



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2017 – 03:01 PM EST

PDB ID : 5V5X  
Title : Protocadherin gammaB7 EC3-6 cis-dimer structure  
Authors : Goodman, K.M.; Mannepalli, S.; Bahna, F.; Honig, B.; Shapiro, L.  
Deposited on : unknown  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345

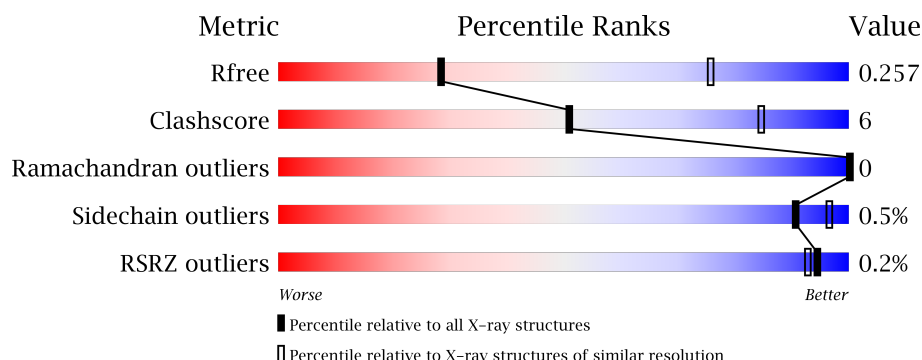
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (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  $\geq 3$ , 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	439	
1	B	439	
1	C	439	
1	D	439	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	A	714	-	-	-	X
3	MAN	A	715	-	-	-	X
3	MAN	C	714	-	-	-	X
3	MAN	C	715	-	-	-	X
4	NAG	C	716	-	-	-	X
4	NAG	D	716	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13104 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 MCG133388, isoform CRA\_y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3197	1988	550	653	6			
1	B	415	Total	C	N	O	S	0	1	0
			3102	1938	532	628	4			
1	C	415	Total	C	N	O	S	0	0	0
			3111	1943	527	636	5			
1	D	427	Total	C	N	O	S	0	0	0
			3209	1994	554	656	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	639	HIS	-	expression tag	UNP Q91XX3
A	640	HIS	-	expression tag	UNP Q91XX3
A	641	HIS	-	expression tag	UNP Q91XX3
A	642	HIS	-	expression tag	UNP Q91XX3
A	643	HIS	-	expression tag	UNP Q91XX3
A	644	HIS	-	expression tag	UNP Q91XX3
A	645	HIS	-	expression tag	UNP Q91XX3
A	646	HIS	-	expression tag	UNP Q91XX3
B	639	HIS	-	expression tag	UNP Q91XX3
B	640	HIS	-	expression tag	UNP Q91XX3
B	641	HIS	-	expression tag	UNP Q91XX3
B	642	HIS	-	expression tag	UNP Q91XX3
B	643	HIS	-	expression tag	UNP Q91XX3
B	644	HIS	-	expression tag	UNP Q91XX3
B	645	HIS	-	expression tag	UNP Q91XX3
B	646	HIS	-	expression tag	UNP Q91XX3
C	639	HIS	-	expression tag	UNP Q91XX3
C	640	HIS	-	expression tag	UNP Q91XX3
C	641	HIS	-	expression tag	UNP Q91XX3
C	642	HIS	-	expression tag	UNP Q91XX3
C	643	HIS	-	expression tag	UNP Q91XX3

