



# Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 08:12 PM GMT

PDB ID : 1BCR  
Title : COMPLEX OF THE WHEAT SERINE CARBOXYPEPTIDASE, CPDW-II,  
WITH THE MICROBIAL PEPTIDE ALDEHYDE INHIBITOR, ANTIPAIN,  
AND ARGININE AT ROOM TEMPERATURE  
Authors : Bullock, T.L.; Remington, S.J.  
Deposited on : 1995-11-03  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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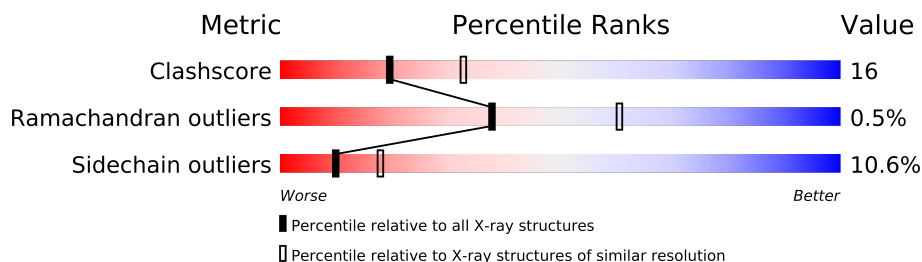
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	263	
2	B	160	
3	C	4	

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 3489 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1991	1274	333	377	7			

- Molecule 2 is a protein called SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1196	768	205	217	6			

- Molecule 3 is a protein called ANTIPAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			18	11	5	2			

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

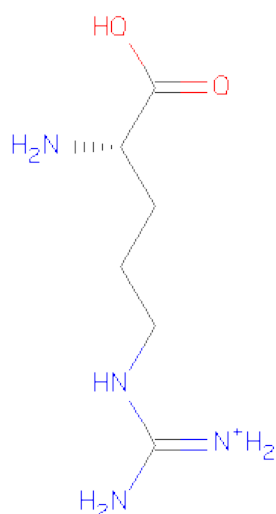


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is ARGININE (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	113	Total	O	0	0
			113	113		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	76	Total 76	O 76	0	0
8	C	3	Total 3	O 3	0	0

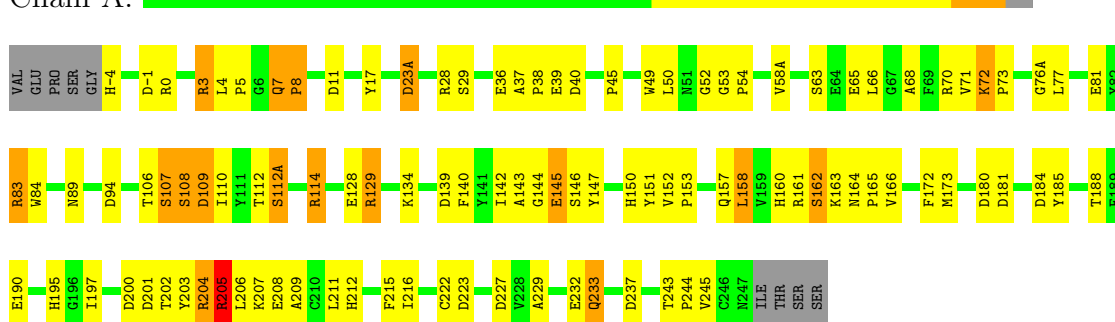
### 3 Residue-property plots

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.

Note EDS was not executed.

