



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2016 – 05:03 PM EDT

PDB ID : 5DZV  
Title : Protocadherin alpha 7 extracellular cadherin domains 1-5  
Authors : Goodman, K.M.; Bahna, F.; Honig, B.; Shapiro, L.  
Deposited on : 2015-09-26  
Resolution : 3.60 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](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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
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-20027674

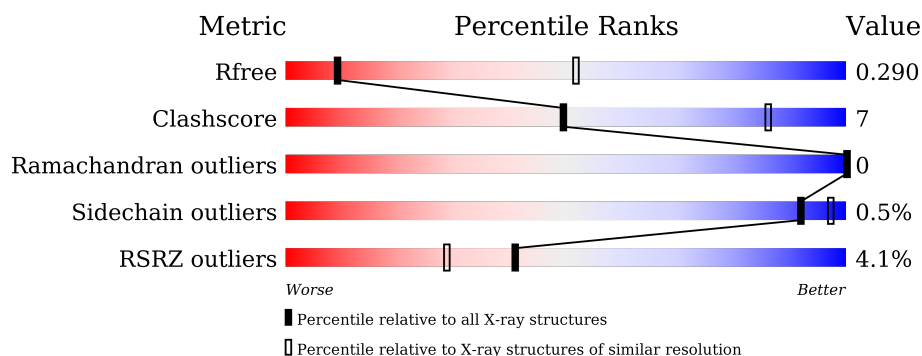
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	539	<div> <div>6%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	B	539	<div> <div>%</div> <div>77%</div> <div>19%</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
2	CA	A	605	-	-	-	X
2	CA	B	606	-	-	-	X
2	CA	B	607	-	-	-	X
2	CA	B	611	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7876 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 Protein Pcdha7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	1	0
			3735	2324	635	769	7			
1	B	522	Total	C	N	O	S	0	1	0
			3867	2435	648	776	8			

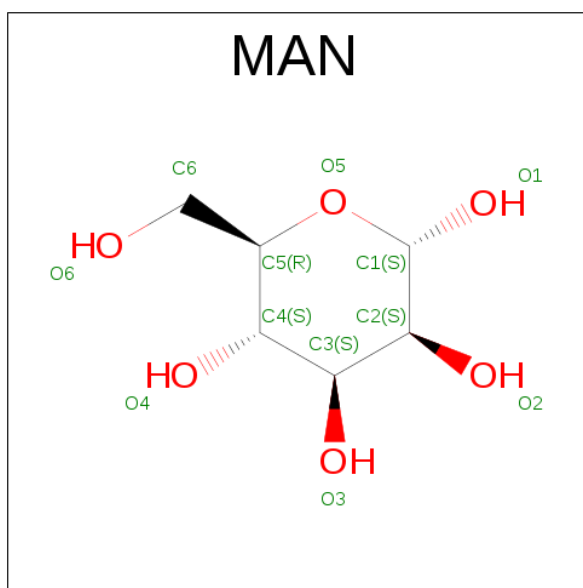
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	532	HIS	-	expression tag	UNP Q91Y13
A	533	HIS	-	expression tag	UNP Q91Y13
A	534	HIS	-	expression tag	UNP Q91Y13
A	535	HIS	-	expression tag	UNP Q91Y13
A	536	HIS	-	expression tag	UNP Q91Y13
A	537	HIS	-	expression tag	UNP Q91Y13
A	538	HIS	-	expression tag	UNP Q91Y13
A	539	HIS	-	expression tag	UNP Q91Y13
B	532	HIS	-	expression tag	UNP Q91Y13
B	533	HIS	-	expression tag	UNP Q91Y13
B	534	HIS	-	expression tag	UNP Q91Y13
B	535	HIS	-	expression tag	UNP Q91Y13
B	536	HIS	-	expression tag	UNP Q91Y13
B	537	HIS	-	expression tag	UNP Q91Y13
B	538	HIS	-	expression tag	UNP Q91Y13
B	539	HIS	-	expression tag	UNP Q91Y13

