



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 9, 2019 – 04:59 PM EST

PDB ID : 6N4Y
Title : Metabotropic Glutamate Receptor 5 Extracellular Domain with Nb43
Authors : Koehl, A.; Hu, H.; Feng, D.; Sun, B.; Chu, M.; Weis, W.I.; Mathiesen, J.M.;
Skinotis, G.; Kobilka, B.K.
Deposited on : 2018-11-20
Resolution : 3.26 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

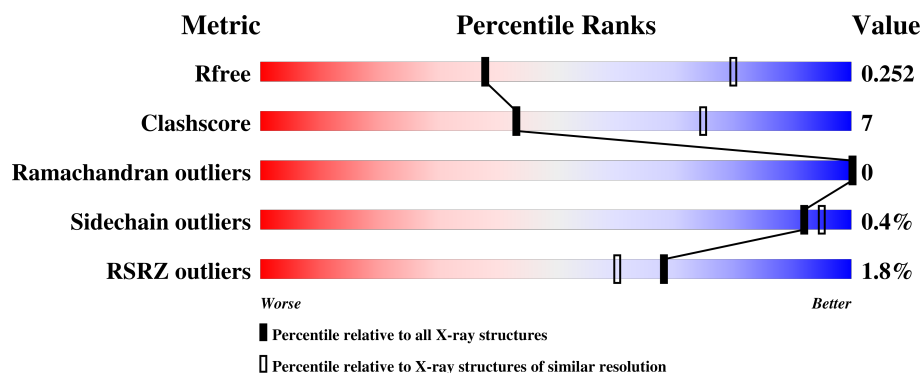
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	111664	1008 (3.30-3.22)
Clashscore	122126	1066 (3.30-3.22)
Ramachandran outliers	120053	1046 (3.30-3.22)
Sidechain outliers	120020	1045 (3.30-3.22)
RSRZ outliers	108989	1993 (3.32-3.20)

