



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:19 PM GMT

PDB ID : 3ES6  
Title : Crystal structure of the novel complex formed between Zinc 2-glycoprotein (ZAG) and Prolactin inducible protein (PIP) from human seminal plasma  
Authors : Hassan, M.I.; Bilgrami, S.; Kumar, V.; Singh, N.; Yadav, S.; Kaur, P.; Singh, T.P.  
Deposited on : 2008-10-04  
Resolution : 3.23 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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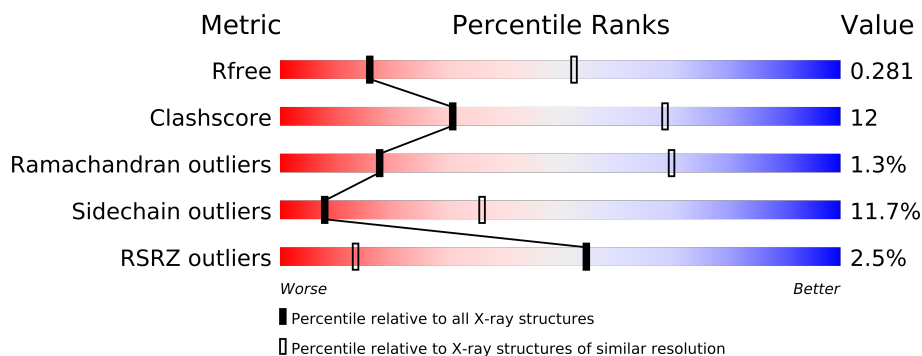
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 3.23 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))
$R_{free}$	66092	1080 (3.30-3.18)
Clashscore	79885	1369 (3.30-3.18)
Ramachandran outliers	78287	1342 (3.30-3.18)
Sidechain outliers	78261	1340 (3.30-3.18)
RSRZ outliers	66119	1081 (3.30-3.18)

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.

Mol	Chain	Length	Quality of chain
1	A	278	
2	B	118	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	CO3	A	688	-	X
6	P6G	A	701	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3354 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 Zinc-alpha-2-glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2266	1444	385	430	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	GLN	MODIFIED RESIDUE	UNP P25311

- Molecule 2 is a protein called Prolactin-inducible protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	118	Total	C	N	O	S	0	0	0
			951	612	155	179	5			

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	4	Total	C	N	O	0	0
			50	28	2	20		

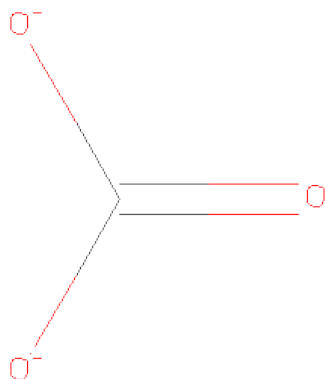
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			64	36	3	25		

There is a discrepancy between the modelled and reference sequences:

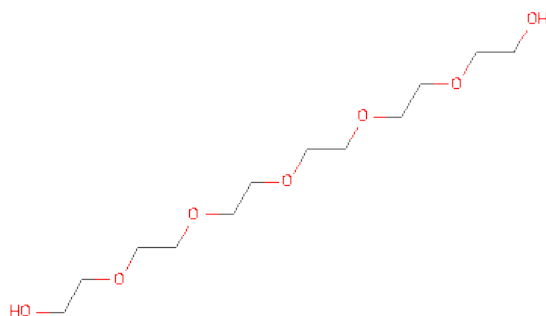
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	GLN	MODIFIED RESIDUE	UNP P25311

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).

