



# Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 08:12 PM GMT

PDB ID : 1BCS  
Title : COMPLEX OF THE WHEAT SERINE CARBOXYPEPTIDASE, CPDW-II,  
WITH THE MICROBIAL PEPTIDE ALDEHYDE INHIBITOR, CHYMO-  
STATIN, AND ARGININE AT 100 DEGREES KELVIN  
Authors : Bullock, T.L.; Remington, S.J.  
Deposited on : 1995-11-03  
Resolution : 2.08 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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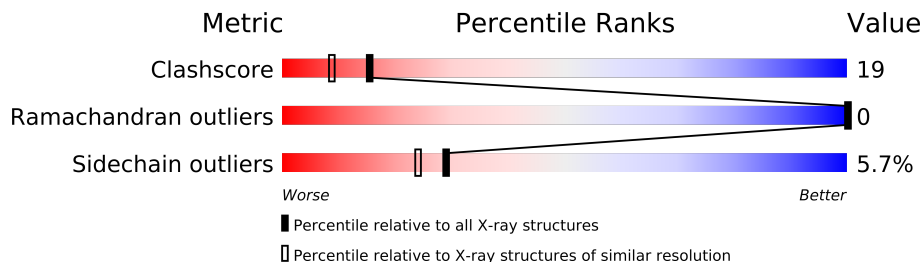
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.08 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	4085 (2.10-2.06)
Ramachandran outliers	78287	4045 (2.10-2.06)
Sidechain outliers	78261	4046 (2.10-2.06)

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

There are 10 unique types of molecules in this entry. The entry contains 3731 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	255	Total	C	N	O	S	0	0	0
			1999	1280	334	378	7			

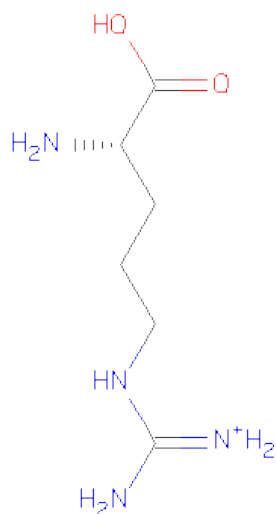
- Molecule 2 is a protein called SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1202	771	207	218	6			

- Molecule 3 is a protein called CHYMOSTATIN A.

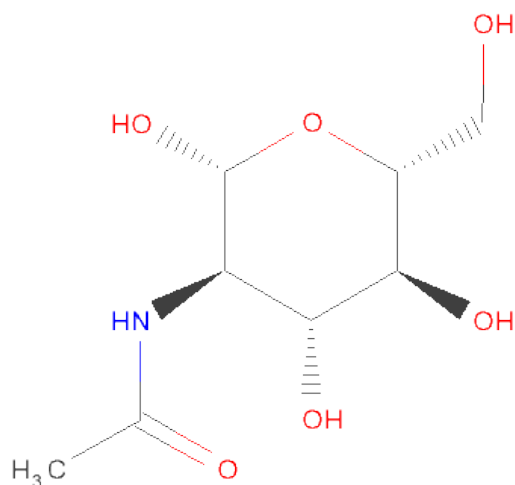
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			44	31	7	6			

- Molecule 4 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

- 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 ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	157	Total 157	O 157	0	0
10	C	1	Total 1	O 1	0	0
10	A	226	Total 226	O 226	0	0

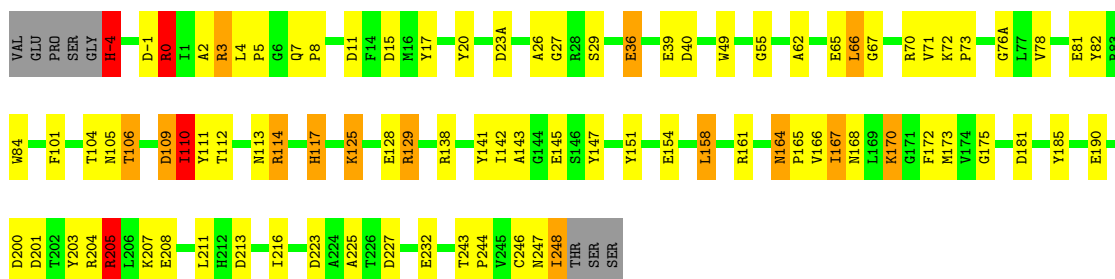
### 3 Residue-property plots

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.