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	596	<div> <div>69%</div> <div>15%</div> <div>15%</div> </div>
1	B	596	<div> <div>2%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div>
1	C	596	<div> <div>2%</div> <div>68%</div> <div>12%</div> <div>19%</div> </div>
1	D	596	<div> <div>71%</div> <div>14%</div> <div>14%</div> </div>
2	E	123	<div> <div>3%</div> <div>87%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	123	<div> <div></div> <div>86%</div> <div>14%</div> </div>
2	G	123	<div> <div></div> <div>83%</div> <div>17%</div> </div>
2	H	123	<div> <div></div> <div>78%</div> <div>19%</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
3	NAG	A	601	-	-	-	X
4	FUC	A	604	-	-	-	X
6	MAN	B	604	-	-	-	X
6	MAN	B	607	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19626 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 Metabotropic glutamate receptor 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			3937	2485	671	745	36			
1	B	517	Total	C	N	O	S	0	0	0
			4018	2537	689	754	38			
1	C	480	Total	C	N	O	S	0	0	0
			3737	2363	638	702	34			
1	D	511	Total	C	N	O	S	0	0	0
			3947	2490	671	748	38			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P41594
A	-15	LEU	-	expression tag	UNP P41594
A	-14	LEU	-	expression tag	UNP P41594
A	-13	VAL	-	expression tag	UNP P41594
A	-12	ASN	-	expression tag	UNP P41594
A	-11	GLN	-	expression tag	UNP P41594
A	-10	SER	-	expression tag	UNP P41594
A	-9	HIS	-	expression tag	UNP P41594
A	-8	GLN	-	expression tag	UNP P41594
A	-7	GLY	-	expression tag	UNP P41594
A	-6	PHE	-	expression tag	UNP P41594
A	-5	ASN	-	expression tag	UNP P41594
A	-4	LYS	-	expression tag	UNP P41594
A	-3	GLU	-	expression tag	UNP P41594
A	-2	HIS	-	expression tag	UNP P41594
A	-1	THR	-	expression tag	UNP P41594
A	0	SER	-	expression tag	UNP P41594
A	1	LYS	-	expression tag	UNP P41594
A	2	MET	-	expression tag	UNP P41594
A	3	VAL	-	expression tag	UNP P41594
A	4	SER	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	-	expression tag	UNP P41594
A	6	ILE	-	expression tag	UNP P41594
A	7	VAL	-	expression tag	UNP P41594
A	8	LEU	-	expression tag	UNP P41594
A	9	TYR	-	expression tag	UNP P41594
A	10	VAL	-	expression tag	UNP P41594
A	11	LEU	-	expression tag	UNP P41594
A	12	LEU	-	expression tag	UNP P41594
A	13	ALA	-	expression tag	UNP P41594
A	14	ALA	-	expression tag	UNP P41594
A	15	ALA	-	expression tag	UNP P41594
A	16	ALA	-	expression tag	UNP P41594
A	17	HIS	-	expression tag	UNP P41594
A	18	SER	-	expression tag	UNP P41594
A	19	ALA	-	expression tag	UNP P41594
A	20	PHE	-	expression tag	UNP P41594
A	572	HIS	-	expression tag	UNP P41594
A	573	HIS	-	expression tag	UNP P41594
A	574	HIS	-	expression tag	UNP P41594
A	575	HIS	-	expression tag	UNP P41594
A	576	HIS	-	expression tag	UNP P41594
A	577	HIS	-	expression tag	UNP P41594
A	578	HIS	-	expression tag	UNP P41594
A	579	HIS	-	expression tag	UNP P41594
B	-16	MET	-	initiating methionine	UNP P41594
B	-15	LEU	-	expression tag	UNP P41594
B	-14	LEU	-	expression tag	UNP P41594
B	-13	VAL	-	expression tag	UNP P41594
B	-12	ASN	-	expression tag	UNP P41594
B	-11	GLN	-	expression tag	UNP P41594
B	-10	SER	-	expression tag	UNP P41594
B	-9	HIS	-	expression tag	UNP P41594
B	-8	GLN	-	expression tag	UNP P41594
B	-7	GLY	-	expression tag	UNP P41594
B	-6	PHE	-	expression tag	UNP P41594
B	-5	ASN	-	expression tag	UNP P41594
B	-4	LYS	-	expression tag	UNP P41594
B	-3	GLU	-	expression tag	UNP P41594
B	-2	HIS	-	expression tag	UNP P41594
B	-1	THR	-	expression tag	UNP P41594
B	0	SER	-	expression tag	UNP P41594
B	1	LYS	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	expression tag	UNP P41594
B	3	VAL	-	expression tag	UNP P41594
B	4	SER	-	expression tag	UNP P41594
B	5	ALA	-	expression tag	UNP P41594
B	6	ILE	-	expression tag	UNP P41594
B	7	VAL	-	expression tag	UNP P41594
B	8	LEU	-	expression tag	UNP P41594
B	9	TYR	-	expression tag	UNP P41594
B	10	VAL	-	expression tag	UNP P41594
B	11	LEU	-	expression tag	UNP P41594
B	12	LEU	-	expression tag	UNP P41594
B	13	ALA	-	expression tag	UNP P41594
B	14	ALA	-	expression tag	UNP P41594
B	15	ALA	-	expression tag	UNP P41594
B	16	ALA	-	expression tag	UNP P41594
B	17	HIS	-	expression tag	UNP P41594
B	18	SER	-	expression tag	UNP P41594
B	19	ALA	-	expression tag	UNP P41594
B	20	PHE	-	expression tag	UNP P41594
B	572	HIS	-	expression tag	UNP P41594
B	573	HIS	-	expression tag	UNP P41594
B	574	HIS	-	expression tag	UNP P41594
B	575	HIS	-	expression tag	UNP P41594
B	576	HIS	-	expression tag	UNP P41594
B	577	HIS	-	expression tag	UNP P41594
B	578	HIS	-	expression tag	UNP P41594
B	579	HIS	-	expression tag	UNP P41594
C	-16	MET	-	initiating methionine	UNP P41594
C	-15	LEU	-	expression tag	UNP P41594
C	-14	LEU	-	expression tag	UNP P41594
C	-13	VAL	-	expression tag	UNP P41594
C	-12	ASN	-	expression tag	UNP P41594
C	-11	GLN	-	expression tag	UNP P41594
C	-10	SER	-	expression tag	UNP P41594
C	-9	HIS	-	expression tag	UNP P41594
C	-8	GLN	-	expression tag	UNP P41594
C	-7	GLY	-	expression tag	UNP P41594
C	-6	PHE	-	expression tag	UNP P41594
C	-5	ASN	-	expression tag	UNP P41594
C	-4	LYS	-	expression tag	UNP P41594
C	-3	GLU	-	expression tag	UNP P41594
C	-2	HIS	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	THR	-	expression tag	UNP P41594
C	0	SER	-	expression tag	UNP P41594
C	1	LYS	-	expression tag	UNP P41594
C	2	MET	-	expression tag	UNP P41594
C	3	VAL	-	expression tag	UNP P41594
C	4	SER	-	expression tag	UNP P41594
C	5	ALA	-	expression tag	UNP P41594
C	6	ILE	-	expression tag	UNP P41594
C	7	VAL	-	expression tag	UNP P41594
C	8	LEU	-	expression tag	UNP P41594
C	9	TYR	-	expression tag	UNP P41594
C	10	VAL	-	expression tag	UNP P41594
C	11	LEU	-	expression tag	UNP P41594
C	12	LEU	-	expression tag	UNP P41594
C	13	ALA	-	expression tag	UNP P41594
C	14	ALA	-	expression tag	UNP P41594
C	15	ALA	-	expression tag	UNP P41594
C	16	ALA	-	expression tag	UNP P41594
C	17	HIS	-	expression tag	UNP P41594
C	18	SER	-	expression tag	UNP P41594
C	19	ALA	-	expression tag	UNP P41594
C	20	PHE	-	expression tag	UNP P41594
C	572	HIS	-	expression tag	UNP P41594
C	573	HIS	-	expression tag	UNP P41594
C	574	HIS	-	expression tag	UNP P41594
C	575	HIS	-	expression tag	UNP P41594
C	576	HIS	-	expression tag	UNP P41594
C	577	HIS	-	expression tag	UNP P41594
C	578	HIS	-	expression tag	UNP P41594
C	579	HIS	-	expression tag	UNP P41594
D	-16	MET	-	initiating methionine	UNP P41594
D	-15	LEU	-	expression tag	UNP P41594
D	-14	LEU	-	expression tag	UNP P41594
D	-13	VAL	-	expression tag	UNP P41594
D	-12	ASN	-	expression tag	UNP P41594
D	-11	GLN	-	expression tag	UNP P41594
D	-10	SER	-	expression tag	UNP P41594
D	-9	HIS	-	expression tag	UNP P41594
D	-8	GLN	-	expression tag	UNP P41594
D	-7	GLY	-	expression tag	UNP P41594
D	-6	PHE	-	expression tag	UNP P41594
D	-5	ASN	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	LYS	-	expression tag	UNP P41594
D	-3	GLU	-	expression tag	UNP P41594
D	-2	HIS	-	expression tag	UNP P41594
D	-1	THR	-	expression tag	UNP P41594
D	0	SER	-	expression tag	UNP P41594
D	1	LYS	-	expression tag	UNP P41594
D	2	MET	-	expression tag	UNP P41594
D	3	VAL	-	expression tag	UNP P41594
D	4	SER	-	expression tag	UNP P41594
D	5	ALA	-	expression tag	UNP P41594
D	6	ILE	-	expression tag	UNP P41594
D	7	VAL	-	expression tag	UNP P41594
D	8	LEU	-	expression tag	UNP P41594
D	9	TYR	-	expression tag	UNP P41594
D	10	VAL	-	expression tag	UNP P41594
D	11	LEU	-	expression tag	UNP P41594
D	12	LEU	-	expression tag	UNP P41594
D	13	ALA	-	expression tag	UNP P41594
D	14	ALA	-	expression tag	UNP P41594
D	15	ALA	-	expression tag	UNP P41594
D	16	ALA	-	expression tag	UNP P41594
D	17	HIS	-	expression tag	UNP P41594
D	18	SER	-	expression tag	UNP P41594
D	19	ALA	-	expression tag	UNP P41594
D	20	PHE	-	expression tag	UNP P41594
D	572	HIS	-	expression tag	UNP P41594
D	573	HIS	-	expression tag	UNP P41594
D	574	HIS	-	expression tag	UNP P41594
D	575	HIS	-	expression tag	UNP P41594
D	576	HIS	-	expression tag	UNP P41594
D	577	HIS	-	expression tag	UNP P41594
D	578	HIS	-	expression tag	UNP P41594
D	579	HIS	-	expression tag	UNP P41594