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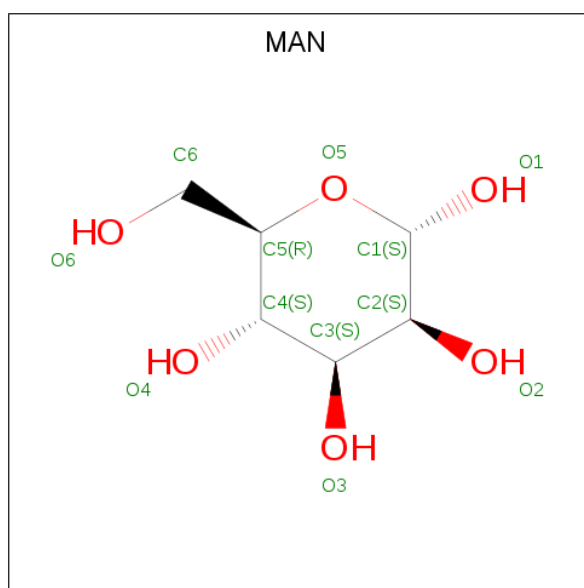
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Chain	Residue	Modelled	Actual	Comment	Reference
C	644	HIS	-	expression tag	UNP Q91XX3
C	645	HIS	-	expression tag	UNP Q91XX3
C	646	HIS	-	expression tag	UNP Q91XX3
D	639	HIS	-	expression tag	UNP Q91XX3
D	640	HIS	-	expression tag	UNP Q91XX3
D	641	HIS	-	expression tag	UNP Q91XX3
D	642	HIS	-	expression tag	UNP Q91XX3
D	643	HIS	-	expression tag	UNP Q91XX3
D	644	HIS	-	expression tag	UNP Q91XX3
D	645	HIS	-	expression tag	UNP Q91XX3
D	646	HIS	-	expression tag	UNP Q91XX3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	9	Total 9 Ca 9	0	0
2	A	9	Total 9 Ca 9	0	0
2	D	9	Total 9 Ca 9	0	0
2	C	9	Total 9 Ca 9	0	0

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



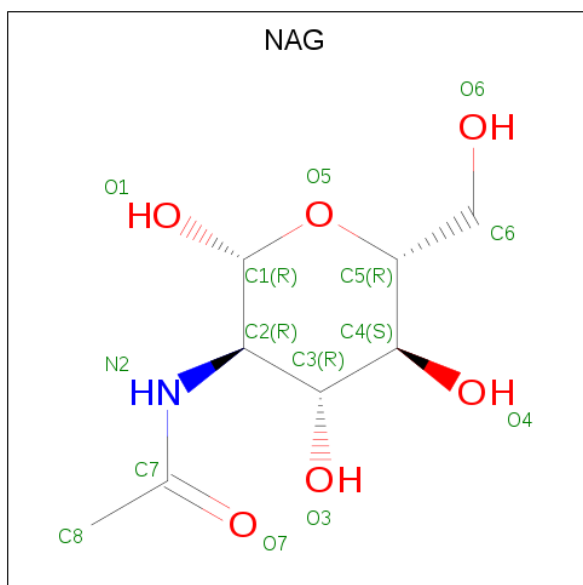
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3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

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

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



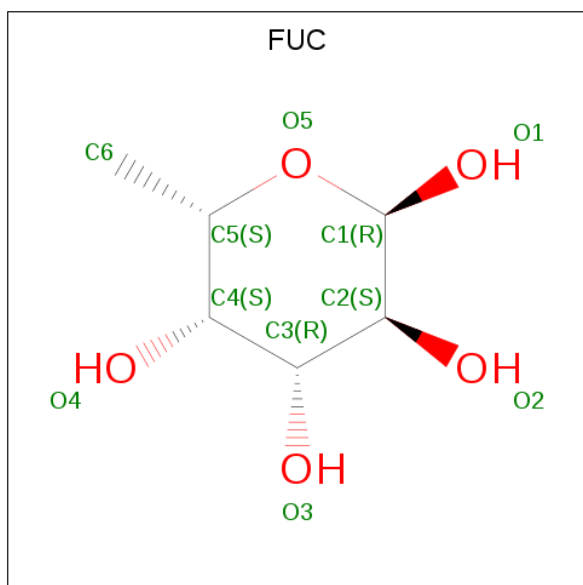
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1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

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

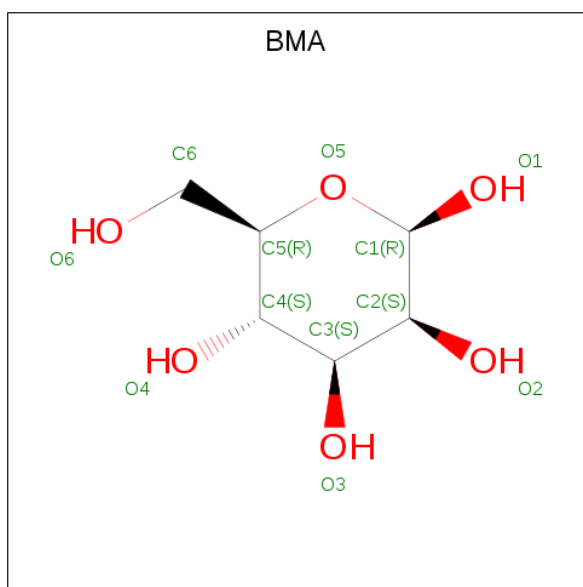
- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