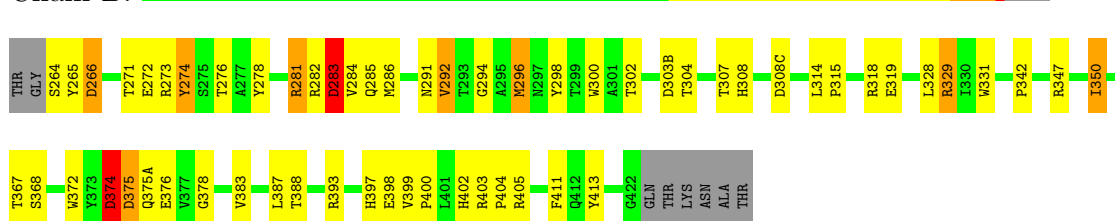
#### • Molecule 1: SERINE CARBOXYPEPTIDASE II

Chain A:



#### • Molecule 2: SERINE CARBOXYPEPTIDASE II

Chain B:



#### • Molecule 3: ANTIPAIN

Chain C:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.40Å 98.40Å 209.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (21.00-2.50)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3489	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, OAR, 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	1.09	6/2054 (0.3%)	1.50	43/2803 (1.5%)
2	B	1.02	3/1236 (0.2%)	1.43	17/1693 (1.0%)
3	C	1.53	0/6	2.13	0/7
All	All	1.07	9/3296 (0.3%)	1.48	60/4503 (1.3%)

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
5	A	1	0
7	B	1	0
All	All	2	0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLU	CD-OE1	7.52	1.33	1.25
1	A	208	GLU	CD-OE1	7.50	1.33	1.25
1	A	39	GLU	CD-OE1	7.29	1.33	1.25
2	B	376	GLU	CD-OE2	6.85	1.33	1.25
1	A	128	GLU	CD-OE2	5.66	1.31	1.25
2	B	272	GLU	CD-OE1	5.55	1.31	1.25
2	B	398	GLU	CD-OE2	5.54	1.31	1.25
1	A	232	GLU	CD-OE2	-5.51	1.19	1.25
1	A	190	GLU	CD-OE1	5.09	1.31	1.25

All (60) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH1	15.69	128.14	120.30
1	A	114	ARG	NE-CZ-NH2	-12.20	114.20	120.30
2	B	266	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	A	129	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	203	TYR	CB-CG-CD2	-8.57	115.86	121.00
1	A	223	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	A	139	ASP	CB-CG-OD1	-7.84	111.25	118.30
1	A	200	ASP	CB-CG-OD1	7.65	125.18	118.30
2	B	347	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	A	205	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	B	283	ASP	N-CA-CB	-7.52	97.07	110.60
1	A	204	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	94	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	145	GLU	CB-CA-C	-7.15	96.11	110.40
2	B	266	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	200	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	A	140	PHE	N-CA-CB	-6.96	98.08	110.60
1	A	11	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	23(A)	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	-1	ASP	CB-CG-OD1	-6.83	112.15	118.30
2	B	413	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	A	23(A)	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	139	ASP	CB-CG-OD2	6.46	124.11	118.30
2	B	393	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	203	TYR	CB-CG-CD1	6.34	124.80	121.00
1	A	180	ASP	CB-CG-OD1	-6.32	112.62	118.30
1	A	11	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	223	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	227	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	A	151	TYR	CB-CG-CD1	6.16	124.69	121.00
1	A	181	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	201	ASP	CB-CG-OD1	-6.08	112.83	118.30
2	B	374	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	A	180	ASP	CB-CG-OD2	6.03	123.73	118.30
2	B	308(C)	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	40	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	17	TYR	CB-CA-C	-5.92	98.57	110.40
2	B	294	GLY	C-N-CA	5.92	136.49	121.70
2	B	307	THR	CA-CB-CG2	-5.89	104.16	112.40
1	A	114	ARG	CD-NE-CZ	5.87	131.81	123.60
2	B	283	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	A	151	TYR	CB-CG-CD2	-5.86	117.48	121.00
2	B	303(B)	ASP	CB-CG-OD2	-5.84	113.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	GLU	CB-CG-CD	-5.73	98.72	114.20
1	A	94	ASP	CB-CG-OD1	5.57	123.31	118.30
2	B	375	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	83	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	184	ASP	CB-CG-OD2	5.39	123.15	118.30
2	B	329	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	109	ASP	CB-CG-OD1	5.30	123.07	118.30
2	B	273	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	109	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	45	PRO	N-CA-CB	5.20	109.54	103.30
1	A	201	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	274	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	81	GLU	CB-CA-C	-5.12	100.17	110.40
1	A	237	ASP	CB-CG-OD1	-5.12	113.70	118.30
2	B	347	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	181	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	0	ARG	NE-CZ-NH1	5.03	122.81	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1132	FUC	C5
7	B	2912	NAG	C2