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	12	Total	Ca	0	0
			12	12		
2	A	12	Total	Ca	0	0
			12	12		

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



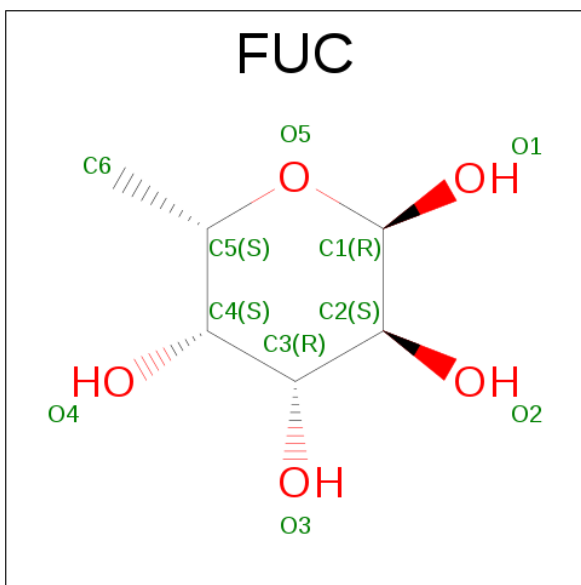
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

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



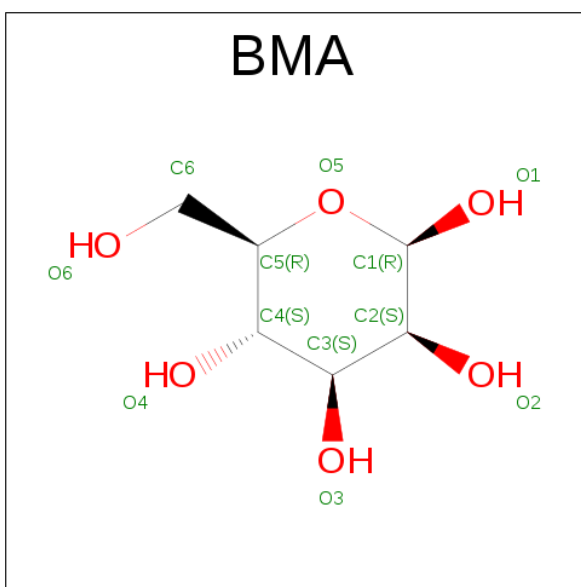
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

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



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

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

- Molecule 7 is water.

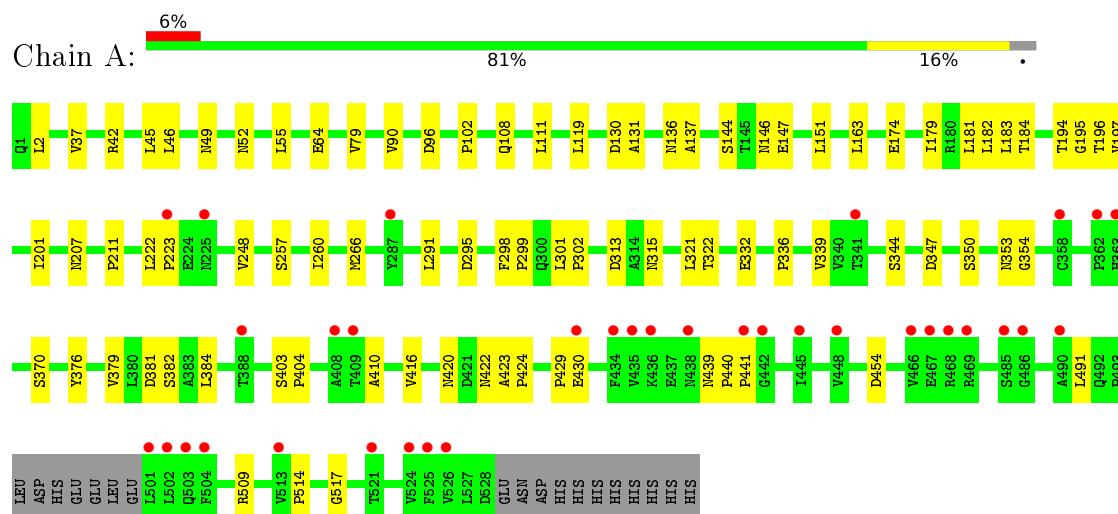
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	O	0	0
			8	8		
7	B	4	Total	O	0	0
			4	4		



