



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 AM GMT

PDB ID : 2ODQ  
Title : Complement component C2a, the catalytic fragment of C3- and C5-convertase of human complement  
Authors : Narayana, S.V.L.; Krishnan, V.  
Deposited on : 2006-12-25  
Resolution : 2.30 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

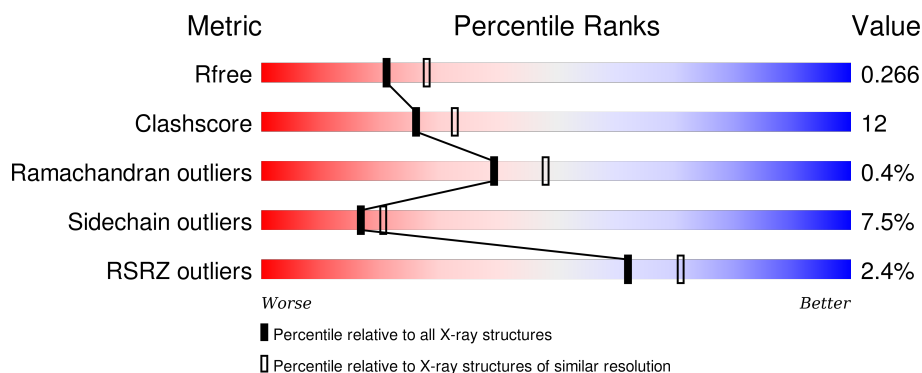
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

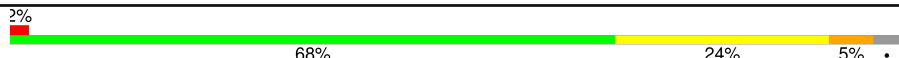
The reported resolution of this entry is 2.30 Å.

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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	509	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4129 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 Complement C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3883	2447	687	723	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	ALA	CYS	ENGINEERED	UNP P06681

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			42	24	3	15		
2	A	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

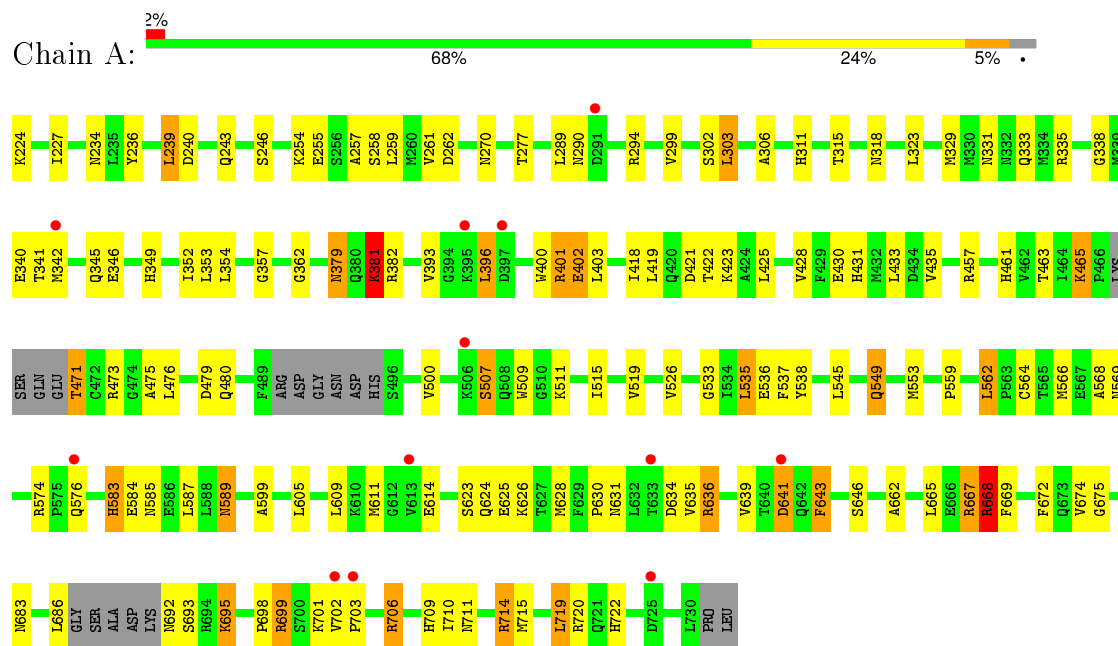
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total	O	0	0
			134	134		