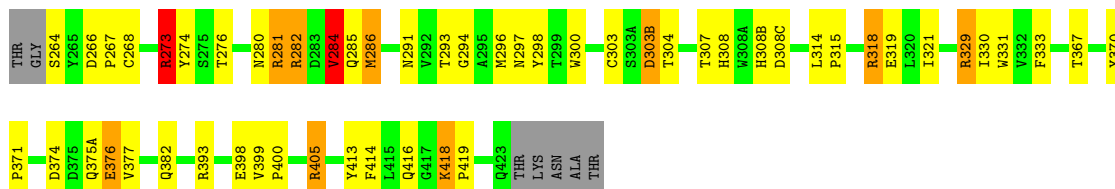
#### • Molecule 1: SERINE CARBOXYPEPTIDASE II

Chain A: 



#### • Molecule 2: SERINE CARBOXYPEPTIDASE II

Chain B: 



#### • Molecule 3: CHYMOSTATIN A

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, $\alpha$ , $\beta$ , $\gamma$	95.40Å 95.40Å 208.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.08	Depositor
% Data completeness (in resolution range)	(Not available) (33.00-2.08)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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: GOL, CSI, NAG, PHA, NDG, FUC, ACT

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	1.13	11/2062 (0.5%)	1.63	36/2814 (1.3%)
2	B	1.10	4/1242 (0.3%)	1.83	30/1702 (1.8%)
3	C	1.10	0/19	1.36	0/21
All	All	1.12	15/3323 (0.5%)	1.71	66/4537 (1.5%)

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
3	C	1	0
6	A	1	0
7	B	3	0
All	All	5	0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLU	CD-OE1	8.44	1.34	1.25
2	B	398	GLU	CD-OE2	7.63	1.34	1.25
1	A	81	GLU	CD-OE1	7.49	1.33	1.25
1	A	232	GLU	CD-OE1	6.67	1.32	1.25
1	A	154	GLU	CD-OE2	6.63	1.32	1.25
1	A	128	GLU	CD-OE2	6.56	1.32	1.25
1	A	65	GLU	CD-OE2	6.28	1.32	1.25
2	B	376	GLU	CD-OE2	5.98	1.32	1.25
1	A	39	GLU	CD-OE2	5.96	1.32	1.25
1	A	36	GLU	CD-OE2	5.95	1.32	1.25
2	B	319	GLU	CD-OE2	5.79	1.32	1.25
1	A	190	GLU	CD-OE1	5.77	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ASN	C-N	-5.30	1.24	1.34
1	A	36	GLU	CD-OE1	-5.29	1.19	1.25
2	B	416	GLN	CG-CD	5.07	1.62	1.51