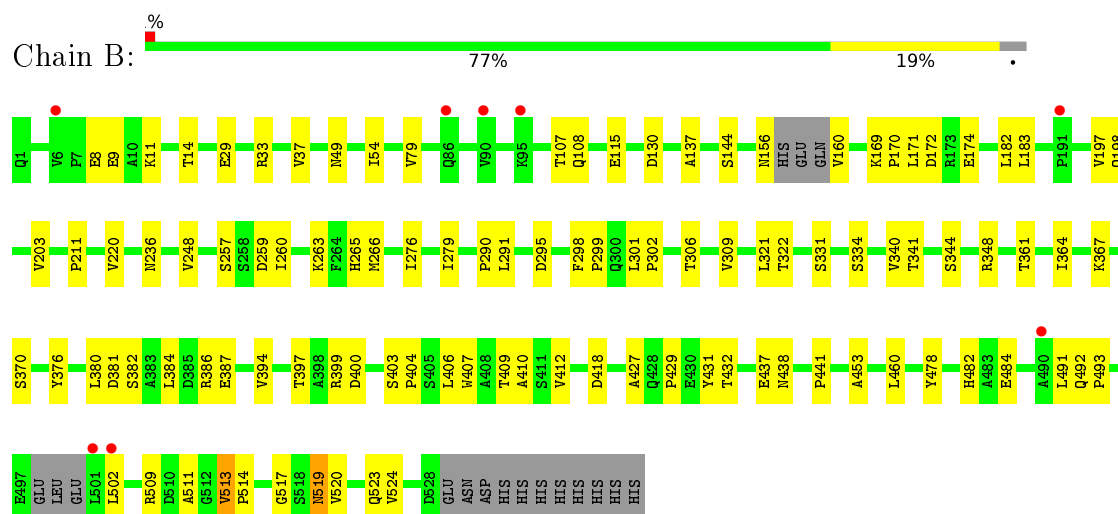
### 3 Residue-property plots

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: Protein Pcdha7



#### • Molecule 1: Protein Pcdha7



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.44Å 106.45Å 558.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.31 – 3.60 43.31 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (43.31-3.60) 95.7 (43.31-3.50)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.254 , 0.290 0.254 , 0.290	Depositor DCC
$R_{free}$ test set	1114 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	92.4	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, FUC

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	0.20	0/3800	0.40	0/5207
1	B	0.21	0/3942	0.41	0/5391
All	All	0.21	0/7742	0.40	0/10598

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

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	3735	0	3420	47	0
1	B	3867	0	3676	60	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
3	A	22	0	20	1	0
3	B	66	0	60	1	0
4	A	28	0	24	0	0
4	B	70	0	60	1	0
5	A	20	0	20	0	0
5	B	10	0	10	0	0
6	B	22	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	8	0	0	2	0
7	B	4	0	0	0	0
All	All	7876	0	7308	107	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.