### 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: Complement C2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.35Å 84.20Å 74.43Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 19.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.30) 98.8 (19.48-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.39 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.214 , 0.274 0.207 , 0.266	Depositor DCC
$R_{free}$ test set	1397 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.0	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 27855 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	1.25	12/3959 (0.3%)	1.14	25/5351 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	GLU	CD-OE2	7.57	1.33	1.25
1	A	402	GLU	CB-CG	6.37	1.64	1.52
1	A	435	VAL	CB-CG1	-6.32	1.39	1.52
1	A	674	VAL	CB-CG2	6.14	1.65	1.52
1	A	576	GLN	C-O	6.12	1.34	1.23
1	A	538	TYR	CD2-CE2	5.51	1.47	1.39
1	A	352	ILE	CB-CG2	5.45	1.69	1.52
1	A	549	GLN	CG-CD	5.19	1.62	1.51
1	A	299	VAL	CB-CG2	-5.16	1.42	1.52
1	A	475	ALA	CA-CB	5.12	1.63	1.52
1	A	662	ALA	CA-CB	5.11	1.63	1.52
1	A	720	ARG	CZ-NH1	5.02	1.39	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	714	ARG	NE-CZ-NH2	-10.02	115.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	706	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	720	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	A	706	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	A	720	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	714	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	479	ASP	CB-CG-OD1	6.96	124.57	118.30
1	A	668	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	240	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	715	MET	CG-SD-CE	-6.74	89.42	100.20
1	A	634	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	714	ARG	CG-CD-NE	-6.19	98.80	111.80
1	A	381	LYS	CD-CE-NZ	6.12	125.78	111.70
1	A	641	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	403	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	A	706	ARG	CD-NE-CZ	5.62	131.46	123.60
1	A	719	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	476	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	614	GLU	OE1-CD-OE2	-5.40	116.83	123.30
1	A	401	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	699	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	479	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	401	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	303	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	576	GLN	N-CA-C	5.06	124.66	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	643	PHE	Peptide

## 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	3883	0	3825	96	1
2	A	84	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	26	0	0
4	A	134	0	0	8	0
All	All	4129	0	3925	96	1

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 12.