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

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



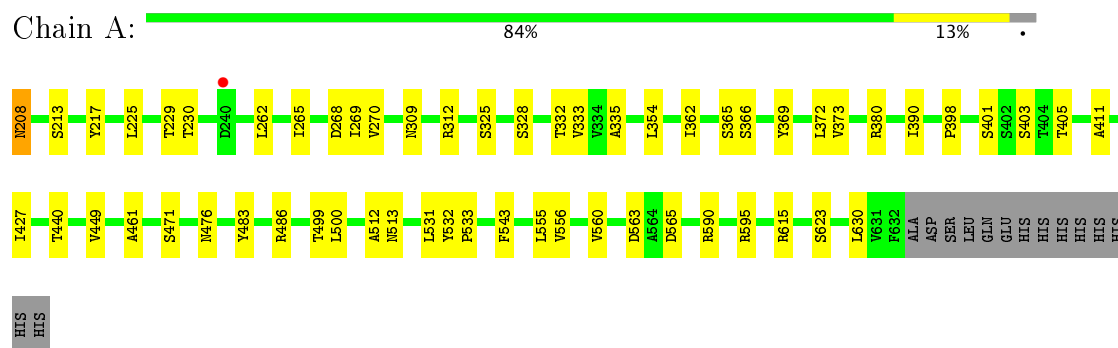


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			11	6	5		

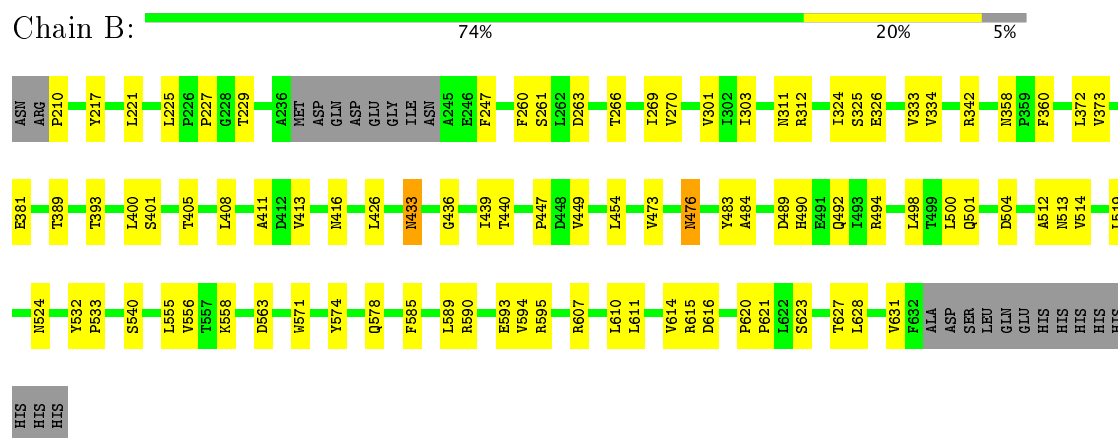
### 3 Residue-property plots

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

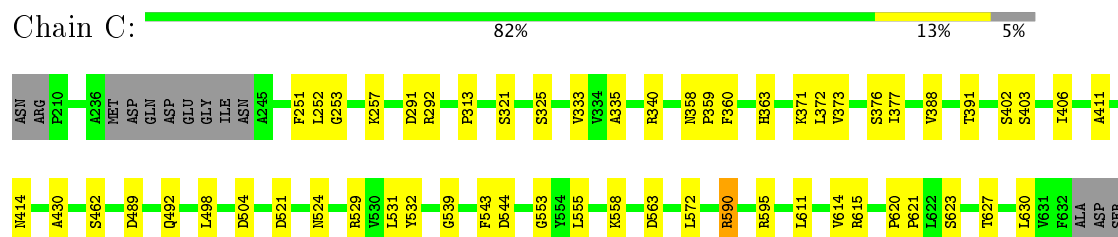
- Molecule 1: MCG133388, isoform CRA\_y



- Molecule 1: MCG133388, isoform CRA\_y



- Molecule 1: MCG133388, isoform CRA\_y



R607	R395	D208
L611	S401	R209
V614	S402	P210
R615	S403	V211
S623	T406	P212
V631	A411	D215
D634	D412	R233
SER	V413	P247
LEU	M414	F260
GLN	A417	S261
GLU	V425	D268
HIS	G436	T269
HIS	P447	V270
HIS	T460	T271
HIS	A468	R272
HIS	F472	I285
HIS	A484	L295
HIS	H490	C299
HIS	I493	I316
	L498	D322
	T499	S325
	L500	R340
	Q501	V351
	D504	L354
	L510	N357
	S511	N358
	A512	P359
	M516	P360
	R529	K361
	V530	I362
	L531	L372
	M571	S376
	L572	I377
	S573	R380
	Q578	E381
	R590	V388
	L598	T389
	R598	I390
	V599	T391
		A392

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.24Å 91.76Å 452.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.50 19.96 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.96-3.50) 98.0 (19.96-3.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.52Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.208 , 0.257 0.205 , 0.257	Depositor DCC
$R_{free}$ test set	1781 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.7	Xtriage
Anisotropy	0.827	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CA, 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	0/3254	0.46	0/4447