All (107) 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:B:519:ASN:H	1:B:519:ASN:HD22	1.33	0.75
1:B:263:LYS:HD3	1:B:279:ILE:HG22	1.71	0.71
1:A:332:GLU:OE2	7:A:701:HOH:O	2.09	0.70
1:B:236:ASN:OD1	4:B:621:NAG:N2	2.27	0.68
1:B:380:LEU:HD11	1:B:384:LEU:HD11	1.77	0.66
1:A:111:LEU:HB2	1:A:201:ILE:HG22	1.76	0.66
1:B:331:SER:HG	1:B:334:SER:HG	1.45	0.65
1:B:37:VAL:HG12	1:B:79:VAL:HG22	1.83	0.61
1:A:257:SER:HB2	1:A:260:ILE:HG12	1.84	0.60
1:A:509:ARG:HD2	1:A:517:GLY:HA3	1.84	0.60
1:B:29:GLU:OE2	1:B:33:ARG:NH1	2.35	0.59
1:B:107:THR:HG22	1:B:108:GLN:HG3	1.84	0.59
1:B:171:LEU:HD21	1:B:203:VAL:HG22	1.86	0.58
1:B:290:PRO:HA	1:B:306:THR:HG22	1.86	0.58
1:B:519:ASN:N	1:B:519:ASN:HD22	2.02	0.57
1:B:460:LEU:HD22	1:B:511:ALA:HB2	1.86	0.57
1:A:313:ASP:OD2	1:A:350:SER:N	2.27	0.57
1:B:484:GLU:N	1:B:484:GLU:OE1	2.39	0.56
1:A:420:ASN:ND2	1:A:514:PRO:O	2.39	0.56
1:B:321:LEU:HD11	1:B:410:ALA:HB2	1.87	0.56
1:A:441:PRO:HA	1:A:491:LEU:HA	1.89	0.54
1:A:422:ASN:ND2	1:A:454:ASP:OD1	2.40	0.54
1:A:37:VAL:HG12	1:A:79:VAL:HG22	1.88	0.54
1:B:397:THR:HG22	1:B:409:THR:HG22	1.88	0.54
1:A:298:PHE:HB3	1:A:299:PRO:HD3	1.89	0.53
1:A:339:VAL:HA	1:A:379:VAL:HA	1.91	0.53
1:B:156:ASN:HB3	1:B:160:VAL:HG11	1.89	0.53
1:A:108:GLN:NE2	7:A:702:HOH:O	2.35	0.53
1:A:336:PRO:HB3	1:A:382:SER:H	1.74	0.52
1:B:259:ASP:OD1	1:B:263:LYS:NZ	2.42	0.52
1:B:115:GLU:HG3	1:B:172:ASP:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:THR:OG1	1:A:344:SER:OG	2.28	0.52
1:A:144:SER:HB2	1:A:182:LEU:HG	1.91	0.52
1:A:266:MET:HE1	1:A:291:LEU:HD13	1.92	0.52
1:A:151:LEU:HD11	1:A:163:LEU:HD13	1.92	0.51
1:B:370:SER:HB2	1:B:376:TYR:CD2	2.46	0.51
1:A:49:ASN:ND2	1:A:52:ASN:OD1	2.44	0.51
1:B:11:LYS:O	1:B:14:THR:OG1	2.23	0.50
1:A:42:ARG:HD3	1:A:45:LEU:HD21	1.93	0.50
1:B:361:THR:HB	1:B:364:ILE:HD12	1.93	0.50
1:B:441:PRO:HA	1:B:491:LEU:HA	1.93	0.50
1:B:220:VAL:HB	1:B:309:VAL:HG12	1.93	0.50
1:B:513:VAL:HG23	1:B:514:PRO:HD3	1.94	0.50
1:B:348:ARG:HA	1:B:348:ARG:HH11	1.77	0.49
1:B:169:LYS:HG2	1:B:170:PRO:HD2	1.93	0.49
1:B:394:VAL:HG13	1:B:412:VAL:HB	1.94	0.49
1:B:437:GLU:HG3	1:B:438:ASN:H	1.78	0.49
1:A:211:PRO:HB3	1:A:248:VAL:HG11	1.95	0.49