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1991	0	1839	65	0
2	B	1196	0	1130	41	0
3	C	18	0	20	6	0
4	A	14	0	13	2	0
5	A	38	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	12	0	12	7	0
7	B	28	0	24	4	0
8	A	113	0	0	7	0
8	B	76	0	0	4	0
8	C	3	0	0	0	0
All	All	3489	0	3072	103	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (103) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:THR:HG23	1:A:114:ARG:HH22	1.08	1.08
1:A:5:PRO:HG2	2:B:284:VAL:HG22	1.47	0.94
1:A:3:ARG:HB3	1:A:3:ARG:HH11	1.40	0.85
1:A:112:THR:CG2	1:A:114:ARG:HH22	1.90	0.82
1:A:112:THR:HG23	1:A:114:ARG:NH2	1.92	0.82
1:A:5:PRO:HG2	2:B:284:VAL:CG2	2.13	0.78
1:A:134:LYS:HD3	1:A:166:VAL:HG11	1.66	0.76
1:A:164:ASN:OD1	1:A:166:VAL:HG22	1.92	0.69
1:A:53:GLY:H	3:C:4:OAR:HO	1.39	0.69
1:A:36:GLU:HB3	1:A:89:ASN:OD1	1.92	0.68
1:A:134:LYS:HD3	1:A:166:VAL:CG1	2.23	0.68
1:A:108:SER:O	1:A:112:THR:HG22	1.95	0.67
2:B:296:MET:HE2	7:B:2911:NAG:O7	1.96	0.66
1:A:3:ARG:HH11	1:A:3:ARG:CB	2.09	0.64
1:A:229:ALA:O	1:A:233:GLN:HG3	1.97	0.64
2:B:281:ARG:O	2:B:285:GLN:HG3	1.97	0.64
1:A:7:GLN:HG2	1:A:8:PRO:O	1.98	0.62
2:B:291:ASN:OD1	2:B:296:MET:HG3	1.99	0.62
1:A:152:VAL:HB	1:A:153:PRO:HD3	1.82	0.62
1:A:205:ARG:NH1	8:A:1216:HOH:O	2.31	0.62
1:A:71:VAL:HG12	1:A:72:LYS:O	2.01	0.61
6:A:426:ARG:N	3:C:4:OAR:HO	1.98	0.61
1:A:173:MET:HA	2:B:331:TRP:O	2.00	0.61
1:A:84:TRP:HB3	2:B:411:PHE:CE2	2.36	0.60
2:B:329:ARG:HD3	8:B:129:HOH:O	2.03	0.59
2:B:374:ASP:HB3	8:B:178:HOH:O	2.02	0.59
2:B:282:ARG:O	2:B:286:MET:HB2	2.03	0.59
1:A:4:LEU:H	1:A:7:GLN:NE2	2.01	0.58
2:B:300:TRP:HB2	7:B:2911:NAG:H81	1.84	0.58
1:A:209:ALA:HB1	1:A:222:CYS:HA	1.84	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:52:GLY:N	6:A:426:ARG:O	2.35	0.57
1:A:243:THR:HB	1:A:244:PRO:HD2	1.85	0.57
1:A:150:HIS:O	1:A:153:PRO:HD2	2.06	0.56
1:A:195:HIS:NE2	8:A:1148:HOH:O	2.32	0.56
1:A:70:ARG:HG3	1:A:70:ARG:HH11	1.69	0.56
4:A:1131:NAG:C3	4:A:1131:NAG:H82	2.36	0.56
4:A:1131:NAG:O3	4:A:1131:NAG:H82	2.05	0.56
1:A:114:ARG:HD2	8:A:1170:HOH:O	2.08	0.54
2:B:387:LEU:C	2:B:387:LEU:HD23	2.28	0.54
1:A:109:ASP:HA	1:A:112:THR:CG2	2.40	0.52
1:A:188:THR:HA	2:B:342:PRO:HG2	1.92	0.52
6:A:426:ARG:N	3:C:4:OAR:HC1	2.25	0.52
1:A:146:SER:OG	1:A:147:TYR:N	2.43	0.51
1:A:72:LYS:HD3	1:A:76(A):GLY:C	2.31	0.51
1:A:65:GLU:OE1	1:A:145:GLU:OE2	2.28	0.50
1:A:58(A):VAL:HB	8:A:1178:HOH:O	2.11	0.50
2:B:278:TYR:O	2:B:281:ARG:HG3	2.12	0.49
2:B:399:VAL:HB	2:B:400:PRO:HD3	1.95	0.49
2:B:300:TRP:HB2	7:B:2911:NAG:C8	2.42	0.49
2:B:265:TYR:CE1	2:B:402:HIS:CE1	3.01	0.49
1:A:72:LYS:HB3	1:A:73:PRO:HD2	1.94	0.49
1:A:-4:HIS:N	8:A:1242:HOH:O	2.45	0.49
