



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:54 PM GMT

PDB ID : 1OQO  
Title : Complex between G0 version of an Fc bound to a minimized version of Protein A called Mini-Z  
Authors : Raju, T.S.; Mulkerrin, M.G.; Parker, M.; De Vos, A.M.; Gazzano-Santoro, H.; Totpal, K.; Ultsch, M.H.  
Deposited on : 2003-03-10  
Resolution : 2.30 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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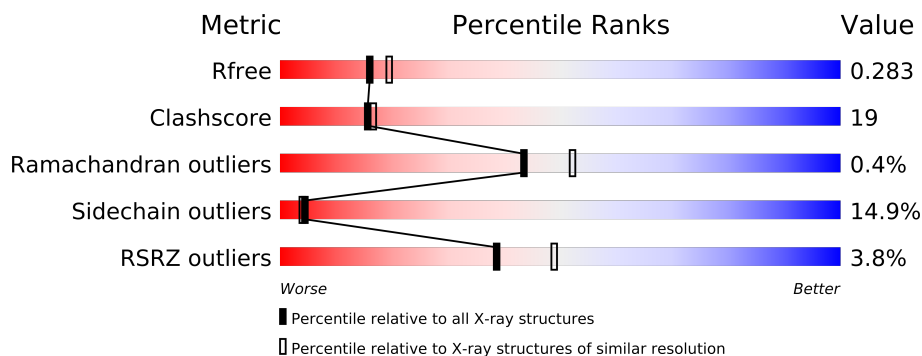
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. 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	212	
1	B	212	
2	C	34	
2	D	34	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4246 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 immunoglobulin gamma-1 heavy chain constant region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			
1	B	208	Total	C	N	O	S	0	0	0
			1662	1058	280	318	6			

- Molecule 2 is a protein called Minimized version of Protein A (Z34C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	34	Total	C	N	O	S	0	0	0
			291	176	57	55	3			
2	D	34	Total	C	N	O	S	0	0	0
			291	176	57	55	3			

- Molecule 3 is a polymer of unknown type called SUGAR (nag-nag-man-man-nag-man-fuc-nag).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	8	Total	C	N	O	0	0
			99	56	4	39		

- Molecule 4 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	8	Total	C	N	O	0	0
			99	56	4	39		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		

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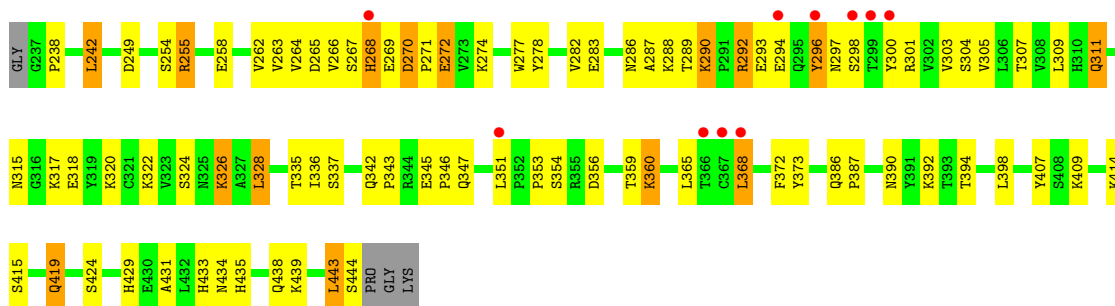
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	58	Total 58	O 58	0	0
5	C	13	Total 13	O 13	0	0
5	D	10	Total 10	O 10	0	0

### 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.

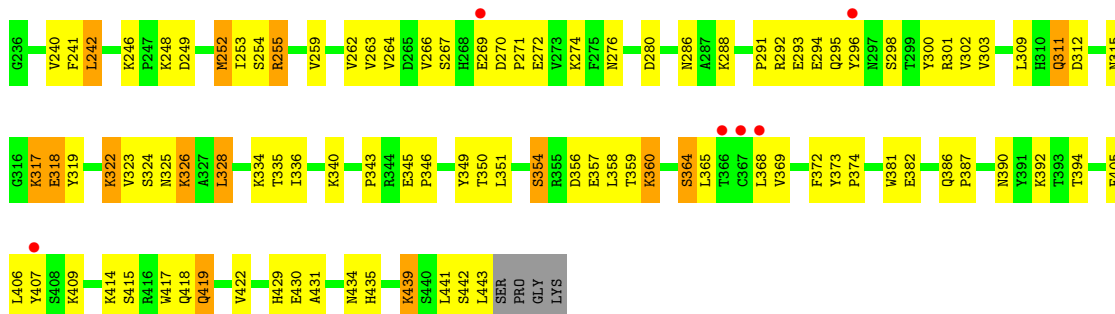
- Molecule 1: immunoglobulin gamma-1 heavy chain constant region

Chain A: 



- Molecule 1: immunoglobulin gamma-1 heavy chain constant region

Chain B: 



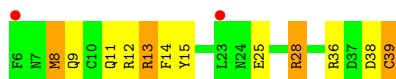
- Molecule 2: Minimized version of Protein A (Z34C)