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH1	19.18	129.89	120.30
2	B	393	ARG	NE-CZ-NH2	-16.96	111.82	120.30
2	B	329	ARG	NE-CZ-NH1	16.47	128.54	120.30
2	B	393	ARG	NE-CZ-NH1	16.37	128.49	120.30
2	B	329	ARG	NE-CZ-NH2	-16.15	112.22	120.30
1	A	114	ARG	NE-CZ-NH2	-15.97	112.31	120.30
2	B	405	ARG	NE-CZ-NH1	13.32	126.96	120.30
1	A	205	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	A	205	ARG	NE-CZ-NH2	-10.22	115.19	120.30
2	B	266	ASP	CB-CG-OD2	-8.99	110.21	118.30
2	B	405	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	129	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	11	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	A	200	ASP	CB-CG-OD1	8.43	125.88	118.30
1	A	181	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	A	200	ASP	CB-CG-OD2	-8.14	110.98	118.30
2	B	303(B)	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	A	-4	HIS	N-CA-CB	7.98	124.96	110.60
2	B	393	ARG	CD-NE-CZ	7.92	134.69	123.60
2	B	329	ARG	CD-NE-CZ	7.88	134.64	123.60
2	B	273	ARG	NE-CZ-NH1	7.63	124.11	120.30
2	B	266	ASP	CB-CG-OD1	7.62	125.16	118.30
2	B	303(B)	ASP	CB-CG-OD1	7.48	125.03	118.30
2	B	318	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	110	ILE	N-CA-CB	-7.31	93.98	110.80
1	A	161	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	40	ASP	CB-CG-OD1	-7.26	111.77	118.30
1	A	114	ARG	CD-NE-CZ	7.25	133.75	123.60
1	A	11	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	181	ASP	CB-CG-OD1	7.03	124.62	118.30
1	A	110	ILE	CB-CG1-CD1	-6.88	94.64	113.90
1	A	201	ASP	CB-CG-OD2	-6.80	112.18	118.30
2	B	286	MET	CG-SD-CE	6.70	110.91	100.20
2	B	398	GLU	CA-CB-CG	-6.60	98.88	113.40
1	A	151	TYR	CB-CG-CD1	6.34	124.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	TYR	CB-CG-CD1	-6.29	117.23	121.00
2	B	282	ARG	CB-CA-C	6.20	122.80	110.40
1	A	201	ASP	CB-CG-OD1	6.07	123.76	118.30
2	B	405	ARG	CD-NE-CZ	6.04	132.06	123.60
1	A	15	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	205	ARG	CD-NE-CZ	6.01	132.01	123.60
2	B	281	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	161	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	-1	ASP	CB-CG-OD1	-5.82	113.07	118.30
1	A	147	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	A	40	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	223	ASP	CB-CG-OD1	-5.72	113.15	118.30
2	B	273	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	B	281	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	B	284	VAL	CA-CB-CG1	5.61	119.31	110.90
2	B	284	VAL	CA-CB-CG2	5.54	119.21	110.90
1	A	-1	ASP	CB-CG-OD2	5.47	123.23	118.30
2	B	375(A)	GLN	CB-CA-C	5.47	121.34	110.40
2	B	413	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	A	0	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	A	227	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	106	THR	N-CA-CB	-5.37	100.11	110.30
2	B	416	GLN	CA-CB-CG	5.33	125.12	113.40
2	B	308(C)	ASP	CB-CG-OD1	5.30	123.07	118.30
2	B	318	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	117	HIS	CA-CB-CG	-5.28	104.62	113.60
2	B	318	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	109	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	213	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	158	LEU	CB-CA-C	-5.15	100.42	110.20
2	B	307	THR	CA-CB-CG2	-5.06	105.31	112.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1134	NDG	C2
7	B	2912	NAG	C2,C5,C1
3	C	2	CSI	CB

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	1999	0	1853	74	0
2	B	1202	0	1135	55	0
3	C	44	0	36	3	0
4	A	12	0	12	1	0
5	A	14	0	13	7	0
6	A	38	0	34	9	0
7	B	28	0	24	10	0
8	B	4	0	3	1	0
9	A	6	0	8	1	0
10	A	226	0	0	5	0
10	B	157	0	0	6	0
10	C	1	0	0	0	0
All	All	3731	0	3118	121	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 19.