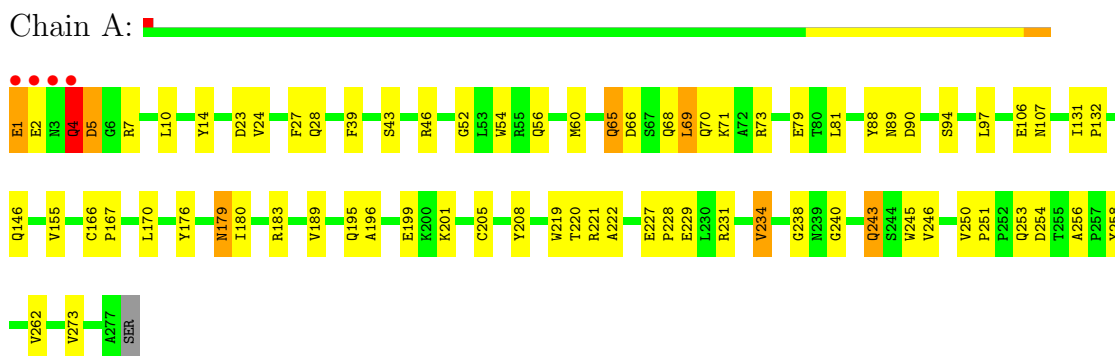


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			19	12	7		

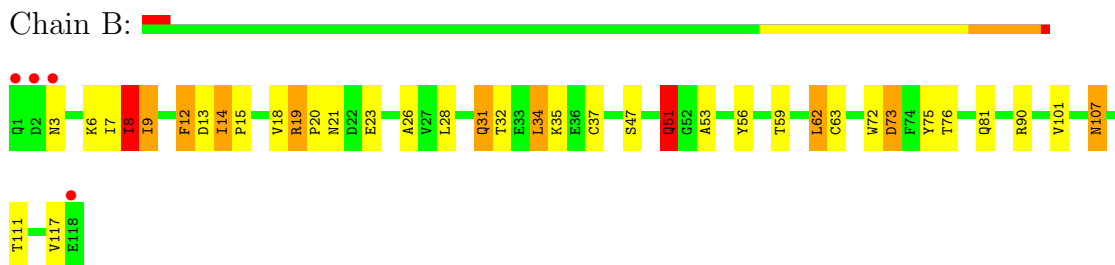
### 3 Residue-property plots

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: Zinc-alpha-2-glycoprotein



#### • Molecule 2: Prolactin-inducible protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.30Å 132.30Å 73.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.23 24.91 – 3.23	Depositor EDS
% Data completeness (in resolution range)	98.8 (25.00-3.23) 98.8 (24.91-3.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.23Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.196 , 0.240 0.226 , 0.281	Depositor DCC
$R_{free}$ test set	515 reflections (4.77%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 6.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 10811 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	3354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, BMA, NAG, NDG, P6G, PCA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.42	3/2325 (0.1%)	0.57	3/3160 (0.1%)
2	B	0.51	1/969 (0.1%)	0.94	8/1318 (0.6%)
All	All	0.45	4/3294 (0.1%)	0.70	11/4478 (0.2%)

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
2	B	0	2
3	B	2	0
All	All	2	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	ARG	CZ-NH2	6.26	1.41	1.33
1	A	2	GLU	C-N	5.49	1.46	1.34
1	A	1	PCA	C-N	5.45	1.46	1.34
2	B	8	ILE	C-N	5.22	1.46	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	ILE	N-CA-C	12.78	145.49	111.00
2	B	73	ASP	CA-CB-CG	11.01	137.62	113.40
2	B	23	GLU	CA-CB-CG	9.35	133.96	113.40
1	A	2	GLU	O-C-N	-8.08	109.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	ILE	N-CA-CB	-6.87	95.01	110.80
2	B	75	TYR	CA-CB-CG	6.80	126.32	113.40
2	B	12	PHE	CA-CB-CG	6.77	130.15	113.90
1	A	69	LEU	CA-CB-CG	6.72	130.76	115.30
2	B	35	LYS	CD-CE-NZ	6.28	126.14	111.70
2	B	51	GLN	CB-CG-CD	5.89	126.90	111.60
1	A	2	GLU	CA-C-N	5.25	128.75	117.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	300	NDG	C1
3	B	303	MAN	C1

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PCA	Peptide
2	B	8	ILE	Mainchain,Peptide

## 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	2266	0	2153	46	0
2	B	951	0	963	30	0
3	B	50	0	41	4	0
4	A	64	0	55	8	0
5	A	4	0	0	0	0
6	A	19	0	26	3	0
All	All	3354	0	3238	78	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 12.