All (96) 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:631:ASN:HD21	2:A:801:NAG:C1	1.32	1.41
1:A:569:ASN:HD22	1:A:583:HIS:HE1	1.07	0.97
1:A:589:ASN:HD22	1:A:589:ASN:H	0.99	0.95
1:A:564:CYS:H	1:A:583:HIS:HD2	1.09	0.94
1:A:589:ASN:N	1:A:589:ASN:HD22	1.68	0.91
1:A:357:GLY:O	1:A:402:GLU:HG2	1.72	0.89
1:A:589:ASN:ND2	1:A:589:ASN:H	1.72	0.87
1:A:457:ARG:HD2	4:A:57:HOH:O	1.74	0.86
1:A:631:ASN:HD21	2:A:801:NAG:C2	1.89	0.85
1:A:457:ARG:CD	4:A:57:HOH:O	2.24	0.85
1:A:564:CYS:H	1:A:583:HIS:CD2	1.95	0.84
1:A:471:THR:HG23	1:A:473:ARG:HH12	1.42	0.83
1:A:569:ASN:HD22	1:A:583:HIS:CE1	1.95	0.83
1:A:257:ALA:O	1:A:261:VAL:HG23	1.78	0.82
1:A:471:THR:CG2	1:A:473:ARG:HH12	1.94	0.81
1:A:471:THR:HG23	1:A:473:ARG:NH1	1.96	0.80
1:A:243:GLN:HB2	1:A:315:THR:HB	1.64	0.79
1:A:589:ASN:ND2	4:A:82:HOH:O	2.15	0.78
1:A:234:ASN:HD21	1:A:333:GLN:HE22	1.30	0.77
1:A:224:LYS:HE3	1:A:431:HIS:O	1.89	0.72
1:A:686:LEU:O	1:A:695:LYS:HE2	1.92	0.70
1:A:584:GLU:OE2	1:A:714:ARG:NH2	2.22	0.68
1:A:636:ARG:HD2	1:A:639:VAL:O	1.94	0.67
1:A:270:ASN:HD22	1:A:294:ARG:NH2	1.92	0.67
1:A:270:ASN:ND2	1:A:294:ARG:HH22	1.95	0.65
1:A:609:LEU:HB3	1:A:611:MET:HE2	1.79	0.65
1:A:270:ASN:HD22	1:A:294:ARG:HH22	1.45	0.64
1:A:236:TYR:OH	1:A:349:HIS:HD2	1.82	0.62
1:A:277:THR:OG1	1:A:311:HIS:HE1	1.82	0.62
1:A:574:ARG:HD3	4:A:55:HOH:O	2.00	0.61
1:A:692:ASN:N	4:A:99:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LEU:HB3	1:A:628:MET:HE3	1.82	0.61
1:A:589:ASN:N	1:A:589:ASN:ND2	2.41	0.61
1:A:587:LEU:HD22	1:A:665:LEU:HD11	1.82	0.60
1:A:254:LYS:HE3	1:A:306:ALA:HB3	1.84	0.58
1:A:533:GLY:O	1:A:630:PRO:HD2	2.04	0.58
1:A:698:PRO:HG2	1:A:701:LYS:HB2	1.86	0.58
1:A:255:GLU:HG2	1:A:422:THR:OG1	2.04	0.57
1:A:533:GLY:HA3	1:A:631:ASN:HB3	1.88	0.56
1:A:553:MET:SD	1:A:559:PRO:HD3	2.45	0.56
1:A:357:GLY:O	1:A:402:GLU:CG	2.50	0.56
1:A:519:VAL:HG11	1:A:722:HIS:CD2	2.40	0.56
1:A:536:GLU:CD	1:A:628:MET:HE1	2.27	0.55
1:A:430:GLU:OE1	2:A:804:NAG:H82	2.07	0.55
1:A:234:ASN:ND2	1:A:333:GLN:HE22	2.04	0.54
1:A:667:ARG:NH2	1:A:668:ARG:NH2	2.55	0.54
1:A:400:TRP:HB2	1:A:418:ILE:HD11	1.89	0.54
1:A:500:VAL:HG23	1:A:515:ILE:HD11	1.90	0.54
1:A:569:ASN:ND2	1:A:583:HIS:HE1	1.90	0.53
1:A:609:LEU:HB3	1:A:611:MET:CE	2.37	0.53
1:A:641:ASP:O	1:A:714:ARG:HG3	2.10	0.52
1:A:646:SER:OG	1:A:709:HIS:HE1	1.91	0.52
1:A:624:GLN:HB3	1:A:702:VAL:HG13	1.93	0.51
1:A:341:THR:O	1:A:345:GLN:HG3	2.12	0.50
1:A:631:ASN:ND2	2:A:801:NAG:C2	2.64	0.50
1:A:631:ASN:CG	2:A:801:NAG:C1	2.78	0.49
1:A:236:TYR:OH	1:A:349:HIS:CD2	2.64	0.49
1:A:609:LEU:CB	1:A:611:MET:HE2	2.42	0.48
1:A:262:ASP:HB2	1:A:669:PHE:HE2	1.78	0.48
1:A:461:HIS:HE1	4:A:123:HOH:O	1.96	0.48
1:A:623:SER:O	1:A:626:LYS:HE2	2.13	0.48
1:A:393:VAL:HA	1:A:419:LEU:O	2.13	0.48
1:A:585:ASN:O	1:A:589:ASN:HB3	2.14	0.47
1:A:471:THR:HG21	1:A:473:ARG:HH12	1.77	0.47
1:A:625:GLU:HB2	1:A:703:PRO:HG3	1.96	0.47
1:A:463:THR:CG2	1:A:465:LYS:HE2	2.45	0.47
1:A:463:THR:HG22	1:A:465:LYS:HE2	1.95	0.46
1:A:342:MET:O	1:A:346:GLU:HG2	2.14	0.46
1:A:683:ASN:C	1:A:683:ASN:OD1	2.54	0.46
1:A:311:HIS:HD2	4:A:60:HOH:O	1.99	0.46
1:A:686:LEU:O	1:A:695:LYS:CE	2.61	0.45
1:A:227:ILE:HD11	1:A:433:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ALA:HB2	1:A:605:LEU:HD11	1.99	0.45
1:A:239:LEU:N	1:A:239:LEU:HD23	2.32	0.45
1:A:675:GLY:HA2	1:A:710:ILE:O	2.17	0.44
1:A:323:LEU:HD21	1:A:353:LEU:HD11	1.99	0.44
1:A:536:GLU:HG3	1:A:628:MET:CE	2.47	0.44
1:A:643:PHE:HA	1:A:709:HIS:O	2.18	0.44
1:A:379:ASN:ND2	1:A:381:LYS:HD2	2.32	0.44
1:A:270:ASN:ND2	4:A:16:HOH:O	2.51	0.44
1:A:562:LEU:O	1:A:568:ALA:HB2	2.17	0.44
1:A:536:GLU:CG	1:A:628:MET:HE1	2.49	0.43
1:A:289:LEU:HD23	1:A:329:MET:HG3	2.00	0.43
1:A:511:LYS:NZ	1:A:549:GLN:HE22	2.17	0.43
1:A:507:SER:C	1:A:509:TRP:H	2.21	0.42
1:A:379:ASN:H	1:A:382:ARG:HB2	1.85	0.41
1:A:609:LEU:CB	1:A:611:MET:CE	2.99	0.41
1:A:331:ASN:HD21	1:A:335:ARG:HH21	1.67	0.41
1:A:536:GLU:CG	1:A:628:MET:CE	2.99	0.41
1:A:239:LEU:HD22	1:A:354:LEU:HD12	2.01	0.41
1:A:672:PHE:CD1	1:A:672:PHE:N	2.89	0.41
1:A:526:VAL:HA	1:A:537:PHE:O	2.21	0.41
1:A:507:SER:HB2	1:A:509:TRP:H	1.86	0.41
1:A:338:GLY:C	1:A:340:GLU:H	2.24	0.41
1:A:419:LEU:HD21	1:A:428:VAL:HG21	2.02	0.40
1:A:318:ASN:OD1	1:A:362:GLY:HA3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLU:OE1	1:A:699:ARG:NH2[2_545]	1.98	0.22