1	B	0.27	0/3161	0.46	0/4326
1	C	0.26	0/3167	0.44	0/4332
1	D	0.26	0/3266	0.46	0/4466
All	All	0.26	0/12848	0.46	0/17571

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	3197	0	3058	36	0
1	B	3102	0	2960	61	0
1	C	3111	0	2978	39	0
1	D	3209	0	3062	42	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	9	0	0	0	0
3	A	66	0	60	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	66	0	60	0	0
3	C	66	0	60	0	0
3	D	66	0	60	0	0
4	A	28	0	26	1	0
4	B	56	0	49	2	0
4	C	42	0	37	0	0
4	D	28	0	25	0	0
5	B	10	0	10	0	0
5	D	10	0	10	0	0
6	C	11	0	10	0	0
All	All	13104	0	12465	165	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 6.

The worst 5 of 165 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:461:ALA:HB3	1:A:499:THR:HB	1.60	0.81
1:B:490:HIS:O	1:C:590:ARG:NH1	2.24	0.70
1:A:230:THR:HA	1:A:270:VAL:HG22	1.74	0.70
1:D:351:MET:SD	1:D:395:ARG:NH2	2.65	0.69
1:C:555:LEU:HA	1:C:595:ARG:HG2	1.76	0.67

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	423/439 (96%)	410 (97%)	13 (3%)	0	100	100
1	B	412/439 (94%)	396 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	411/439 (94%)	395 (96%)	16 (4%)	0	100	100
1	D	425/439 (97%)	413 (97%)	12 (3%)	0	100	100
All	All	1671/1756 (95%)	1614 (97%)	57 (3%)	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	351/380 (92%)	350 (100%)	1 (0%)	94	98
1	B	336/380 (88%)	334 (99%)	2 (1%)	89	96
1	C	342/380 (90%)	341 (100%)	1 (0%)	94	98
1	D	351/380 (92%)	348 (99%)	3 (1%)	82	93
All	All	1380/1520 (91%)	1373 (100%)	7 (0%)	91	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	590	ARG
1	D	598	ARG
1	D	215	ASP
1	B	433	ASN
1	D	322	ASP