All (78) close contacts within the same asymmetric unit are listed below.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:303:MAN:O3	3:B:303:MAN:C3	1.78	1.30
2:B:18:VAL:HG12	2:B:19:ARG:H	1.13	1.08
4:A:321:NAG:O3	4:A:322:BMA:H2	1.55	1.05
2:B:14:ILE:HB	2:B:15:PRO:HD2	1.37	1.00
1:A:196:ALA:HB3	1:A:199:GLU:HB3	1.44	0.98
4:A:321:NAG:H4	4:A:322:BMA:O2	1.74	0.88
2:B:18:VAL:HG12	2:B:19:ARG:N	1.93	0.83
1:A:189:VAL:HG11	1:A:262:VAL:HG21	1.63	0.80
2:B:18:VAL:CG1	2:B:19:ARG:H	1.95	0.78
2:B:14:ILE:HB	2:B:15:PRO:CD	2.15	0.75
1:A:251:PRO:HG2	1:A:254:ASP:HB2	1.69	0.75
4:A:327:MAN:O3	4:A:328:NDG:C1	2.36	0.74
1:A:245:TRP:HH2	2:B:56:TYR:CD1	2.06	0.74
1:A:24:VAL:HG21	2:B:81:GLN:HG3	1.68	0.73
1:A:60:MET:HE2	1:A:176:TYR:HB2	1.75	0.69
1:A:180:ILE:O	1:A:183:ARG:HG3	1.93	0.68
2:B:32:THR:OG1	2:B:34:LEU:HB2	1.93	0.68
4:A:320:NAG:O3	4:A:321:NAG:O5	2.12	0.67
1:A:52:GLY:HA2	1:A:238:GLY:HA2	1.76	0.66
2:B:14:ILE:HG21	2:B:26:ALA:HA	1.78	0.65
1:A:73:ARG:NH1	6:A:701:P6G:H61	2.13	0.64
3:B:302:BMA:O2	3:B:303:MAN:O2	2.18	0.61
1:A:196:ALA:HB3	1:A:199:GLU:CB	2.26	0.61
2:B:8:ILE:HG22	2:B:9:ILE:H	1.64	0.61
2:B:26:ALA:HB3	2:B:72:TRP:HB2	1.83	0.60
1:A:73:ARG:HH11	6:A:701:P6G:H61	1.67	0.60
1:A:245:TRP:CH2	2:B:56:TYR:CE1	2.91	0.58
1:A:183:ARG:NH2	1:A:240:GLY:O	2.37	0.58
2:B:14:ILE:CG2	2:B:26:ALA:HA	2.35	0.57
1:A:245:TRP:CH2	2:B:56:TYR:CD1	2.92	0.56
4:A:327:MAN:HO3	4:A:328:NDG:C1	2.16	0.56
2:B:14:ILE:CB	2:B:15:PRO:HD2	2.24	0.56
4:A:320:NAG:O3	4:A:321:NAG:C1	2.54	0.55
1:A:166:CYS:HB3	1:A:167:PRO:HD3	1.90	0.54
2:B:8:ILE:O	2:B:32:THR:HA	2.09	0.53
1:A:73:ARG:HH11	6:A:701:P6G:C6	2.22	0.51
1:A:179:ASN:H	1:A:179:ASN:HD22	1.59	0.51
1:A:222:ALA:HB2	1:A:256:ALA:HB1	1.94	0.50
1:A:228:PRO:HB3	1:A:246:VAL:HG13	1.93	0.49
1:A:27:PHE:HB3	1:A:43:SER:HB3	1.94	0.49
1:A:7:ARG:HB3	1:A:106:GLU:HG3	1.95	0.49
3:B:302:BMA:O2	3:B:303:MAN:C2	2.60	0.49