- Molecule 2 is a protein called Nanobody 43.

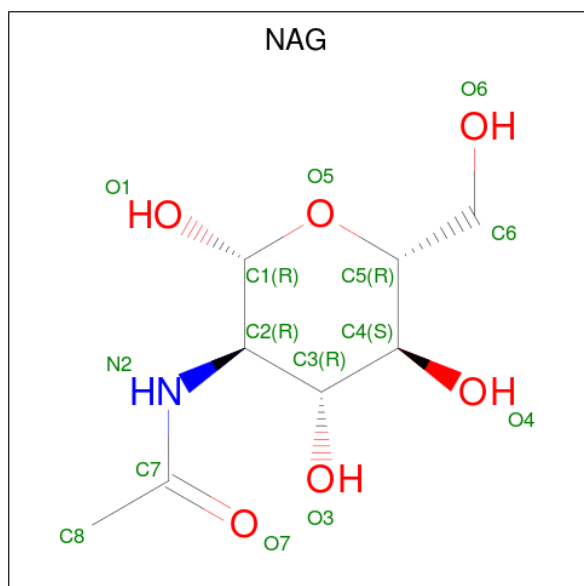
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	123	Total	C	N	O	S	0	0	0
			933	580	161	187	5			
2	F	123	Total	C	N	O	S	0	0	0
			927	577	158	187	5			
2	G	123	Total	C	N	O	S	0	0	0
			929	577	160	187	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	119	Total	C	N	O	S	0	0	0
			893	558	152	178	5			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



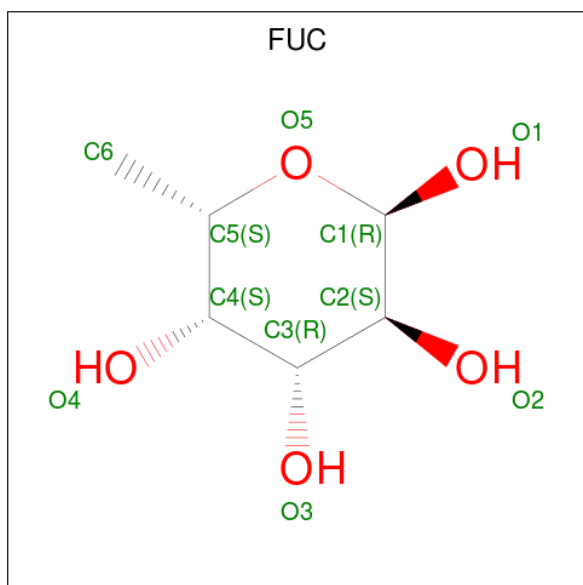
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	B	1	Total	C	N	O		0	0
			14	8	1	5			
3	B	1	Total	C	N	O		0	0
			14	8	1	5			
3	B	1	Total	C	N	O		0	0
			14	8	1	5			
3	C	1	Total	C	N	O		0	0
			14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