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

Mol	Chain	Res	Type
1	A	497	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 74 ligands modelled in this entry, 36 are monoatomic - leaving 38 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$
3	MAN	A	710	1	11,11,12	0.79	1 (9%)	13,15,17	1.07	2 (15%)
3	MAN	A	711	1	11,11,12	0.72	0	13,15,17	1.13	2 (15%)
3	MAN	A	712	1	11,11,12	0.66	0	13,15,17	1.45	3 (23%)
3	MAN	A	713	1	11,11,12	0.82	0	13,15,17	1.13	2 (15%)
3	MAN	A	714	1	11,11,12	0.73	0	13,15,17	1.12	2 (15%)
3	MAN	A	715	1	11,11,12	0.70	0	13,15,17	0.99	1 (7%)
4	NAG	A	716	1	14,14,15	0.15	0	15,19,21	0.46	0
4	NAG	A	717	1	14,14,15	0.46	0	15,19,21	0.63	0
3	MAN	B	710	1	11,11,12	0.74	0	13,15,17	1.24	2 (15%)
3	MAN	B	711	1	11,11,12	0.74	0	13,15,17	1.06	2 (15%)
3	MAN	B	712	1	11,11,12	0.63	0	13,15,17	1.26	2 (15%)
3	MAN	B	713	1	11,11,12	0.65	0	13,15,17	1.39	3 (23%)
3	MAN	B	714	1	11,11,12	0.82	0	13,15,17	1.25	2 (15%)
3	MAN	B	715	1	11,11,12	0.74	0	13,15,17	1.08	2 (15%)
4	NAG	B	716	1,5,4	14,14,15	0.24	0	15,19,21	0.47	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	717	4	14,14,15	0.33	0	15,19,21	0.44	0
5	FUC	B	718	4	9,10,11	0.76	0	13,14,16	1.05	2 (15%)
4	NAG	B	719	1,4	14,14,15	0.35	0	15,19,21	0.82	1 (6%)
4	NAG	B	720	4	14,14,15	0.51	0	15,19,21	0.42	0
3	MAN	C	710	1	11,11,12	0.92	0	13,15,17	1.17	2 (15%)
3	MAN	C	711	1	11,11,12	0.76	0	13,15,17	1.25	2 (15%)
3	MAN	C	712	1	11,11,12	0.62	0	13,15,17	1.37	3 (23%)
3	MAN	C	713	1	11,11,12	0.71	0	13,15,17	1.27	3 (23%)
3	MAN	C	714	1	11,11,12	0.78	0	13,15,17	1.10	2 (15%)
3	MAN	C	715	1	11,11,12	0.90	0	13,15,17	1.15	1 (7%)
4	NAG	C	716	1,4	14,14,15	0.49	0	15,19,21	0.56	0
4	NAG	C	717	4,6	14,14,15	0.32	0	15,19,21	0.54	0
6	BMA	C	718	4	11,11,12	0.71	0	13,15,17	0.77	0
4	NAG	C	719	1	14,14,15	0.26	0	15,19,21	0.46	0
3	MAN	D	710	1	11,11,12	0.84	0	13,15,17	1.20	2 (15%)
3	MAN	D	711	1	11,11,12	0.94	0	13,15,17	1.04	1 (7%)
3	MAN	D	712	1	11,11,12	0.59	0	13,15,17	1.29	2 (15%)
3	MAN	D	713	1	11,11,12	0.78	0	13,15,17	1.21	2 (15%)
3	MAN	D	714	1	11,11,12	0.75	0	13,15,17	1.13	2 (15%)
3	MAN	D	715	1	11,11,12	0.62	0	13,15,17	1.15	2 (15%)
4	NAG	D	716	1	14,14,15	0.32	0	15,19,21	0.63	0
4	NAG	D	717	1,5	14,14,15	0.21	0	15,19,21	0.44	0
5	FUC	D	718	4	9,10,11	0.68	0	13,14,16	1.13	1 (7%)

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	MAN	A	710	1	-	0/2/19/22	0/1/1/1
3	MAN	A	711	1	-	0/2/19/22	0/1/1/1
3	MAN	A	712	1	-	0/2/19/22	0/1/1/1
3	MAN	A	713	1	-	0/2/19/22	0/1/1/1
3	MAN	A	714	1	-	0/2/19/22	0/1/1/1
3	MAN	A	715	1	-	0/2/19/22	0/1/1/1
4	NAG	A	716	1	-	0/6/23/26	0/1/1/1
4	NAG	A	717	1	-	0/6/23/26	0/1/1/1
3	MAN	B	710	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	B	711	1	-	0/2/19/22	0/1/1/1
3	MAN	B	712	1	-	0/2/19/22	0/1/1/1
3	MAN	B	713	1	-	0/2/19/22	0/1/1/1
3	MAN	B	714	1	-	0/2/19/22	0/1/1/1
3	MAN	B	715	1	-	0/2/19/22	0/1/1/1
4	NAG	B	716	1,5,4	-	0/6/23/26	0/1/1/1
4	NAG	B	717	4	-	0/6/23/26	0/1/1/1
5	FUC	B	718	4	-	0/0/17/20	0/1/1/1
4	NAG	B	719	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	720	4	-	0/6/23/26	0/1/1/1
3	MAN	C	710	1	-	0/2/19/22	0/1/1/1
3	MAN	C	711	1	-	0/2/19/22	0/1/1/1
3	MAN	C	712	1	-	0/2/19/22	0/1/1/1
3	MAN	C	713	1	-	0/2/19/22	0/1/1/1
3	MAN	C	714	1	-	0/2/19/22	0/1/1/1
3	MAN	C	715	1	-	0/2/19/22	0/1/1/1
4	NAG	C	716	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	717	4,6	-	0/6/23/26	0/1/1/1
6	BMA	C	718	4	-	0/2/19/22	0/1/1/1
4	NAG	C	719	1	-	0/6/23/26	0/1/1/1
3	MAN	D	710	1	-	0/2/19/22	0/1/1/1
3	MAN	D	711	1	-	0/2/19/22	0/1/1/1
3	MAN	D	712	1	-	0/2/19/22	0/1/1/1
3	MAN	D	713	1	-	0/2/19/22	0/1/1/1
3	MAN	D	714	1	-	0/2/19/22	0/1/1/1
3	MAN	D	715	1	-	0/2/19/22	0/1/1/1
4	NAG	D	716	1	-	0/6/23/26	0/1/1/1
4	NAG	D	717	1,5	-	0/6/23/26	0/1/1/1
5	FUC	D	718	4	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	710	MAN	O5-C1	-2.11	1.40	1.43