1:A:4:GLN:HB2	1:A:107:ASN:HD21	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:31:GLN:HA	2:B:62:LEU:HD21	1.94	0.48
1:A:189:VAL:HG23	1:A:273:VAL:HG21	1.95	0.47
1:A:201:LYS:HB3	1:A:250:VAL:HG13	1.97	0.47
2:B:53:ALA:HB3	2:B:73:ASP:O	2.13	0.47
2:B:107:ASN:H	2:B:107:ASN:HD22	1.63	0.47
1:A:54:TRP:CD1	1:A:60:MET:HE1	2.50	0.46
3:B:301:NAG:H61	3:B:302:BMA:H2	1.96	0.46
1:A:81:LEU:HD13	1:A:97:LEU:HB2	1.98	0.46
1:A:28:GLN:NE2	2:B:47:SER:O	2.44	0.45
1:A:234:VAL:HG21	2:B:56:TYR:CE1	2.52	0.45
1:A:179:ASN:N	1:A:179:ASN:HD22	2.14	0.45
1:A:245:TRP:HH2	2:B:56:TYR:CE1	2.29	0.45
1:A:208:TYR:CE2	4:A:321:NAG:H61	2.52	0.44
1:A:234:VAL:HG21	2:B:56:TYR:HE1	1.82	0.44
2:B:107:ASN:N	2:B:107:ASN:HD22	2.14	0.44
1:A:65:GLN:O	1:A:68:GLN:HB2	2.18	0.44
2:B:8:ILE:HG22	2:B:9:ILE:HG13	2.00	0.43
1:A:131:ILE:HB	1:A:132:PRO:C	2.37	0.43
1:A:14:TYR:HD2	1:A:27:PHE:CZ	2.37	0.43
1:A:88:TYR:C	1:A:90:ASP:H	2.22	0.43
4:A:321:NAG:HO3	4:A:322:BMA:H2	1.75	0.43
1:A:65:GLN:HE21	1:A:65:GLN:HB2	1.59	0.43
2:B:20:PRO:HD3	2:B:117:VAL:HG12	2.00	0.43
1:A:208:TYR:CB	1:A:243:GLN:HG3	2.50	0.42
1:A:10:LEU:HB2	1:A:170:LEU:HD13	2.01	0.42
1:A:189:VAL:CG2	1:A:273:VAL:HG21	2.50	0.42
1:A:60:MET:HE2	1:A:176:TYR:CB	2.47	0.41
2:B:51:GLN:H	2:B:51:GLN:HG3	1.19	0.41
1:A:54:TRP:NE1	1:A:60:MET:HE1	2.36	0.41
1:A:205:CYS:HB2	1:A:219:TRP:CZ2	2.56	0.40
2:B:14:ILE:CB	2:B:15:PRO:CD	2.86	0.40
1:A:234:VAL:CG2	2:B:56:TYR:CE1	3.05	0.40
2:B:31:GLN:HE21	2:B:31:GLN:HB3	1.65	0.40
1:A:221:ARG:HG3	1:A:258:TYR:CZ	2.56	0.40
1:A:66:ASP:O	1:A:70:GLN:HG2	2.22	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	275/278 (99%)	261 (95%)	11 (4%)	3 (1%)	21	74
2	B	116/118 (98%)	102 (88%)	12 (10%)	2 (2%)	14	63
All	All	391/396 (99%)	363 (93%)	23 (6%)	5 (1%)	18	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
2	B	8	ILE
1	A	89	ASN
1	A	4	GLN
2	B	6	LYS