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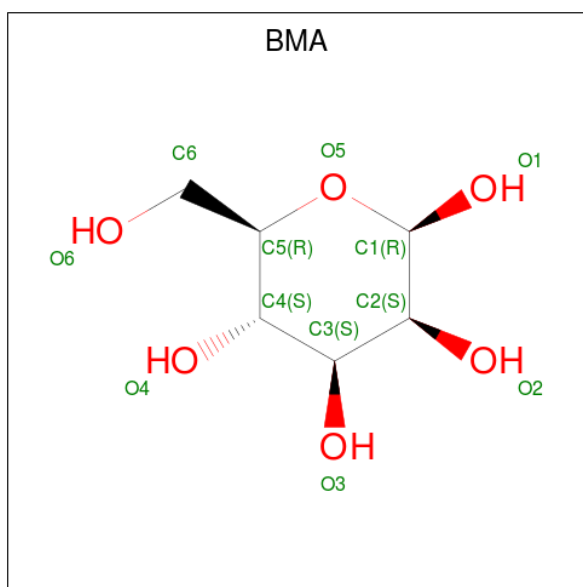
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



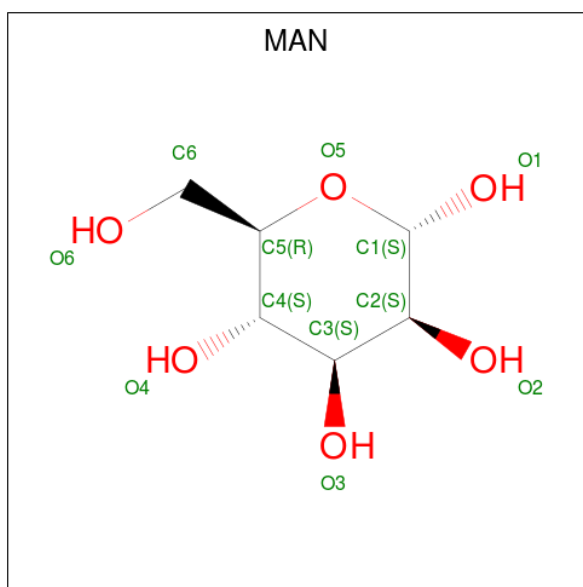
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		

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



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

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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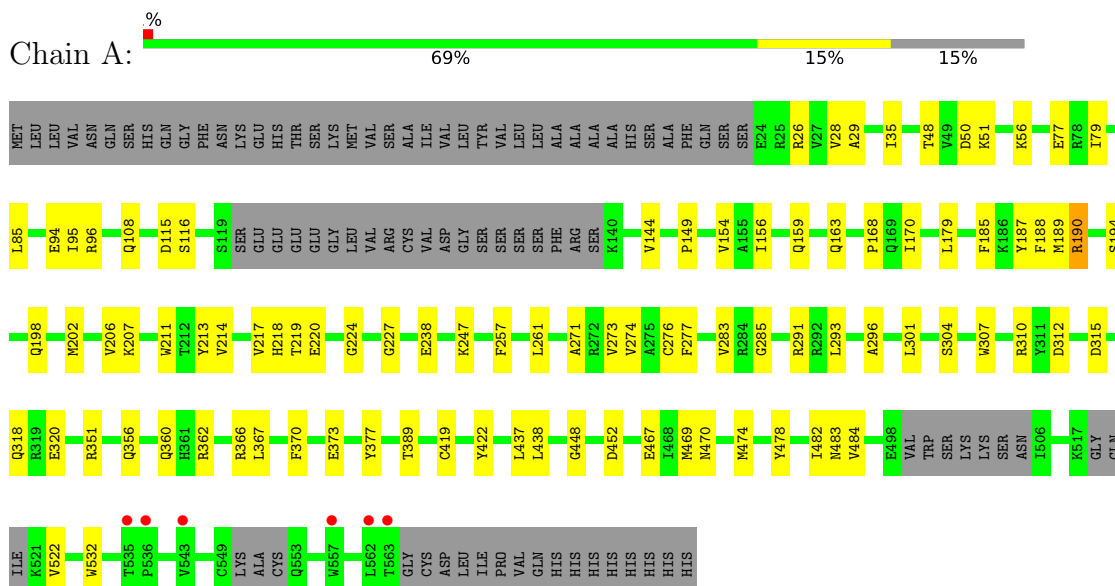
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		