All (121) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:MET:HE1	2:B:414:PHE:HB2	1.42	1.01
1:A:0:ARG:HG3	1:A:17:TYR:CE2	2.08	0.88
1:A:113:ASN:ND2	5:A:1131:NAG:N2	2.26	0.83
1:A:5:PRO:HG2	2:B:284:VAL:HG12	1.64	0.78
2:B:374:ASP:HB3	10:B:3066:HOH:O	1.85	0.76
1:A:105:ASN:HD21	6:A:1133:NAG:C1	2.02	0.73
2:B:296:MET:O	7:B:2911:NAG:H3	1.89	0.72
1:A:4:LEU:H	1:A:7:GLN:NE2	1.87	0.72
2:B:303(B):ASP:HA	3:C:1:PHE:CD2	2.25	0.71
2:B:285:GLN:HE22	7:B:2911:NAG:H83	1.54	0.70
1:A:105:ASN:HD21	6:A:1133:NAG:C2	2.04	0.70
7:B:2911:NAG:O3	7:B:2912:NAG:H61	1.90	0.70
1:A:110:ILE:HG22	1:A:111:TYR:CD1	2.27	0.69
1:A:3:ARG:NH1	1:A:7:GLN:O	2.26	0.68
1:A:-4:HIS:HB3	1:A:129:ARG:O	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:318:ARG:HD3	10:B:3007:HOH:O	1.92	0.68
2:B:291:ASN:HD21	2:B:294:GLY:HA2	1.59	0.67
4:A:426:ARG:N	3:C:4:PHA:O	2.27	0.67
6:A:1134:NDG:H8C3	2:B:293:THR:HG21	1.78	0.65
2:B:304:THR:O	2:B:308:HIS:HD2	1.77	0.65
1:A:164:ASN:OD1	1:A:166:VAL:HG22	1.97	0.65
1:A:71:VAL:HG12	1:A:72:LYS:O	1.98	0.64
2:B:291:ASN:OD1	2:B:296:MET:HB2	1.97	0.63
6:A:1132:FUC:H5	6:A:1134:NDG:C1	2.28	0.63
1:A:0:ARG:HG3	1:A:17:TYR:CZ	2.32	0.63
1:A:125:LYS:HD2	1:A:125:LYS:N	2.13	0.63
1:A:173:MET:HE1	2:B:414:PHE:CB	2.26	0.62
1:A:173:MET:HE3	2:B:414:PHE:CD1	2.35	0.61
1:A:3:ARG:HD2	10:A:1156:HOH:O	2.00	0.61
1:A:205:ARG:HD2	1:A:225:ALA:HB2	1.81	0.61
2:B:297:ASN:HB3	10:B:3033:HOH:O	2.01	0.60
1:A:4:LEU:H	1:A:7:GLN:HE21	1.51	0.59
1:A:248:ILE:HD11	2:B:273:ARG:HG2	1.84	0.59
1:A:207:LYS:O	1:A:211:LEU:HG	2.02	0.59
2:B:300:TRP:HB2	7:B:2911:NAG:H81	1.83	0.58
1:A:105:ASN:HD21	6:A:1133:NAG:H2	1.67	0.58
1:A:104:THR:HG21	1:A:109:ASP:HB2	1.84	0.58
1:A:106:THR:O	1:A:109:ASP:HB2	2.03	0.58
1:A:72:LYS:HD3	1:A:76(A):GLY:C	2.24	0.58
2:B:282:ARG:O	2:B:286:MET:HG3	2.04	0.58
2:B:297:ASN:N	2:B:297:ASN:OD1	2.31	0.57
1:A:173:MET:HE3	2:B:331:TRP:HB2	1.86	0.56
2:B:298:TYR:O	7:B:2911:NAG:N2	2.39	0.56
2:B:291:ASN:ND2	2:B:294:GLY:HA2	2.19	0.56
2:B:321:ILE:HG13	2:B:330:ILE:HD12	1.87	0.56
1:A:205:ARG:HD2	1:A:225:ALA:CB	2.35	0.56
2:B:329:ARG:HD3	10:B:3012:HOH:O	2.06	0.55
1:A:36:GLU:OE1	9:A:450:GOL:H32	2.07	0.55
1:A:105:ASN:ND2	6:A:1133:NAG:H83	2.21	0.55
2:B:281:ARG:HB2	2:B:284:VAL:HG13	1.90	0.54
1:A:105:ASN:ND2	6:A:1133:NAG:C1	2.70	0.54
6:A:1133:NAG:H61	6:A:1134:NDG:H2	1.90	0.53
1:A:101:PHE:HD1	2:B:296:MET:HE1	1.73	0.53
1:A:70:ARG:HB2	1:A:78:VAL:HG23	1.91	0.53
1:A:246:CYS:HA	2:B:267:PRO:HG2	1.89	0.53
1:A:20:TYR:HB3	1:A:29:SER:OG	2.10	0.52
1:A:167:ILE:HA	10:A:1197:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:GLY:HA3	1:A:105:ASN:HB2	1.91	0.52
1:A:203:TYR:O	1:A:207:LYS:HG3	2.11	0.51
2:B:376:GLU:HG3	10:B:3066:HOH:O	2.11	0.51
7:B:2911:NAG:C3	7:B:2912:NAG:H61	2.42	0.50
2:B:374:ASP:CG	2:B:405:ARG:HH11	2.11	0.50
2:B:374:ASP:OD2	2:B:405:ARG:NH1	2.27	0.50
2:B:303(B):ASP:HA	3:C:1:PHE:CE2	2.46	0.50
1:A:113:ASN:ND2	5:A:1131:NAG:C2	2.76	0.49