Chain C: 



- Molecule 2: Minimized version of Protein A (Z34C)

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.78Å 126.41Å 54.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 24.25 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.30) 99.6 (24.25-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.31Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, $R_{free}$	0.216 , 0.286 0.218 , 0.283	Depositor DCC
$R_{free}$ test set	2673 reflections (11.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26861 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.58% 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: BMA, NAG, NDG, FUC, FUL, 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	0.52	0/1710	0.70	0/2330
1	B	0.50	0/1708	0.69	0/2327
2	C	0.49	0/295	0.58	0/393
2	D	0.51	0/295	0.64	0/393
All	All	0.51	0/4008	0.69	0/5443

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
4	B	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	8	FUC	C1

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	1664	0	1630	63	0
1	B	1662	0	1628	77	0
2	C	291	0	272	9	0
2	D	291	0	272	10	0
3	A	99	0	85	0	0
4	B	99	0	85	4	0
5	A	59	0	0	1	0
5	B	58	0	0	5	0
5	C	13	0	0	1	0
5	D	10	0	0	1	0
All	All	4246	0	3972	150	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 (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:252:MET:HG2	5:B:496:HOH:O	1.69	0.93
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.52	0.88
1:A:292:ARG:HD3	1:A:300:TYR:CE2	2.10	0.87
1:B:269:GLU:O	1:B:271:PRO:HD3	1.75	0.85
1:A:386:GLN:HG3	1:A:387:PRO:HD2	1.59	0.81
2:C:8:MET:O	2:C:12:ARG:HG3	1.80	0.81
1:B:359:THR:HG23	1:B:360:LYS:HD2	1.63	0.79
1:A:356:ASP:O	1:A:359:THR:HG22	1.86	0.75
1:A:429:HIS:CD2	1:A:431:ALA:H	2.04	0.75
1:A:429:HIS:HD2	1:A:431:ALA:H	1.33	0.74
1:A:270:ASP:N	1:A:271:PRO:HD3	2.07	0.70
1:B:240:VAL:HG22	1:B:263:VAL:HG22	1.74	0.69
2:C:28:ARG:HD3	5:C:47:HOH:O	1.92	0.68
1:A:292:ARG:HD3	1:A:300:TYR:CD2	2.27	0.68
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.74	0.68
1:B:415:SER:O	1:B:419:GLN:HB2	1.94	0.68
1:B:248:LYS:NZ	1:B:255:ARG:HH12	1.91	0.68
1:B:359:THR:HG23	1:B:360:LYS:CD	2.24	0.67
2:D:38:ASP:O	2:D:39:CYS:HB3	1.94	0.67
1:A:359:THR:HG23	1:A:360:LYS:HE2	1.76	0.66
1:B:270:ASP:HA	1:B:326:LYS:HZ3	1.60	0.66
1:A:443:LEU:O	1:A:444:SER:HB2	1.95	0.66
2:D:8:MET:O	2:D:12:ARG:HG3	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:ASP:OD1	1:A:255:ARG:HD2	1.97	0.65
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.78	0.64
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.78	0.64
1:A:311:GLN:HG2	2:C:32:ILE:CD1	2.28	0.64
1:B:386:GLN:HG3	1:B:387:PRO:HD2	1.81	0.63
1:A:311:GLN:HG2	2:C:32:ILE:HD13	1.80	0.62
1:B:360:LYS:HD2	1:B:360:LYS:N	2.14	0.62
1:A:415:SER:O	1:A:419:GLN:HB2	1.99	0.62
1:A:255:ARG:HH11	1:A:255:ARG:HG2	1.65	0.61
1:B:259:VAL:HG13	1:B:336:ILE:HD11	1.81	0.61
1:B:381:TRP:O	1:B:382:GLU:HG3	2.01	0.60
1:B:269:GLU:C	1:B:271:PRO:HD3	2.22	0.60
1:A:290:LYS:HE3	1:A:305:VAL:HG23	1.83	0.60
1:B:262:VAL:HG22	1:B:303:VAL:HG22	1.84	0.58
1:A:360:LYS:O	1:A:414:LYS:HE2	2.03	0.58