## 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	484/509 (95%)	463 (96%)	19 (4%)	2 (0%)	39	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	LEU
1	A	635	VAL

### 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	428/447 (96%)	396 (92%)	32 (8%)	17	21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	LEU
1	A	246	SER
1	A	258	SER
1	A	259	LEU
1	A	290	ASN
1	A	302	SER
1	A	303	LEU
1	A	379	ASN
1	A	381	LYS
1	A	396	LEU
1	A	401	ARG
1	A	421	ASP
1	A	423	LYS
1	A	425	LEU
1	A	465	LYS
1	A	471	THR
1	A	480	GLN
1	A	507	SER

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Mol	Chain	Res	Type
1	A	535	LEU
1	A	545	LEU
1	A	562	LEU
1	A	566	MET
1	A	583	HIS
1	A	589	ASN
1	A	636	ARG
1	A	667	ARG
1	A	668	ARG
1	A	693	SER
1	A	695	LYS
1	A	706	ARG
1	A	711	ASN
1	A	719	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	290	ASN
1	A	311	HIS
1	A	331	ASN
1	A	332	ASN
1	A	333	GLN
1	A	349	HIS
1	A	379	ASN
1	A	426	HIS
1	A	461	HIS
1	A	480	GLN
1	A	532	GLN
1	A	549	GLN
1	A	569	ASN
1	A	583	HIS
1	A	589	ASN
1	A	591	GLN
1	A	608	ASN
1	A	631	ASN
1	A	709	HIS
1	A	711	ASN
1	A	722	HIS