1:A:142:ILE:O	1:A:172:PHE:HA	2.13	0.49
1:A:216:ILE:HG22	10:A:1236:HOH:O	2.11	0.49
1:A:7:GLN:HG2	1:A:8:PRO:O	2.13	0.49
1:A:66:LEU:HB2	1:A:84:TRP:CG	2.48	0.49
1:A:138:ARG:O	1:A:168:ASN:HB3	2.12	0.49
2:B:274:TYR:N	2:B:274:TYR:CD1	2.75	0.48
1:A:72:LYS:HB3	1:A:73:PRO:HD2	1.96	0.47
2:B:314:LEU:N	2:B:315:PRO:CD	2.77	0.47
2:B:308(B):HIS:N	2:B:308(B):HIS:CD2	2.81	0.47
7:B:2911:NAG:O3	7:B:2912:NAG:O5	2.28	0.47
2:B:291:ASN:ND2	7:B:2911:NAG:C1	2.78	0.47
1:A:114:ARG:HD2	10:A:1165:HOH:O	2.13	0.47
1:A:145:GLU:HA	1:A:175:GLY:O	2.14	0.47
2:B:370:TYR:HB2	2:B:371:PRO:HD2	1.95	0.47
1:A:173:MET:HA	2:B:331:TRP:O	2.15	0.46
1:A:243:THR:HB	1:A:244:PRO:HD2	1.96	0.46
1:A:175:GLY:HA3	2:B:333:PHE:CZ	2.51	0.46
1:A:164:ASN:OD1	1:A:165:PRO:HD2	2.16	0.46
1:A:141:TYR:CE2	1:A:170:LYS:HB2	2.51	0.46
2:B:377:VAL:H	8:B:461:ACT:H2	1.79	0.46
2:B:291:ASN:ND2	7:B:2911:NAG:O5	2.49	0.46
1:A:72:LYS:HD3	1:A:76(A):GLY:CA	2.46	0.46
1:A:113:ASN:HD21	5:A:1131:NAG:HN2	1.65	0.45
2:B:280:ASN:OD1	2:B:300:TRP:N	2.42	0.45
5:A:1131:NAG:C8	5:A:1131:NAG:C1	2.95	0.45
1:A:66:LEU:H	1:A:66:LEU:HD23	1.81	0.45
1:A:26:ALA:O	1:A:105:ASN:HB2	2.17	0.45
7:B:2911:NAG:H2	7:B:2912:NAG:O6	2.17	0.45
1:A:173:MET:HE2	2:B:331:TRP:HE3	1.82	0.45
2:B:318:ARG:NH2	10:B:2984:HOH:O	2.50	0.44
2:B:367:THR:O	2:B:382:GLN:HG3	2.16	0.44
1:A:173:MET:HE2	2:B:331:TRP:CE3	2.52	0.44
1:A:173:MET:HE2	2:B:331:TRP:HB3	1.98	0.44
2:B:418:LYS:HE3	2:B:418:LYS:HB3	1.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:113:ASN:O	1:A:117:HIS:HD2	2.01	0.44
2:B:304:THR:O	2:B:308:HIS:CD2	2.65	0.44
1:A:55:GLY:O	2:B:303:CYS:HA	2.18	0.43
1:A:173:MET:CE	2:B:331:TRP:CE3	3.02	0.43
1:A:110:ILE:HD12	1:A:110:ILE:HG21	1.18	0.43
1:A:248:ILE:HD11	2:B:273:ARG:CG	2.47	0.43
1:A:113:ASN:HD22	5:A:1131:NAG:C7	2.32	0.42
1:A:49:TRP:HA	1:A:143:ALA:O	2.19	0.42
1:A:173:MET:CE	2:B:331:TRP:CB	2.97	0.42
2:B:268:CYS:O	2:B:273:ARG:HB2	2.20	0.42
2:B:303(B):ASP:OD1	2:B:304:THR:N	2.52	0.42
6:A:1132:FUC:C1	6:A:1133:NAG:N2	2.82	0.41
2:B:276:THR:HA	2:B:300:TRP:CZ3	2.56	0.41
1:A:142:ILE:O	1:A:172:PHE:HB2	2.19	0.41
1:A:113:ASN:ND2	5:A:1131:NAG:C1	2.84	0.41
2:B:399:VAL:HB	2:B:400:PRO:HD3	2.02	0.41
1:A:113:ASN:ND2	5:A:1131:NAG:C7	2.83	0.41
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.80	0.41
1:A:2:ALA:HB3	10:A:1326:HOH:O	2.20	0.40
1:A:62:ALA:O	1:A:67:GLY:HA3	2.20	0.40
1:A:23(A):ASP:OD1	1:A:26:ALA:N	2.40	0.40
1:A:110:ILE:HG23	1:A:110:ILE:HD13	1.21	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	253/263 (96%)	243 (96%)	10 (4%)	0	100	100
2	B	151/160 (94%)	142 (94%)	9 (6%)	0	100	100
3	C	1/4 (25%)	1 (100%)	0	0	100	100
All	All	405/427 (95%)	386 (95%)	19 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/215 (95%)	191 (93%)	14 (7%)	22	18
2	B	123/133 (92%)	118 (96%)	5 (4%)	41	40
3	C	2/2 (100%)	2 (100%)	0	100	100
All	All	330/350 (94%)	311 (94%)	19 (6%)	29	23