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	711	MAN	O2-C2-C3	-2.65	104.98	110.17
3	D	715	MAN	O2-C2-C3	-2.47	105.31	110.17
3	D	712	MAN	O2-C2-C3	-2.45	105.36	110.17
3	D	713	MAN	O2-C2-C3	-2.42	105.42	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	710	MAN	O2-C2-C3	-2.35	105.57	110.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	716	NAG	1	0
4	B	716	NAG	2	0
4	B	717	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/439 (96%)	-0.53	1 (0%) 94 93	47, 92, 148, 183	0
1	B	415/439 (94%)	-0.49	0 100 100	43, 90, 175, 219	0
1	C	415/439 (94%)	-0.49	0 100 100	55, 99, 151, 209	0
1	D	427/439 (97%)	-0.52	2 (0%) 90 86	44, 88, 154, 187	0
All	All	1682/1756 (95%)	-0.51	3 (0%) 94 93	43, 93, 157, 219	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	ASP	2.8
1	D	599	ALA	2.6
1	D	598	ARG	2.1

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	D	716	14/15	0.82	0.48	5.53	115,126,135,137	0
3	MAN	C	715	11/12	0.91	0.42	4.52	79,97,115,120	0
3	MAN	C	714	11/12	0.88	0.38	3.10	105,117,128,137	0
3	MAN	A	714	11/12	0.89	0.36	2.74	104,130,144,145	0
4	NAG	C	716	14/15	0.89	0.25	2.32	63,94,129,148	0
3	MAN	A	715	11/12	0.88	0.37	2.00	91,109,124,146	0
3	MAN	D	715	11/12	0.90	0.26	1.67	98,106,133,145	0
3	MAN	B	715	11/12	0.94	0.28	1.24	88,115,129,136	0
3	MAN	C	713	11/12	0.89	0.30	1.18	87,112,122,122	0
3	MAN	D	713	11/12	0.91	0.21	0.94	77,97,123,124	0
3	MAN	A	713	11/12	0.84	0.27	0.72	81,106,124,125	0
2	CA	C	706	1/1	0.99	0.18	0.59	75,75,75,75	0
2	CA	D	709	1/1	0.97	0.16	-0.79	74,74,74,74	0
2	CA	A	704	1/1	0.99	0.14	-0.99	63,63,63,63	0
2	CA	D	706	1/1	0.99	0.13	-1.06	39,39,39,39	0
2	CA	A	703	1/1	0.96	0.11	-1.09	53,53,53,53	0
2	CA	D	708	1/1	0.97	0.10	-1.19	87,87,87,87	0
2	CA	D	704	1/1	0.98	0.12	-1.32	52,52,52,52	0
2	CA	C	709	1/1	0.98	0.10	-1.32	93,93,93,93	0
2	CA	B	703	1/1	0.95	0.13	-1.37	48,48,48,48	0
2	CA	B	708	1/1	0.96	0.10	-1.38	86,86,86,86	0
2	CA	A	707	1/1	1.00	0.14	-1.44	98,98,98,98	0
2	CA	B	709	1/1	0.98	0.11	-1.47	92,92,92,92	0
2	CA	C	704	1/1	0.94	0.13	-1.48	96,96,96,96	0
2	CA	C	705	1/1	0.99	0.13	-1.63	65,65,65,65	0
2	CA	C	703	1/1	1.00	0.12	-1.64	40,40,40,40	0
2	CA	A	709	1/1	0.96	0.16	-1.64	98,98,98,98	0
2	CA	D	703	1/1	0.99	0.13	-1.75	58,58,58,58	0