2:B:274:TYR:N	2:B:274:TYR:CD1	2.75	0.49
1:A:202:THR:HG22	1:A:206:LEU:HD11	1.95	0.49
1:A:112(A):SER:HB3	8:A:1230:HOH:O	2.12	0.48
2:B:342:PRO:HA	8:B:2:HOH:O	2.13	0.48
1:A:7:GLN:HB2	1:A:77:LEU:HD12	1.95	0.48
2:B:283:ASP:O	2:B:286:MET:HB3	2.14	0.48
1:A:160:HIS:HE1	8:B:128:HOH:O	1.96	0.47
2:B:298:TYR:O	7:B:2911:NAG:H3	2.14	0.47
1:A:207:LYS:O	1:A:211:LEU:HG	2.14	0.46
2:B:276:THR:HA	2:B:300:TRP:HZ3	1.79	0.46
1:A:70:ARG:HG3	1:A:70:ARG:NH1	2.30	0.46
2:B:374:ASP:O	2:B:375:ASP:HB2	2.15	0.46
6:A:426:ARG:N	3:C:4:OAR:C	2.79	0.46
1:A:28:ARG:HD3	1:A:109:ASP:OD2	2.17	0.45
2:B:367:THR:HB	2:B:383:VAL:HB	1.99	0.45
2:B:266:ASP:O	2:B:271:THR:HG23	2.17	0.45
1:A:145:GLU:OE1	6:A:426:ARG:OXT	2.35	0.44
2:B:403:ARG:N	2:B:404:PRO:HD3	2.33	0.44
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.62	0.44
2:B:314:LEU:N	2:B:315:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:276:THR:HA	2:B:300:TRP:CZ3	2.53	0.44
2:B:314:LEU:O	2:B:318:ARG:HG3	2.18	0.44
2:B:296:MET:HE3	2:B:296:MET:HB3	1.77	0.43
1:A:152:VAL:N	1:A:153:PRO:CD	2.81	0.43
1:A:53:GLY:HA3	1:A:54:PRO:C	2.38	0.43
1:A:209:ALA:CB	1:A:222:CYS:HA	2.48	0.43
1:A:146:SER:HB2	2:B:397:HIS:NE2	2.33	0.43
1:A:53:GLY:N	6:A:426:ARG:N	2.67	0.43
1:A:164:ASN:OD1	1:A:165:PRO:HD2	2.19	0.43
2:B:375:ASP:HB3	2:B:375(A):GLN:H	1.46	0.43
1:A:162:SER:O	1:A:163:LYS:HB2	2.19	0.42
1:A:157:GLN:NE2	2:B:319:GLU:OE1	2.39	0.42
1:A:72:LYS:O	2:B:274:TYR:HB3	2.20	0.42
2:B:403:ARG:N	2:B:404:PRO:CD	2.80	0.41
1:A:142:ILE:O	1:A:172:PHE:HB2	2.20	0.41
1:A:37:ALA:HB1	1:A:38:PRO:HD2	2.03	0.41
2:B:350:ILE:N	2:B:350:ILE:HD13	2.35	0.41
6:A:426:ARG:N	3:C:4:OAR:O	2.53	0.41
1:A:106:THR:O	1:A:108:SER:N	2.52	0.41
1:A:53:GLY:N	3:C:4:OAR:HO	2.11	0.41
2:B:271:THR:HG23	2:B:271:THR:H	1.61	0.41
2:B:304:THR:O	2:B:308:HIS:HD2	2.04	0.41
1:A:68:ALA:HA	1:A:83:ARG:HB3	2.03	0.41
2:B:387:LEU:HD23	2:B:388:THR:N	2.36	0.40
1:A:50:LEU:O	1:A:144:GLY:HA3	2.21	0.40
1:A:-4:HIS:HB3	1:A:129:ARG:HG2	2.02	0.40
1:A:212:HIS:HB2	8:A:1214:HOH:O	2.22	0.40
1:A:49:TRP:HA	1:A:143:ALA:O	2.20	0.40
1:A:209:ALA:HB1	1:A:222:CYS:CA	2.51	0.40
2:B:372:TRP:CH2	2:B:378:GLY:HA3	2.57	0.40
1:A:71:VAL:HG12	2:B:274:TYR:HB3	2.03	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	252/263 (96%)	238 (94%)	13 (5%)	1 (0%)	43	66
2	B	150/160 (94%)	140 (93%)	9 (6%)	1 (1%)	30	50
All	All	402/423 (95%)	378 (94%)	22 (6%)	2 (0%)	38	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	SER
2	B	292	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	204/215 (95%)	181 (89%)	23 (11%)	9	15
2	B	123/133 (92%)	112 (91%)	11 (9%)	14	26
3	C	1/2 (50%)	1 (100%)	0	100	100
All	All	328/350 (94%)	294 (90%)	34 (10%)	10	18