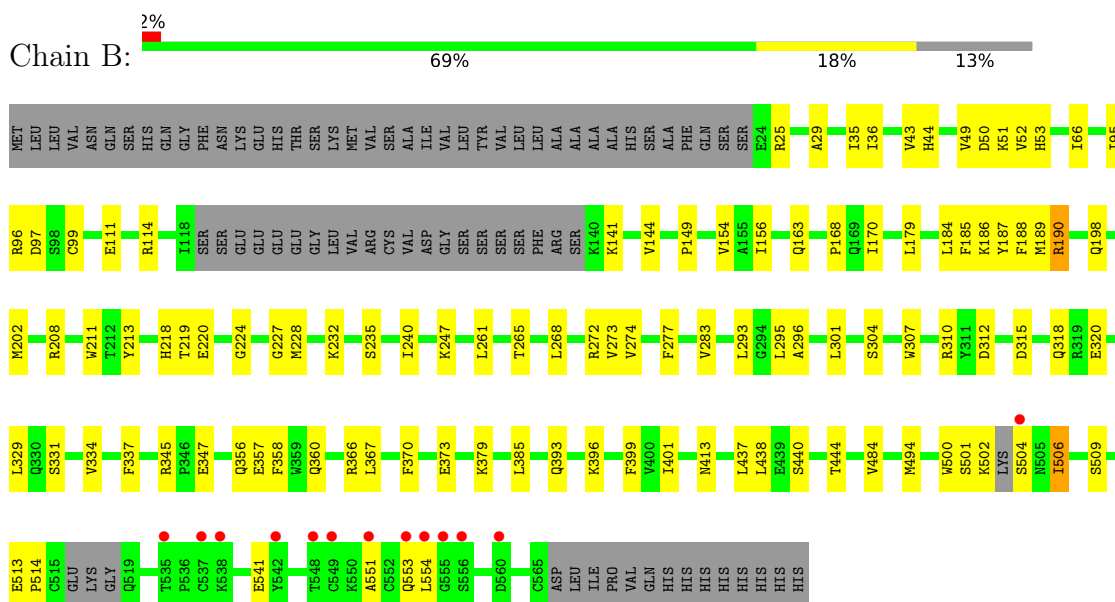
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

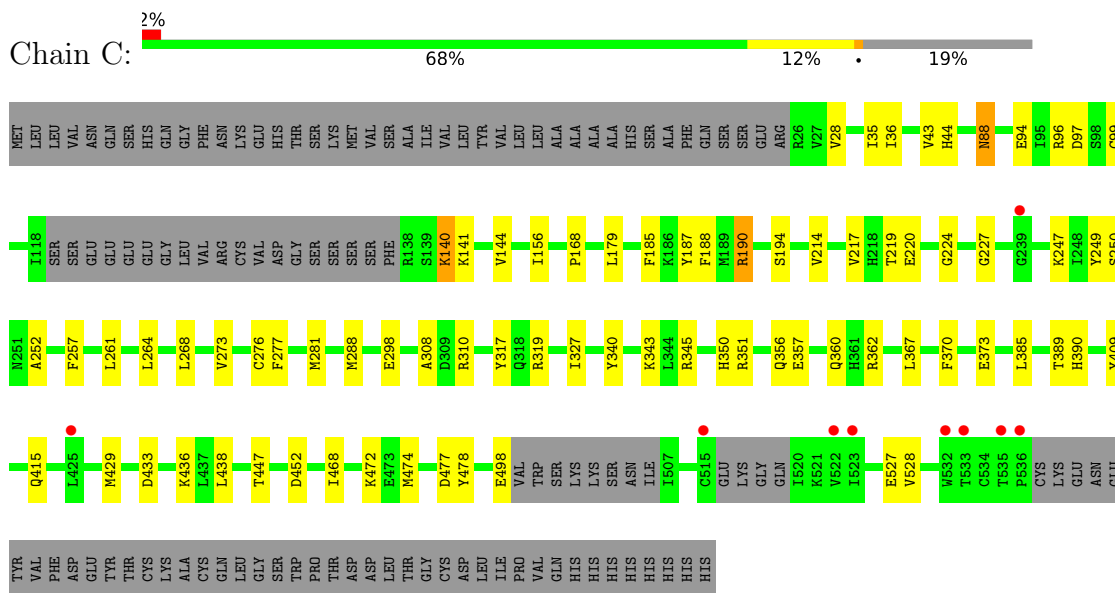
• Molecule 1: Metabotropic glutamate receptor 5



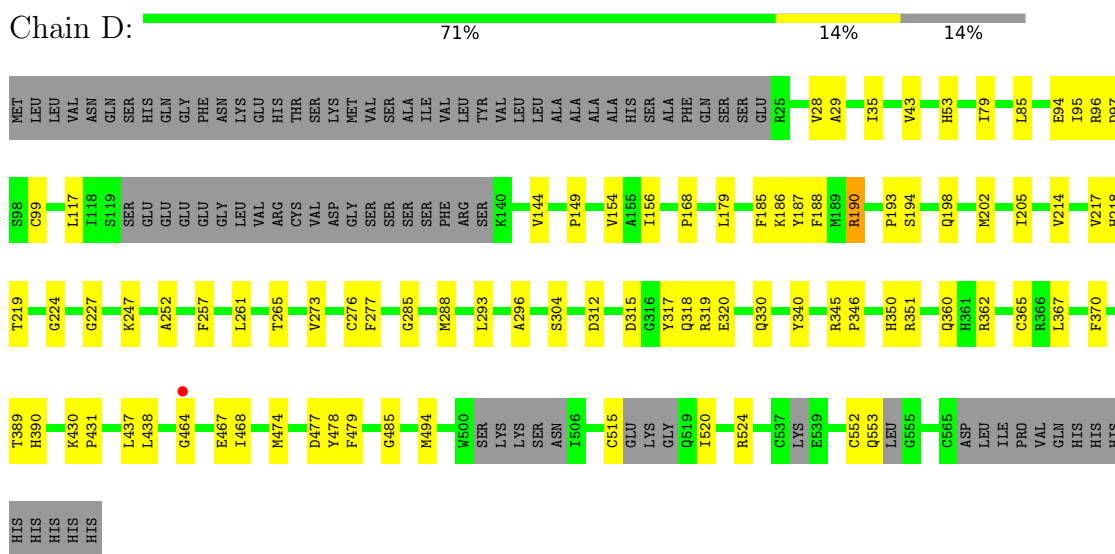
• Molecule 1: Metabotropic glutamate receptor 5