2	CA	C	707	1/1	0.94	0.12	-1.80	91,91,91,91	0
2	CA	D	705	1/1	0.97	0.09	-2.03	56,56,56,56	0
2	CA	A	701	1/1	0.99	0.11	-2.08	44,44,44,44	0
2	CA	B	706	1/1	0.99	0.11	-2.09	46,46,46,46	0
2	CA	C	708	1/1	0.97	0.09	-2.09	72,72,72,72	0
2	CA	D	701	1/1	0.98	0.11	-2.15	43,43,43,43	0
2	CA	D	707	1/1	0.96	0.06	-2.31	93,93,93,93	0
2	CA	B	705	1/1	0.98	0.12	-2.35	49,49,49,49	0
2	CA	A	705	1/1	0.99	0.11	-2.38	62,62,62,62	0
2	CA	B	707	1/1	0.97	0.07	-2.54	87,87,87,87	0
2	CA	C	701	1/1	0.98	0.10	-2.55	43,43,43,43	0
2	CA	A	708	1/1	0.99	0.11	-2.61	80,80,80,80	0
2	CA	A	706	1/1	0.99	0.11	-2.83	49,49,49,49	0
2	CA	A	702	1/1	0.99	0.05	-2.91	39,39,39,39	0
2	CA	B	702	1/1	0.99	0.10	-3.02	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	B	701	1/1	0.99	0.10	-3.28	58,58,58,58	0
2	CA	D	702	1/1	0.97	0.07	-3.44	34,34,34,34	0
2	CA	B	704	1/1	0.98	0.08	-3.56	66,66,66,66	0
2	CA	C	702	1/1	0.98	0.08	-3.60	30,30,30,30	0
4	NAG	B	716	14/15	0.87	0.26	-	112,127,149,156	0
3	MAN	D	712	11/12	0.94	0.16	-	55,79,90,95	0
3	MAN	D	711	11/12	0.90	0.27	-	84,95,105,107	0
3	MAN	D	714	11/12	0.86	0.40	-	100,122,127,128	0
4	NAG	B	719	14/15	0.85	0.26	-	80,109,126,138	0
3	MAN	C	711	11/12	0.95	0.35	-	59,83,97,102	0
3	MAN	C	712	11/12	0.91	0.23	-	47,68,88,90	0
5	FUC	B	718	10/11	0.93	0.32	-	130,143,150,157	0
3	MAN	B	714	11/12	0.83	0.39	-	71,111,124,130	0
3	MAN	B	711	11/12	0.94	0.34	-	73,87,103,107	0
4	NAG	B	717	14/15	0.80	0.46	-	126,155,163,168	0
3	MAN	D	710	11/12	0.94	0.19	-	56,79,92,101	0
6	BMA	C	718	11/12	0.73	0.43	-	125,159,166,167	0
3	MAN	C	710	11/12	0.92	0.21	-	59,91,125,141	0
3	MAN	A	711	11/12	0.95	0.31	-	74,105,116,117	0
4	NAG	C	717	14/15	0.86	0.40	-	117,144,154,157	0
4	NAG	A	717	14/15	0.87	0.36	-	71,100,125,128	0
4	NAG	A	716	14/15	0.73	0.33	-	114,142,153,155	0
4	NAG	D	717	14/15	0.86	0.30	-	111,125,145,147	0
3	MAN	B	710	11/12	0.93	0.24	-	51,70,79,89	0
4	NAG	B	720	14/15	0.82	0.56	-	147,153,163,170	0
3	MAN	A	710	11/12	0.91	0.19	-	67,93,110,111	0
3	MAN	B	713	11/12	0.81	0.27	-	100,120,138,140	0
3	MAN	A	712	11/12	0.91	0.26	-	60,90,100,107	0
4	NAG	C	719	14/15	0.77	0.48	-	121,135,154,158	0
3	MAN	B	712	11/12	0.93	0.19	-	69,87,103,115	0
5	FUC	D	718	10/11	0.81	0.36	-	126,142,147,149	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.