0.22	-	63,71,80,83	0
7	SO4	A	2028	5/5	0.97	0.10	-	61,65,68,68	5
6	MAN	A	2025	11/12	0.59	0.34	-	140,145,150,152	0
5	BMA	A	2009	11/12	0.68	0.28	-	99,115,119,121	0
4	NAG	A	2008	14/15	0.90	0.21	-	84,98,109,115	0
6	MAN	A	2024	11/12	0.88	0.27	-	113,117,125,127	0
6	MAN	A	2014	11/12	0.84	0.20	-	91,98,106,107	0
6	MAN	A	2013	11/12	0.93	0.12	-	67,75,85,86	0

6.5 Other polymers

There are no such residues in this entry.