1:B:49:ASN:OD1	1:B:54:ILE:HG22	2.14	0.48
1:B:502:LEU:HB2	1:B:524:VAL:HG13	1.95	0.48
1:B:432:THR:HG22	1:B:523:GLN:HB2	1.96	0.48
1:A:381:ASP:OD1	1:A:382:SER:N	2.48	0.47
1:B:298:PHE:HB3	1:B:299:PRO:HD3	1.96	0.47
1:B:322:THR:OG1	1:B:344:SER:OG	2.32	0.47
1:A:179:ILE:HB	1:A:201:ILE:HG13	1.97	0.47
1:A:347:ASP:OD2	1:A:354:GLY:HA2	2.16	0.46
1:A:429:PRO:HA	1:A:430:GLU:HA	1.64	0.46
1:A:146:ASN:HD22	1:A:181:LEU:HD21	1.79	0.46
1:A:184:THR:HG22	1:A:196:THR:HG22	1.98	0.46
1:B:400:ASP:HB3	1:B:406:LEU:HB2	1.97	0.46
1:B:381:ASP:OD1	1:B:382:SER:N	2.49	0.45
1:B:509:ARG:HG2	1:B:517:GLY:HA3	1.97	0.45
1:A:370:SER:HB2	1:A:376:TYR:CD2	2.51	0.45
1:B:257:SER:HB3	1:B:260:ILE:HG13	1.98	0.45
1:A:102:PRO:O	1:A:195:GLY:HA3	2.17	0.45
1:B:265:HIS:HB2	1:B:276:ILE:HD13	1.98	0.45
1:B:427:ALA:HB3	1:B:431:TYR:OH	2.17	0.45
1:B:295:ASP:OD1	1:B:295:ASP:N	2.44	0.45
1:A:119:LEU:H	1:A:119:LEU:HD12	1.81	0.45
1:B:386:ARG:HD2	1:B:418:ASP:HA	1.99	0.45
1:A:439:ASN:HA	1:A:440:PRO:HD3	1.82	0.44
1:A:207:ASN:ND2	1:A:295:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HB3	1:B:197:VAL:HG13	1.98	0.44
1:B:429:PRO:HB3	1:B:520:VAL:HG23	1.98	0.44
1:A:96:ASP:OD2	1:A:136:ASN:ND2	2.47	0.44
1:B:399:ARG:NH1	1:B:407:TRP:HB3	2.32	0.44
1:B:340:VAL:HG12	1:B:341:THR:HG23	2.00	0.43
1:A:174:GLU:N	1:A:174:GLU:OE1	2.49	0.43
1:B:130:ASP:OD2	1:B:137:ALA:HA	2.19	0.43
1:A:64:GLU:HG2	1:A:131:ALA:HB1	1.99	0.43
1:B:174:GLU:OE1	1:B:174:GLU:N	2.48	0.43
1:B:144:SER:HB2	1:B:182:LEU:HG	1.99	0.43
1:A:315:ASN:HD22	1:A:353:ASN:HB2	1.82	0.43
1:A:2:LEU:HB3	1:A:90:VAL:HG13	2.00	0.43
1:A:194:THR:HB	3:A:614:MAN:H2	1.55	0.43
1:A:46:LEU:HB3	1:A:55:LEU:HD11	2.01	0.42
1:B:409:THR:HB	3:B:625:MAN:H2	1.77	0.42
1:B:54:ILE:HD12	1:B:54:ILE:HA	1.94	0.42
1:A:301:LEU:HA	1:A:302:PRO:HD3	1.82	0.42
1:B:301:LEU:HA	1:B:302:PRO:HD3	1.83	0.42
1:A:183:LEU:HB3	1:A:197:VAL:HG13	2.02	0.42
1:B:108:GLN:HG2	1:B:198:GLN:HG3	2.00	0.42
1:A:420:ASN:HB3	1:A:514:PRO:HG2	2.01	0.41
1:A:130:ASP:OD2	1:A:137:ALA:HA	2.20	0.41
1:B:211:PRO:HB3	1:B:248:VAL:HG11	2.02	0.41
1:B:367:LYS:HD3	1:B:381:ASP:OD2	2.20	0.41
1:B:403:SER:HA	1:B:404:PRO:HA	1.86	0.41
1:A:222:LEU:HA	1:A:223:PRO:HD3	1.95	0.41