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	HIS
1	A	0	ARG
1	A	3	ARG
1	A	66	LEU
1	A	110	ILE
1	A	112	THR
1	A	125	LYS
1	A	167	ILE
1	A	170	LYS
1	A	185	TYR
1	A	204	ARG
1	A	205	ARG
1	A	247	ASN
1	A	248	ILE
2	B	264	SER
2	B	273	ARG
2	B	284	VAL
2	B	418	LYS
2	B	419	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN

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Mol	Chain	Res	Type
1	A	105	ASN
1	A	117	HIS
1	A	217	HIS
1	A	233	GLN
1	A	247	ASN
2	B	285	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	PHA	C	4	1,3	11,11,11	2.35	2 (18%)	13,13,13	2.45	2 (15%)

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	PHA	C	4	1,3	-	0/5/6/6	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	PHA	CA-C	6.29	1.56	1.50
3	C	4	PHA	O-C	4.18	1.40	1.19

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	PHA	O-C-CA	-8.13	106.91	125.12
3	C	4	PHA	CG-CB-CA	-2.38	110.01	113.68

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$
6	FUC	A	1132	6	9,10,11	2.01	2 (22%)	10,14,16	4.32	7 (70%)
6	NAG	A	1133	6	12,14,15	1.22	2 (16%)	15,19,21	2.70	6 (40%)
6	NDG	A	1134	6	12,14,15	0.91	0	15,19,21	3.79	5 (33%)
7	NAG	B	2911	7	12,14,15	0.65	0	15,19,21	2.57	7 (46%)
7	NAG	B	2912	7	12,14,15	2.04	3 (25%)	15,19,21	4.05	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
6	FUC	A	1132	6	-	0/0/17/20	0/1/1/1
6	NAG	A	1133	6	-	0/6/23/26	0/1/1/1
6	NDG	A	1134	6	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	B	2911	7	-	0/6/23/26	0/1/1/1
7	NAG	B	2912	7	3/3/5/7	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1132	FUC	O5-C5	4.70	1.54	1.45
7	B	2912	NAG	C2-N2	4.65	1.51	1.46
7	B	2912	NAG	C3-C2	3.27	1.59	1.52
7	B	2912	NAG	C4-C3	3.07	1.60	1.52
6	A	1133	NAG	C2-N2	-2.53	1.43	1.46
6	A	1133	NAG	C3-C2	-2.43	1.47	1.52
6	A	1132	FUC	C4-C3	2.13	1.58	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2912	NAG	O6-C6-C5	12.05	152.81	111.36
6	A	1134	NDG	O6-C6-C5	11.43	150.68	111.36
6	A	1132	FUC	C4-C3-C2	-8.54	99.04	110.50
6	A	1132	FUC	O3-C3-C2	8.38	125.27	109.94
6	A	1134	NDG	C3-C2-N2	6.70	121.97	111.76
7	B	2912	NAG	O5-C5-C6	6.14	113.42	106.98
6	A	1133	NAG	C3-C2-N2	-6.00	102.62	111.76
7	B	2911	NAG	O3-C3-C4	5.08	121.75	110.35
6	A	1133	NAG	O5-C5-C6	4.57	111.78	106.98
7	B	2912	NAG	C3-C4-C5	4.56	118.35	110.20
7	B	2911	NAG	O6-C6-C5	-4.35	96.38	111.36
6	A	1133	NAG	C3-C4-C5	4.31	117.90	110.20