### 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	242/243 (100%)	221 (91%)	21 (9%)	15	53
2	B	108/108 (100%)	88 (82%)	20 (18%)	2	12
All	All	350/351 (100%)	309 (88%)	41 (12%)	8	36

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	ASP
1	A	23	ASP
1	A	39	PHE

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Mol	Chain	Res	Type
1	A	46	ARG
1	A	56	GLN
1	A	65	GLN
1	A	69	LEU
1	A	71	LYS
1	A	79	GLU
1	A	94	SER
1	A	146	GLN
1	A	155	VAL
1	A	179	ASN
1	A	195	GLN
1	A	220	THR
1	A	227	GLU
1	A	229	GLU
1	A	234	VAL
1	A	243	GLN
1	A	253	GLN
2	B	3	ASN
2	B	7	ILE
2	B	12	PHE
2	B	13	ASP
2	B	14	ILE
2	B	19	ARG
2	B	21	ASN
2	B	28	LEU
2	B	31	GLN
2	B	34	LEU
2	B	37	CYS
2	B	51	GLN
2	B	59	THR
2	B	62	LEU
2	B	63	CYS
2	B	76	THR
2	B	90	ARG
2	B	101	VAL
2	B	107	ASN
2	B	111	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN

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Mol	Chain	Res	Type
1	A	107	ASN
1	A	179	ASN
1	A	184	GLN
1	A	253	GLN
1	A	263	GLN
2	B	31	GLN
2	B	66	ASN
2	B	107	ASN

### 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$
1	PCA	A	1	1	8,8,9	14.98	7 (87%)	8,10,12	10.64	5 (62%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	O-C	39.87	1.39	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	9.22	1.54	1.34
1	A	1	PCA	CB-CA	7.27	1.62	1.53
1	A	1	PCA	CA-C	5.54	1.59	1.48
1	A	1	PCA	OE-CD	3.73	1.31	1.23
1	A	1	PCA	CA-N	3.71	1.54	1.46
1	A	1	PCA	CB-CG	2.78	1.59	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	C-CA-N	21.38	115.54	110.71
1	A	1	PCA	CA-N-CD	-20.07	98.69	114.37
1	A	1	PCA	OE-CD-CG	-5.69	117.77	126.70
1	A	1	PCA	CB-CA-N	2.35	110.49	103.72
1	A	1	PCA	CG-CD-N	2.23	115.76	107.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

9 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
4	NAG	A	320	1,4	12,14,15	0.69	1 (8%)	15,19,21	0.90	1 (6%)
4	NAG	A	321	4	12,14,15	0.64	0	15,19,21	0.83	1 (6%)
4	BMA	A	322	4	10,11,12	0.52	0	11,15,17	1.44	1 (9%)
4	MAN	A	327	4	10,11,12	1.26	1 (10%)	11,15,17	3.12	4 (36%)
4	NDG	A	328	4	12,14,15	1.45	1 (8%)	15,19,21	1.17	2 (13%)
3	NDG	B	300	3,2	12,14,15	0.81	0	15,19,21	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	301	3	12,14,15	0.78	0	15,19,21	0.95	0
3	BMA	B	302	3	10,11,12	2.02	2 (20%)	11,15,17	1.99	3 (27%)
3	MAN	B	303	3	10,11,12	5.25	3 (30%)	11,15,17	4.04	4 (36%)