1:B:482:HIS:CE1	1:B:484:GLU:HB2	2.56	0.41
1:B:266:MET:HE1	1:B:291:LEU:HD13	2.02	0.41
1:A:321:LEU:HD11	1:A:410:ALA:HB2	2.03	0.41
1:B:387:GLU:HG2	1:B:453:ALA:HB1	2.02	0.41
1:B:8:GLU:HG2	1:B:9:GLU:HG3	2.02	0.41
1:A:384:LEU:HD22	1:A:416:VAL:HG11	2.03	0.40
1:B:492:GLN:HA	1:B:493:PRO:HD3	1.98	0.40
1:A:423:ALA:HA	1:A:424:PRO:HD3	1.93	0.40
1:A:403:SER:HA	1:A:404:PRO:HA	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/539 (96%)	490 (95%)	28 (5%)	0	100	100
1	B	517/539 (96%)	488 (94%)	29 (6%)	0	100	100
All	All	1035/1078 (96%)	978 (94%)	57 (6%)	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	383/473 (81%)	382 (100%)	1 (0%)	94	99
1	B	418/473 (88%)	415 (99%)	3 (1%)	88	96
All	All	801/946 (85%)	797 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	GLU
1	B	478	TYR
1	B	513	VAL
1	B	519	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	B	422	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 44 ligands modelled in this entry, 24 are monoatomic - leaving 20 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	613	1	11,11,12	0.92	1 (9%)	15,15,17	0.91	1 (6%)
3	MAN	A	614	1	11,11,12	0.83	1 (9%)	15,15,17	0.87	0
4	NAG	A	615	1,5	14,14,15	0.46	0	15,19,21	0.36	0
5	FUC	A	616	4	10,10,11	0.58	0	13,14,16	0.89	0
4	NAG	A	617	1,5	14,14,15	0.26	0	15,19,21	0.26	0
5	FUC	A	618	4	10,10,11	1.19	1 (10%)	13,14,16	1.07	1 (7%)
3	MAN	B	613	1	11,11,12	0.60	0	15,15,17	1.25	2 (13%)
3	MAN	B	614	1	11,11,12	0.95	0	15,15,17	1.00	0
4	NAG	B	615	1,5,4	14,14,15	0.17	0	15,19,21	0.42	0
5	FUC	B	616	4	10,10,11	0.57	0	13,14,16	0.85	0
4	NAG	B	617	4,6	14,14,15	0.20	0	15,19,21	0.42	0
6	BMA	B	618	3,4	11,11,12	0.82	0	15,15,17	0.99	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	B	619	6	11,11,12	0.70	0	15,15,17	0.98	2 (13%)
3	MAN	B	620	6	11,11,12	1.03	0	15,15,17	2.04	4 (26%)
4	NAG	B	621	1,4	14,14,15	0.59	1 (7%)	15,19,21	0.56	0
4	NAG	B	622	4,6	14,14,15	0.37	0	15,19,21	0.61	1 (6%)
6	BMA	B	623	4	11,11,12	0.51	0	15,15,17	0.82	0
4	NAG	B	624	1	14,14,15	0.19	0	15,19,21	0.30	0
3	MAN	B	625	1	11,11,12	0.80	1 (9%)	15,15,17	0.86	1 (6%)
3	MAN	B	626	1	11,11,12	0.61	0	15,15,17	1.25	3 (20%)