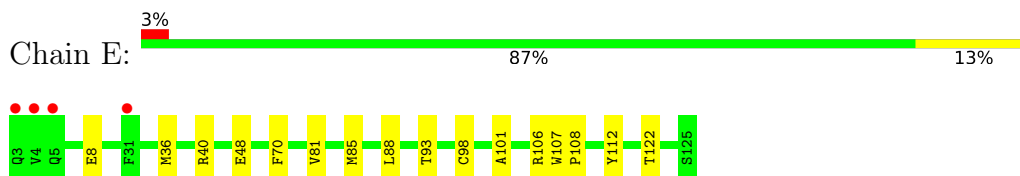
• Molecule 1: Metabotropic glutamate receptor 5



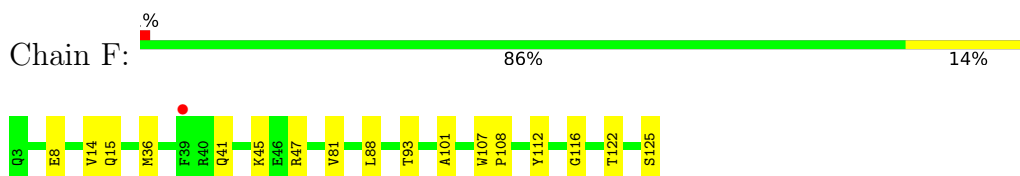
- Molecule 1: Metabotropic glutamate receptor 5



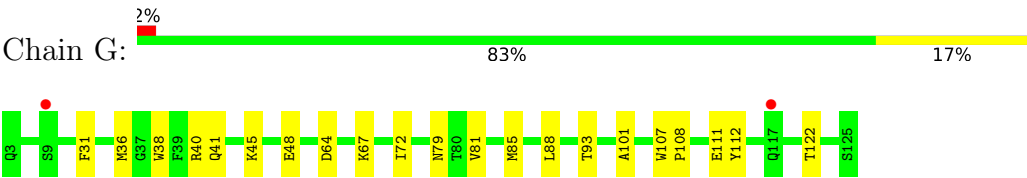
- Molecule 2: Nanobody 43



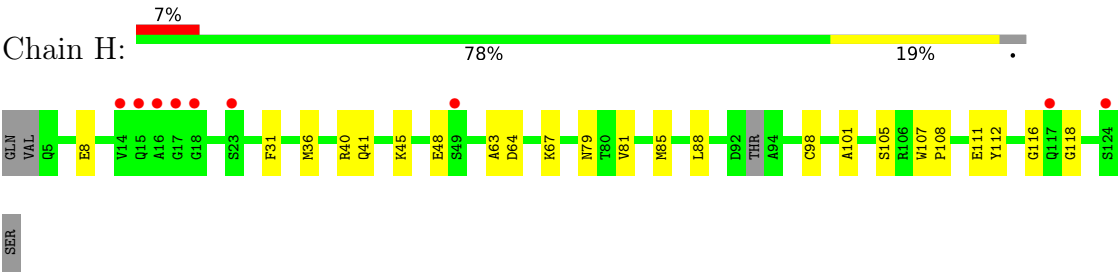
- Molecule 2: Nanobody 43



● Molecule 2: Nanobody 43



● Molecule 2: Nanobody 43



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.53Å 158.39Å 111.96Å 90.00° 101.93° 90.00°	Depositor
Resolution (Å)	38.87 – 3.26 39.60 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.87-3.26) 91.7 (39.60-3.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.199 , 0.251 0.200 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19626	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.41% 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: FUC, BMA, NAG, 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	0.26	0/4023	0.48	0/5446
1	B	0.30	0/4107	0.50	0/5560
1	C	0.25	0/3819	0.48	0/5164
1	D	0.26	0/4032	0.48	0/5457
2	E	0.27	0/955	0.50	0/1293
2	F	0.27	0/949	0.48	0/1286
2	G	0.26	0/951	0.50	0/1289
2	H	0.25	0/914	0.51	0/1238
All	All	0.27	0/19750	0.49	0/26733

There are no bond length outliers.

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	3937	0	3736	56	0
1	B	4018	0	3834	73	0
1	C	3737	0	3585	53	0
1	D	3947	0	3733	54	0
2	E	933	0	869	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	927	0	858	10	0
2	G	929	0	858	14	0
2	H	893	0	822	15	0
3	A	42	0	37	0	0
3	B	42	0	35	0	0
3	C	42	0	36	1	0
3	D	42	0	35	0	0
4	A	10	0	10	0	0
4	B	20	0	20	0	0
4	C	10	0	10	1	0
4	D	20	0	20	0	0
5	B	11	0	8	2	0
5	C	11	0	9	0	0
5	D	11	0	9	0	0
6	B	22	0	20	0	0
6	C	11	0	10	0	0
6	D	11	0	10	0	0
All	All	19626	0	18564	277	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 7.