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	GLN
1	A	8	PRO
1	A	23(A)	ASP
1	A	29	SER
1	A	63	SER
1	A	66	LEU
1	A	72	LYS
1	A	107	SER
1	A	108	SER
1	A	110	ILE
1	A	112(A)	SER
1	A	158	LEU
1	A	161	ARG

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Mol	Chain	Res	Type
1	A	162	SER
1	A	185	TYR
1	A	197	ILE
1	A	204	ARG
1	A	205	ARG
1	A	215	PHE
1	A	216	ILE
1	A	233	GLN
1	A	245	VAL
2	B	264	SER
2	B	281	ARG
2	B	283	ASP
2	B	292	VAL
2	B	296	MET
2	B	302	THR
2	B	328	LEU
2	B	350	ILE
2	B	368	SER
2	B	374	ASP
2	B	405	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	117	HIS
1	A	217	HIS
1	A	233	GLN
2	B	308	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	OAR	C	4	1,3	10,10,10	1.06	0	11,11,11	2.11	2 (18%)

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	OAR	C	4	1,3	-	0/9/9/9	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	OAR	C-CA-N1	5.03	122.16	110.16
3	C	4	OAR	CB-CA-C	-3.41	107.78	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

5 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	$\# Z  > 2$
5	FUC	A	1132	5	9,10,11	2.09	2 (22%)	10,14,16	4.88	7 (70%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1133	1,5	12,14,15	0.87	0	15,19,21	2.07	4 (26%)
5	NAG	A	1134	5	12,14,15	2.00	4 (33%)	15,19,21	3.58	6 (40%)
7	NAG	B	2911	2,7	12,14,15	0.76	0	15,19,21	2.76	5 (33%)
7	NAG	B	2912	7	12,14,15	1.53	2 (16%)	15,19,21	3.49	7 (46%)