### 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 ⓘ

6 carbohydrates 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$
2	NAG	A	801	1,2	14,14,15	0.82	0	15,19,21	1.69	3 (20%)
2	NAG	A	802	2	14,14,15	0.67	0	15,19,21	2.16	1 (6%)
2	NAG	A	803	2	14,14,15	0.74	0	15,19,21	1.31	2 (13%)
2	NAG	A	804	1,2	14,14,15	1.22	2 (14%)	15,19,21	1.44	4 (26%)
2	NAG	A	805	2	14,14,15	1.02	1 (7%)	15,19,21	2.23	5 (33%)
2	NAG	A	806	2	14,14,15	0.76	0	15,19,21	3.32	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
2	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	NAG	A	803	2	-	0/6/23/26	0/1/1/1
2	NAG	A	804	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	805	2	-	0/6/23/26	0/1/1/1
2	NAG	A	806	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	805	NAG	O5-C1	-3.06	1.38	1.43
2	A	804	NAG	C1-C2	2.27	1.55	1.52
2	A	804	NAG	C4-C3	2.29	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	805	NAG	O7-C7-C8	-2.85	116.84	122.06
2	A	805	NAG	O4-C4-C5	-2.82	101.75	109.24
2	A	805	NAG	C3-C4-C5	-2.59	105.69	110.20
2	A	801	NAG	O4-C4-C3	-2.57	104.54	110.34
2	A	801	NAG	O3-C3-C4	-2.56	104.57	110.34
2	A	803	NAG	O7-C7-C8	-2.09	118.22	122.06
2	A	804	NAG	C2-N2-C7	2.04	125.66	123.04
2	A	804	NAG	O4-C4-C5	2.20	115.08	109.24
2	A	804	NAG	C6-C5-C4	2.34	118.78	113.02
2	A	806	NAG	O5-C5-C6	2.59	112.96	107.35
2	A	804	NAG	C1-O5-C5	2.62	115.57	112.25
2	A	805	NAG	O4-C4-C3	2.88	116.81	110.34
2	A	803	NAG	C1-O5-C5	3.09	116.17	112.25
2	A	801	NAG	C3-C4-C5	3.64	116.54	110.20
2	A	805	NAG	C1-O5-C5	5.47	119.19	112.25
2	A	806	NAG	C2-N2-C7	5.57	130.20	123.04
2	A	802	NAG	C1-O5-C5	7.62	121.91	112.25
2	A	806	NAG	C1-O5-C5	10.86	126.03	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	4	0
2	A	804	NAG	1	0

## 5.6 Ligand geometry

2 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	807	1	14,14,15	0.94	1 (7%)	15,19,21	2.06	7 (46%)
3	NAG	A	808	1	14,14,15	1.08	1 (7%)	15,19,21	2.29	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	NAG	A	807	1	-	0/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	807	NAG	O5-C1	-2.33	1.39	1.43
3	A	808	NAG	C1-C2	2.52	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	807	NAG	C3-C4-C5	-3.05	104.87	110.20
3	A	807	NAG	C4-C3-C2	-2.66	107.09	111.23
3	A	807	NAG	O3-C3-C2	-2.45	104.25	109.11
3	A	808	NAG	C8-C7-N2	2.12	120.17	116.11
3	A	807	NAG	C1-O5-C5	2.18	115.02	112.25
3	A	807	NAG	O4-C4-C5	2.28	115.28	109.24
3	A	808	NAG	O3-C3-C4	2.79	116.62	110.34
3	A	807	NAG	O4-C4-C3	3.50	118.21	110.34
3	A	807	NAG	C2-N2-C7	3.81	127.93	123.04
3	A	808	NAG	C1-O5-C5	7.07	121.23	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 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, 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	492/509 (96%)	-0.04	12 (2%) 62 71	15, 28, 48, 59	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	LYS	3.3
1	A	395	LYS	2.8
1	A	725	ASP	2.8
1	A	702	VAL	2.7
1	A	576	GLN	2.6
1	A	703	PRO	2.5
1	A	633	THR	2.3
1	A	291	ASP	2.2
1	A	613	VAL	2.2
1	A	342	MET	2.1
1	A	397	ASP	2.1
1	A	641	ASP	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](#)

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
2	NAG	A	801	14/15	0.89	0.15	-0.39	46,50,55,61	0
2	NAG	A	804	14/15	0.93	0.11	-0.59	23,30,33,34	0
2	NAG	A	803	14/15	0.83	0.27	-	57,61,63,64	0
2	NAG	A	806	14/15	0.65	0.32	-	63,69,76,76	0
2	NAG	A	802	14/15	0.91	0.29	-	64,69,74,76	0
2	NAG	A	805	14/15	0.95	0.14	-	32,35,44,55	0

## 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	808	14/15	0.77	0.23	1.82	46,52,57,58	0
3	NAG	A	807	14/15	0.94	0.19	1.35	36,45,51,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.