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	613	1	-	0/2/19/22	0/1/1/1
3	MAN	A	614	1	-	0/2/19/22	0/1/1/1
4	NAG	A	615	1,5	-	0/6/23/26	0/1/1/1
5	FUC	A	616	4	-	0/0/17/20	0/1/1/1
4	NAG	A	617	1,5	-	0/6/23/26	0/1/1/1
5	FUC	A	618	4	-	0/0/17/20	0/1/1/1
3	MAN	B	613	1	-	0/2/19/22	0/1/1/1
3	MAN	B	614	1	-	0/2/19/22	0/1/1/1
4	NAG	B	615	1,5,4	-	0/6/23/26	0/1/1/1
5	FUC	B	616	4	-	0/0/17/20	0/1/1/1
4	NAG	B	617	4,6	-	0/6/23/26	0/1/1/1
6	BMA	B	618	3,4	-	0/2/19/22	0/1/1/1
3	MAN	B	619	6	-	0/2/19/22	0/1/1/1
3	MAN	B	620	6	-	0/2/19/22	0/1/1/1
4	NAG	B	621	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	622	4,6	-	0/6/23/26	0/1/1/1
6	BMA	B	623	4	-	0/2/19/22	0/1/1/1
4	NAG	B	624	1	-	0/6/23/26	0/1/1/1
3	MAN	B	625	1	-	0/2/19/22	0/1/1/1
3	MAN	B	626	1	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	618	FUC	O5-C1	-3.08	1.38	1.43
3	A	613	MAN	O5-C1	-2.14	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	625	MAN	O5-C1	-2.13	1.40	1.43
3	A	614	MAN	O5-C1	-2.12	1.40	1.43
4	B	621	NAG	O5-C1	-2.09	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	620	MAN	O2-C2-C3	-3.16	103.83	110.19
3	B	613	MAN	O2-C2-C3	-2.75	104.64	110.19
3	A	613	MAN	O2-C2-C3	-2.27	105.61	110.19
3	B	626	MAN	O2-C2-C3	-2.22	105.72	110.19
3	B	619	MAN	O2-C2-C3	-2.21	105.72	110.19
3	B	625	MAN	O2-C2-C3	-2.16	105.83	110.19
3	B	626	MAN	O5-C1-C2	2.10	114.25	110.89
3	B	619	MAN	C1-O5-C5	2.12	115.25	112.14
4	B	622	NAG	C1-O5-C5	2.23	115.42	112.14
5	A	618	FUC	O2-C2-C1	2.33	113.89	109.23
3	B	626	MAN	C1-O5-C5	2.71	116.13	112.14
3	B	613	MAN	C1-O5-C5	3.04	116.61	112.14
3	B	620	MAN	O5-C1-C2	3.10	115.86	110.89
3	B	620	MAN	C1-C2-C3	3.77	114.12	109.55
3	B	620	MAN	C1-O5-C5	4.40	118.61	112.14