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
5	FUC	A	1132	5	1/1/4/5	0/0/17/20	0/1/1/1
5	NAG	A	1133	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1134	5	-	0/6/23/26	0/1/1/1
7	NAG	B	2911	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	2912	7	1/1/5/7	1/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1132	FUC	O5-C5	5.19	1.55	1.45
5	A	1134	NAG	O4-C4	4.81	1.54	1.43
7	B	2912	NAG	C2-N2	3.27	1.50	1.46
5	A	1132	FUC	C4-C3	3.01	1.60	1.52
7	B	2912	NAG	C4-C5	2.64	1.58	1.53
5	A	1134	NAG	C3-C2	2.59	1.57	1.52
5	A	1134	NAG	C4-C5	2.33	1.58	1.53
5	A	1134	NAG	C4-C3	2.22	1.58	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1134	NAG	O6-C6-C5	11.47	150.83	111.36
5	A	1132	FUC	C4-C3-C2	-10.10	96.95	110.50
5	A	1132	FUC	O3-C3-C2	9.84	127.94	109.94
7	B	2912	NAG	C3-C2-N2	8.11	124.11	111.76
7	B	2911	NAG	O6-C6-C5	7.48	137.09	111.36
7	B	2912	NAG	O5-C5-C4	5.77	117.97	110.65
7	B	2912	NAG	O6-C6-C5	5.72	131.06	111.36
7	B	2911	NAG	O5-C5-C4	4.48	116.34	110.65
5	A	1133	NAG	O6-C6-C5	-4.40	96.22	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1133	NAG	O5-C5-C6	-4.20	102.58	106.98
7	B	2912	NAG	C3-C4-C5	4.05	117.43	110.20
7	B	2912	NAG	O7-C7-C8	-4.04	114.15	122.04
7	B	2911	NAG	C3-C4-C5	4.00	117.34	110.20
5	A	1133	NAG	C3-C2-N2	-3.88	105.86	111.76
5	A	1134	NAG	C3-C2-N2	3.83	117.59	111.76
5	A	1134	NAG	O4-C4-C5	3.68	118.97	109.28
5	A	1132	FUC	O2-C2-C3	3.66	118.08	110.18
5	A	1134	NAG	O4-C4-C3	3.53	118.26	110.35
5	A	1132	FUC	C6-C5-C4	2.71	117.47	113.06
5	A	1132	FUC	O3-C3-C4	-2.60	104.53	110.35
7	B	2912	NAG	C2-N2-C7	2.60	127.45	123.09
5	A	1132	FUC	O5-C5-C4	2.29	113.68	110.22
5	A	1134	NAG	C3-C4-C5	2.26	114.25	110.20
7	B	2911	NAG	O4-C4-C5	-2.18	103.54	109.28
5	A	1134	NAG	O5-C5-C4	2.12	113.35	110.65
5	A	1133	NAG	O3-C3-C2	-2.12	104.63	109.09
7	B	2911	NAG	O3-C3-C2	2.04	113.38	109.09
7	B	2912	NAG	O7-C7-N2	2.04	126.16	121.90
5	A	1132	FUC	C3-C4-C5	-2.02	106.47	109.84

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1132	FUC	C5
7	B	2912	NAG	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2912	NAG	C8-C7-N2-C2

There are no ring outliers.

## 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	$\# Z  > 2$
4	NAG	A	1131	1	12,14,15	0.88	0	15,19,21	1.71	5 (33%)
6	ARG	A	426	-	11,11,11	0.80	0	13,13,13	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1131	1	1/1/5/7	0/6/23/26	0/1/1/1
6	ARG	A	426	-	-	0/11/11/11	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1131	NAG	C3-C2-N2	2.94	116.24	111.76
4	A	1131	NAG	O6-C6-C5	2.61	120.35	111.36
4	A	1131	NAG	C4-C3-C2	-2.58	105.00	111.32
4	A	1131	NAG	C2-N2-C7	2.44	127.18	123.09
4	A	1131	NAG	O7-C7-C8	-2.22	117.71	122.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1131	NAG	C2

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.