7	B	2912	NAG	C3-C2-N2	3.76	117.49	111.76
6	A	1133	NAG	O7-C7-C8	3.72	129.31	122.04
7	B	2911	NAG	O3-C3-C2	3.70	116.85	109.09
7	B	2911	NAG	C8-C7-N2	-3.53	109.22	116.11
6	A	1134	NDG	O7-C7-C8	3.53	128.93	122.04
6	A	1132	FUC	O5-C5-C4	3.45	115.43	110.22
6	A	1132	FUC	O4-C4-C5	3.01	116.73	109.78
6	A	1132	FUC	O3-C3-C4	-2.91	103.84	110.35
7	B	2912	NAG	C2-N2-C7	2.78	127.76	123.09
6	A	1134	NDG	C4-C3-C2	-2.65	104.83	111.32
6	A	1133	NAG	C8-C7-N2	-2.64	110.94	116.11
6	A	1132	FUC	C6-C5-C4	2.56	117.21	113.06
6	A	1132	FUC	O2-C2-C3	2.53	115.64	110.18
7	B	2912	NAG	O4-C4-C3	2.49	115.94	110.35
7	B	2911	NAG	O5-C5-C6	2.48	109.58	106.98
7	B	2911	NAG	O7-C7-C8	2.33	126.59	122.04
6	A	1133	NAG	O3-C3-C4	-2.29	105.22	110.35
7	B	2911	NAG	C3-C2-N2	-2.24	108.35	111.76
6	A	1134	NDG	O-C5-C6	2.13	109.22	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2912	NAG	O7-C7-C8	-2.06	118.02	122.04

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	2912	NAG	C2
7	B	2912	NAG	C5
7	B	2912	NAG	C1
6	A	1134	NDG	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2912	NAG	C1-C2-N2-C7

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

4 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
5	NAG	A	1131	-	12,14,15	1.00	1 (8%)	15,19,21	2.46	6 (40%)
4	ARG	A	426	-	11,11,11	1.31	1 (9%)	13,13,13	3.33	4 (30%)
9	GOL	A	450	-	5,5,5	0.44	0	5,5,5	0.60	0
8	ACT	B	461	-	1,3,3	4.28	1 (100%)	0,3,3	0.00	-

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	NAG	A	1131	-	1/1/5/7	0/6/23/26	0/1/1/1
4	ARG	A	426	-	-	0/11/11/11	0/0/0/0
9	GOL	A	450	-	-	0/4/4/4	0/0/0/0
8	ACT	B	461	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	461	ACT	CH3-C	4.28	1.54	1.48
4	A	426	ARG	CA-C	-2.72	1.43	1.53
5	A	1131	NAG	C2-N2	-2.44	1.43	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	426	ARG	OXT-C-O	8.16	142.53	124.07
5	A	1131	NAG	O6-C6-C5	5.84	131.47	111.36
4	A	426	ARG	CB-CA-N	5.69	124.05	110.14
4	A	426	ARG	O-C-CA	-4.71	104.77	118.36
5	A	1131	NAG	O5-C5-C6	-4.16	102.62	106.98
5	A	1131	NAG	C8-C7-N2	3.21	122.39	116.11
4	A	426	ARG	CG-CB-CA	-3.15	101.85	113.11
5	A	1131	NAG	C2-N2-C7	2.64	127.53	123.09
5	A	1131	NAG	O7-C7-C8	-2.32	117.51	122.04
5	A	1131	NAG	C3-C2-N2	-2.22	108.38	111.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	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.