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
3	A	614	MAN	1	0
4	B	621	NAG	1	0
3	B	625	MAN	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	521/539 (96%)	-0.04	35 (6%) 21 13	63, 160, 342, 521	0
1	B	522/539 (96%)	-0.37	8 (1%) 76 64	59, 135, 247, 378	0
All	All	1043/1078 (96%)	-0.20	43 (4%) 41 29	59, 144, 309, 521	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	VAL	14.7
1	A	434	PHE	11.8
1	A	503	GLN	9.0
1	A	525	PHE	6.0
1	A	504	PHE	6.0
1	A	445	ILE	5.2
1	A	486	GLY	5.1
1	A	468	ARG	5.1
1	A	436	LYS	4.9
1	B	501	LEU	4.5
1	A	521	THR	4.3
1	A	448	VAL	3.9
1	A	469	ARG	3.9
1	A	524	VAL	3.8
1	A	502	LEU	3.7
1	B	95	LYS	3.6
1	A	467	GLU	3.5
1	A	441	PRO	3.3
1	A	442	GLY	3.1
1	A	438	ASN	3.0
1	A	430	GLU	2.9
1	A	408	ALA	2.8
1	A	363	HIS	2.8
1	A	388	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	341	THR	2.6
1	B	191	PRO	2.6
1	A	362	PRO	2.5
1	A	466	VAL	2.5
1	A	490	ALA	2.5
1	A	526	VAL	2.4
1	A	223	PRO	2.4
1	B	490	ALA	2.3
1	A	501	LEU	2.3
1	A	485	SER	2.2
1	A	358	CYS	2.2
1	A	513	VAL	2.1
1	B	90	VAL	2.1
1	B	6	VAL	2.1
1	B	86	GLN	2.0
1	A	409	THR	2.0
1	A	225	ASN	2.0
1	A	287	TYR	2.0
1	B	502	LEU	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, 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(Å <sup>2</sup> )	Q<0.9
2	CA	B	607	1/1	0.63	0.33	13.90	231,231,231,231	0
2	CA	B	611	1/1	0.93	0.37	8.05	264,264,264,264	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	B	606	1/1	0.69	0.46	5.86	290,290,290,290	0
2	CA	A	605	1/1	0.94	0.25	3.07	161,161,161,161	0
2	CA	B	610	1/1	0.99	0.21	1.29	71,71,71,71	0
3	MAN	A	613	11/12	0.86	0.21	1.29	133,153,192,208	0
2	CA	B	604	1/1	0.86	0.22	0.57	94,94,94,94	0
2	CA	A	602	1/1	0.94	0.19	0.42	95,95,95,95	0
2	CA	B	612	1/1	0.90	0.20	0.27	75,75,75,75	0
2	CA	A	604	1/1	0.96	0.21	0.15	73,73,73,73	0
3	MAN	B	626	11/12	0.86	0.18	0.05	102,132,175,179	0
2	CA	A	601	1/1	0.95	0.14	-0.04	56,56,56,56	0
4	NAG	B	615	14/15	0.86	0.16	-0.04	103,148,175,183	0
2	CA	A	603	1/1	0.95	0.17	-0.10	85,85,85,85	0
2	CA	B	605	1/1	0.94	0.16	-0.38	93,93,93,93	0
2	CA	A	607	1/1	0.96	0.13	-0.39	108,108,108,108	0
3	MAN	B	614	11/12	0.82	0.17	-0.52	153,183,200,202	0
2	CA	B	602	1/1	1.00	0.13	-0.56	136,136,136,136	0
2	CA	B	603	1/1	0.98	0.10	-0.63	156,156,156,156	0
2	CA	A	609	1/1	0.76	0.11	-0.63	193,193,193,193	0
2	CA	B	608	1/1	0.98	0.13	-0.66	103,103,103,103	0
2	CA	B	601	1/1	0.98	0.11	-0.93	110,110,110,110	0
2	CA	A	610	1/1	0.90	0.08	-1.01	267,267,267,267	0
2	CA	A	608	1/1	0.88	0.10	-1.28	205,205,205,205	0
2	CA	A	611	1/1	0.93	0.06	-1.38	383,383,383,383	0
2	CA	B	609	1/1	0.98	0.11	-1.42	78,78,78,78	0
2	CA	A	612	1/1	0.87	0.04	-1.99	184,184,184,184	0
4	NAG	B	622	14/15	0.88	0.32	-	187,212,232,234	0
3	MAN	B	625	11/12	0.81	0.20	-	96,135,160,192	0
2	CA	A	606	1/1	0.98	0.20	-	106,106,106,106	0
3	MAN	B	613	11/12	0.89	0.23	-	115,139,150,154	0
5	FUC	B	616	10/11	0.78	0.37	-	183,193,204,230	0
5	FUC	A	618	10/11	0.83	0.26	-	211,223,235,236	0
4	NAG	A	617	14/15	0.83	0.17	-	151,175,208,217	0
4	NAG	B	617	14/15	0.84	0.14	-	141,171,189,199	0
6	BMA	B	618	11/12	0.85	0.15	-	149,186,200,200	0
6	BMA	B	623	11/12	0.52	0.44	-	191,207,227,230	0
3	MAN	B	619	11/12	0.76	0.20	-	172,188,194,195	0
4	NAG	B	621	14/15	0.89	0.11	-	162,182,194,205	0
4	NAG	B	624	14/15	0.85	0.13	-	179,211,225,237	0
5	FUC	A	616	10/11	0.81	0.29	-	207,221,231,232	0
3	MAN	A	614	11/12	0.92	0.15	-	76,117,145,162	0
3	MAN	B	620	11/12	0.91	0.14	-	115,144,190,194	0
4	NAG	A	615	14/15	0.82	0.13	-	143,170,188,209	0

## 6.5 Other polymers

There are no such residues in this entry.