The worst 5 of 277 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:D:345:ARG:HD3	1:D:346:PRO:HD2	1.58	0.84
1:C:472:LYS:HD2	1:C:498:GLU:HG3	1.69	0.74
1:C:268:LEU:HD11	1:C:298:GLU:HB3	1.71	0.72
1:D:515:CYS:HB3	1:D:520:ILE:HB	1.70	0.72
1:C:527:GLU:HG2	1:C:528:VAL:HG23	1.71	0.72

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	497/596 (83%)	469 (94%)	28 (6%)	0	100	100
1	B	509/596 (85%)	482 (95%)	27 (5%)	0	100	100
1	C	472/596 (79%)	449 (95%)	23 (5%)	0	100	100
1	D	499/596 (84%)	476 (95%)	23 (5%)	0	100	100
2	E	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	F	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
2	G	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
2	H	115/123 (94%)	113 (98%)	2 (2%)	0	100	100
All	All	2455/2876 (85%)	2340 (95%)	115 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	422/520 (81%)	421 (100%)	1 (0%)	94	97
1	B	432/520 (83%)	430 (100%)	2 (0%)	90	93
1	C	402/520 (77%)	399 (99%)	3 (1%)	85	91
1	D	422/520 (81%)	420 (100%)	2 (0%)	90	93
2	E	96/97 (99%)	96 (100%)	0	100	100
2	F	95/97 (98%)	95 (100%)	0	100	100
2	G	95/97 (98%)	95 (100%)	0	100	100
2	H	90/97 (93%)	90 (100%)	0	100	100
All	All	2054/2468 (83%)	2046 (100%)	8 (0%)	92	95

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	88	ASN
1	D	524	ARG
1	C	190	ARG
1	B	506	ILE
1	C	140	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	413	ASN
1	C	108	GLN
1	D	74	HIS
1	B	350	HIS
1	C	166	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

25 ligands 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	601	1	14,14,15	0.25	0	17,19,21	0.37	0
3	NAG	A	602	1,3,4	14,14,15	0.36	0	17,19,21	0.93	1 (5%)
3	NAG	A	603	3	14,14,15	0.40	0	17,19,21	0.60	0
4	FUC	A	604	3	9,10,11	1.11	0	13,14,16	1.26	1 (7%)
3	NAG	B	601	1,3,4	14,14,15	1.05	1 (7%)	17,19,21	0.75	0
3	NAG	B	602	3,5	14,14,15	0.63	1 (7%)	17,19,21	0.86	1 (5%)
5	BMA	B	603	3,6	11,11,12	1.21	1 (9%)	15,15,17	1.33	2 (13%)
6	MAN	B	604	5	11,11,12	0.73	0	15,15,17	1.00	2 (13%)
4	FUC	B	605	3	9,10,11	1.48	2 (22%)	13,14,16	1.43	3 (23%)
4	FUC	B	606	3	9,10,11	0.79	0	13,14,16	0.90	0
6	MAN	B	607	5	11,11,12	0.60	0	15,15,17	1.06	2 (13%)
3	NAG	B	608	1	14,14,15	0.51	0	17,19,21	0.59	0
3	NAG	C	601	1,3,4	14,14,15	0.33	0	17,19,21	0.81	1 (5%)
3	NAG	C	602	3,5	14,14,15	0.65	1 (7%)	17,19,21	0.63	0
5	BMA	C	603	3,6	11,11,12	0.69	0	15,15,17	0.98	1 (6%)
6	MAN	C	604	5	11,11,12	0.60	0	15,15,17	1.03	2 (13%)
4	FUC	C	605	3	9,10,11	0.71	0	13,14,16	0.82	0
3	NAG	C	606	1	14,14,15	0.62	0	17,19,21	0.62	1 (5%)
3	NAG	D	601	1,3,4	14,14,15	0.30	0	17,19,21	0.59	0
3	NAG	D	602	3,5	14,14,15	0.27	0	17,19,21	0.50	0
5	BMA	D	603	3,6	11,11,12	0.69	0	15,15,17	0.82	0
6	MAN	D	604	5	11,11,12	0.74	0	15,15,17	1.17	2 (13%)
4	FUC	D	605	3	9,10,11	0.90	1 (11%)	13,14,16	0.79	0
4	FUC	D	606	3	9,10,11	0.62	0	13,14,16	0.99	1 (7%)
3	NAG	D	607	1	14,14,15	0.50	0	17,19,21	0.52	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	601	1	-	0/6/23/26	0/1/1/1
3	NAG	A	602	1,3,4	-	2/6/23/26	0/1/1/1
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1
4	FUC	A	604	3	-	-	0/1/1/1
3	NAG	B	601	1,3,4	-	4/6/23/26	0/1/1/1
3	NAG	B	602	3,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	B	603	3,6	-	2/2/19/22	0/1/1/1
6	MAN	B	604	5	-	0/2/19/22	0/1/1/1
4	FUC	B	605	3	-	-	0/1/1/1
4	FUC	B	606	3	-	-	0/1/1/1
6	MAN	B	607	5	-	0/2/19/22	0/1/1/1
3	NAG	B	608	1	-	1/6/23/26	0/1/1/1
3	NAG	C	601	1,3,4	-	2/6/23/26	0/1/1/1
3	NAG	C	602	3,5	-	2/6/23/26	0/1/1/1
5	BMA	C	603	3,6	-	0/2/19/22	0/1/1/1
6	MAN	C	604	5	-	0/2/19/22	0/1/1/1
4	FUC	C	605	3	-	-	0/1/1/1
3	NAG	C	606	1	-	0/6/23/26	0/1/1/1
3	NAG	D	601	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	D	602	3,5	-	0/6/23/26	0/1/1/1
5	BMA	D	603	3,6	-	2/2/19/22	0/1/1/1
6	MAN	D	604	5	-	0/2/19/22	0/1/1/1
4	FUC	D	605	3	-	-	0/1/1/1
4	FUC	D	606	3	-	-	0/1/1/1
3	NAG	D	607	1	-	2/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAG	O5-C1	-3.68	1.37	1.43
4	B	605	FUC	C1-C2	2.84	1.58	1.52
5	B	603	BMA	O3-C3	2.64	1.49	1.43
4	B	605	FUC	C4-C5	2.27	1.57	1.52
3	C	602	NAG	O5-C1	-2.23	1.40	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	603	BMA	O3-C3-C2	3.48	116.49	110.02
3	A	602	NAG	C1-O5-C5	3.42	116.84	112.20
6	B	607	MAN	C1-O5-C5	3.00	116.28	112.20
6	D	604	MAN	C1-O5-C5	2.95	116.21	112.20
4	B	605	FUC	O5-C5-C4	2.90	114.28	109.61