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	320	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	321	4	-	0/6/23/26	0/1/1/1
4	BMA	A	322	4	-	0/2/19/22	0/1/1/1
4	MAN	A	327	4	-	0/2/19/22	0/1/1/1
4	NDG	A	328	4	-	0/6/23/26	0/1/1/1
3	NDG	B	300	3,2	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	B	301	3	-	0/6/23/26	0/1/1/1
3	BMA	B	302	3	-	0/2/19/22	0/1/1/1
3	MAN	B	303	3	1/1/4/5	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	MAN	O3-C3	14.81	1.78	1.43
3	B	303	MAN	O2-C2	-6.48	1.29	1.43
3	B	302	BMA	O3-C3	4.58	1.54	1.43
4	A	328	NDG	C8-C7	3.96	1.58	1.50
3	B	302	BMA	O4-C4	-3.63	1.34	1.43
3	B	303	MAN	O6-C6	2.85	1.54	1.42
4	A	327	MAN	O3-C3	-2.53	1.36	1.43
4	A	320	NAG	O5-C5	-2.10	1.41	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	MAN	O2-C2-C3	-9.64	89.38	110.18
4	A	327	MAN	O3-C3-C2	7.71	124.04	109.94
3	B	303	MAN	O3-C3-C2	7.59	123.81	109.94
4	A	327	MAN	O3-C3-C4	-4.61	100.02	110.35
3	B	302	BMA	O4-C4-C5	4.47	121.06	109.28
3	B	303	MAN	O5-C5-C6	4.37	111.56	106.98
4	A	327	MAN	O5-C5-C6	4.17	111.36	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	BMA	O5-C5-C6	3.49	110.64	106.98
4	A	322	BMA	C3-C4-C5	3.01	115.57	110.20
4	A	328	NDG	O-C5-C6	2.72	109.83	106.98
3	B	302	BMA	O4-C4-C3	2.64	116.27	110.35
3	B	300	NDG	O-C5-C6	2.42	109.52	106.98
4	A	321	NAG	O5-C5-C6	2.35	109.44	106.98
4	A	327	MAN	O5-C5-C4	-2.09	108.00	110.65
3	B	303	MAN	C4-C3-C2	2.08	113.30	110.50
4	A	328	NDG	C3-C2-N2	-2.02	108.69	111.76
4	A	320	NAG	O5-C5-C6	2.01	109.09	106.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	300	NDG	C1
3	B	303	MAN	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	300	NDG	C3-C2-N2-C7

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	$\# Z  > 2$
5	CO3	A	688	-	0,3,3	0.00	-	0,3,3	0.00	-
6	P6G	A	701	-	18,18,18	1.30	3 (16%)	17,17,17	0.57	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
5	CO3	A	688	-	-	0/0/0/0	0/0/0/0
6	P6G	A	701	-	-	0/16/16/16	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	P6G	C9-C8	3.52	1.67	1.48
6	A	701	P6G	C3-C2	2.49	1.63	1.49
6	A	701	P6G	O4-C3	2.13	1.51	1.42

There are no bond angle outliers.

There are no chirality outliers.

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 ⓘ

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	277/278 (99%)	-0.14	4 (1%) 72 24	19, 30, 50, 62	0
2	B	118/118 (100%)	-0.05	4 (3%) 43 10	20, 33, 58, 74	0
All	All	395/396 (99%)	-0.11	8 (2%) 54 18	19, 31, 52, 74	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLU	4.0
1	A	1	PCA	3.4
2	B	1	GLN	3.3
1	A	4	GLN	2.8
2	B	2	ASP	2.7
2	B	118	GLU	2.4
2	B	3	ASN	2.3
1	A	3	ASN	2.1

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	PCA	A	1	8/9	0.79	-	61,61,62,62	0

### 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	320	14/15	0.31	6.64	18,20,22,22	14
4	NDG	A	328	14/15	0.33	4.36	33,35,35,35	14
4	NAG	A	321	14/15	0.29	4.28	22,23,25,27	14
4	MAN	A	327	11/12	0.24	2.15	33,34,34,35	11
3	NDG	B	300	14/15	0.29	0.33	56,58,61,64	14
4	BMA	A	322	11/12	0.20	-0.19	29,30,31,32	11
3	BMA	B	302	11/12	0.69	-	70,70,70,70	11
3	MAN	B	303	11/12	0.67	-	70,70,70,70	11
3	NAG	B	301	14/15	0.62	-	68,70,73,74	0

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	CO3	A	688	4/4	0.35	3.57	56,56,56,56	0
6	P6G	A	701	19/19	0.29	2.24	43,45,49,49	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.