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	603	BMA	O5-C5-C6-O6
3	D	607	NAG	O5-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
5	B	603	BMA	C4-C5-C6-O6
3	D	607	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	603	BMA	2	0
3	C	602	NAG	1	0
4	C	605	FUC	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	507/596 (85%)	-0.10	6 (1%) 79 72	43, 71, 114, 131	0
1	B	517/596 (86%)	-0.06	13 (2%) 57 49	48, 73, 118, 148	0
1	C	480/596 (80%)	-0.16	9 (1%) 66 59	46, 69, 109, 135	0
1	D	511/596 (85%)	-0.09	1 (0%) 94 94	46, 80, 123, 141	0
2	E	123/123 (100%)	0.05	4 (3%) 46 37	63, 77, 102, 121	0
2	F	123/123 (100%)	0.04	1 (0%) 86 81	62, 78, 100, 125	0
2	G	123/123 (100%)	0.03	2 (1%) 72 64	55, 78, 109, 126	0
2	H	119/123 (96%)	0.35	9 (7%) 14 10	67, 95, 122, 128	0
All	All	2503/2876 (87%)	-0.06	45 (1%) 68 60	43, 75, 116, 148	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	VAL	4.1
1	C	536	PRO	4.0
1	B	560	ASP	3.9
1	B	556	SER	3.6
1	B	549	CYS	3.4

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 ⓘ

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. 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	B-factors(Å ²)	Q<0.9
3	NAG	A	603	14/15	0.56	0.40	120,159,165,170	0
3	NAG	A	601	14/15	0.63	0.42	95,135,152,159	0
6	MAN	B	604	11/12	0.69	0.50	116,140,148,149	0
4	FUC	A	604	10/11	0.77	0.46	124,138,147,147	0
6	MAN	B	607	11/12	0.77	0.42	91,118,141,142	0
3	NAG	C	601	14/15	0.77	0.19	121,141,160,162	0
3	NAG	A	602	14/15	0.77	0.30	122,140,155,157	0
3	NAG	C	602	14/15	0.77	0.33	135,147,159,167	0
3	NAG	B	608	14/15	0.79	0.25	93,118,134,138	0
4	FUC	B	606	10/11	0.79	0.23	103,127,136,138	0
6	MAN	D	604	11/12	0.80	0.33	81,96,103,106	0
3	NAG	C	606	14/15	0.82	0.20	108,135,142,144	0
6	MAN	C	604	11/12	0.84	0.47	125,132,140,140	0
3	NAG	D	607	14/15	0.85	0.26	87,113,123,135	0
5	BMA	B	603	11/12	0.86	0.29	109,123,130,139	0
3	NAG	B	602	14/15	0.86	0.30	110,127,132,136	0
5	BMA	C	603	11/12	0.86	0.24	112,129,137,138	0
5	BMA	D	603	11/12	0.86	0.18	90,101,111,113	0
4	FUC	C	605	10/11	0.86	0.29	133,140,143,143	0
3	NAG	D	602	14/15	0.88	0.24	93,102,112,115	0
3	NAG	D	601	14/15	0.89	0.26	93,102,115,120	0
3	NAG	B	601	14/15	0.90	0.12	89,120,129,133	0
4	FUC	D	605	10/11	0.91	0.20	83,95,108,109	0
4	FUC	B	605	10/11	0.92	0.17	106,114,126,131	0
4	FUC	D	606	10/11	0.92	0.42	90,109,123,127	0

6.5 Other polymers ⓘ

There are no such residues in this entry.