1:B:294:GLU:HB3	5:B:492:HOH:O	2.03	0.58
1:B:318:GLU:HG2	1:B:335:THR:CG2	2.34	0.58
1:B:292:ARG:HB2	1:B:300:TYR:HD2	1.69	0.57
1:A:356:ASP:OD1	1:B:439:LYS:NZ	2.37	0.57
1:A:345:GLU:HG3	1:A:431:ALA:O	2.05	0.57
1:B:255:ARG:O	2:D:36:ARG:NH2	2.37	0.57
1:B:292:ARG:HB3	1:B:302:VAL:HG22	1.87	0.57
1:A:311:GLN:CG	2:C:32:ILE:HD13	2.35	0.56
2:D:13:ARG:NH2	5:D:65:HOH:O	2.39	0.56
1:B:358:LEU:HD22	1:B:418:GLN:HE21	1.71	0.55
1:B:345:GLU:HG3	1:B:431:ALA:O	2.06	0.55
1:B:280:ASP:OD2	1:B:317:LYS:HG3	2.06	0.55
1:A:238:PRO:HD2	1:A:328:LEU:HD13	1.88	0.55
1:B:292:ARG:HG3	1:B:300:TYR:CE2	2.42	0.55
1:B:374:PRO:O	1:B:429:HIS:HE1	1.91	0.54
1:A:271:PRO:HD2	1:A:326:LYS:NZ	2.23	0.54
1:A:289:THR:HA	1:A:304:SER:HA	1.90	0.54
1:A:262:VAL:HG13	1:A:303:VAL:HG22	1.89	0.53
1:B:325:ASN:HB3	1:B:328:LEU:HD22	1.91	0.53
1:B:311:GLN:O	1:B:315:ASN:HB2	2.08	0.52
1:B:291:PRO:HA	5:B:484:HOH:O	2.09	0.52
1:B:242:LEU:HD13	1:B:336:ILE:HG12	1.91	0.52
1:A:429:HIS:O	1:A:435:HIS:HA	2.10	0.52
1:A:270:ASP:HA	1:A:326:LYS:HZ3	1.75	0.52
1:B:343:PRO:HA	1:B:373:TYR:O	2.10	0.52
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.45	0.51
1:A:354:SER:CB	1:B:349:TYR:HB3	2.40	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:252:MET:CG	5:B:496:HOH:O	2.42	0.51
1:A:277:TRP:O	1:A:283:GLU:HA	2.11	0.51
2:C:9:GLN:O	2:C:13:ARG:HG3	2.09	0.51
1:A:272:GLU:H	1:A:326:LYS:NZ	2.09	0.51
1:A:292:ARG:HD3	1:A:300:TYR:HE2	1.72	0.51
1:B:418:GLN:HA	1:B:443:LEU:HD22	1.93	0.51
1:A:343:PRO:HA	1:A:373:TYR:O	2.11	0.51
1:B:359:THR:HG23	1:B:360:LYS:CE	2.41	0.50
1:B:292:ARG:HG3	1:B:300:TYR:HE2	1.75	0.50
1:B:356:ASP:O	1:B:359:THR:HG22	2.12	0.50
1:A:351:LEU:HB3	5:B:467:HOH:O	2.12	0.49
2:D:11:GLN:HA	2:D:11:GLN:OE1	2.12	0.49
1:A:266:VAL:HB	1:A:300:TYR:CB	2.40	0.49
1:A:438:GLN:O	1:A:439:LYS:HG2	2.12	0.49
1:A:278:TYR:CE2	1:A:283:GLU:HB2	2.47	0.49
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.95	0.48
1:B:422:VAL:HG22	1:B:442:SER:HB3	1.94	0.48
1:A:297:ASN:O	1:A:298:SER:HB2	2.14	0.48
1:B:429:HIS:CD2	1:B:431:ALA:H	2.32	0.48
1:B:312:ASP:HB3	1:B:319:TYR:OH	2.14	0.48
2:D:9:GLN:O	2:D:13:ARG:HG3	2.14	0.47
1:B:350:THR:O	1:B:351:LEU:HD23	2.12	0.47
1:A:268:HIS:O	1:A:271:PRO:HG3	2.14	0.47
1:B:248:LYS:HZ3	1:B:255:ARG:HH12	1.60	0.47
1:A:433:HIS:O	1:A:434:ASN:HB2	2.14	0.47
1:B:264:VAL:HG12	1:B:301:ARG:HG3	1.97	0.47
1:A:290:LYS:HE3	1:A:305:VAL:CG2	2.44	0.47
1:B:312:ASP:O	1:B:317:LYS:HB2	2.15	0.47
1:B:318:GLU:HG2	1:B:335:THR:HG21	1.96	0.46
1:B:394:THR:HG23	1:B:407:TYR:O	2.15	0.46
1:B:270:ASP:HA	1:B:326:LYS:NZ	2.30	0.46
1:B:241:PHE:CE2	4:B:2:NAG:H4	2.50	0.46
1:B:248:LYS:HZ2	1:B:255:ARG:HH12	1.60	0.46
1:B:269:GLU:N	1:B:269:GLU:OE2	2.47	0.46
1:A:270:ASP:N	1:A:271:PRO:CD	2.73	0.46
1:A:242:LEU:HD13	1:A:336:ILE:HG12	1.98	0.46
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.35	0.45
1:B:295:GLN:OE1	4:B:1:NAG:H62	2.16	0.45
1:B:248:LYS:NZ	1:B:255:ARG:NH1	2.61	0.45
1:A:270:ASP:OD1	1:A:326:LYS:HB2	2.16	0.45
1:A:255:ARG:CG	1:A:255:ARG:HH11	2.28	0.45
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:294:GLU:HG2	1:B:300:TYR:CZ	2.52	0.45
1:B:429:HIS:HD2	1:B:431:ALA:HB3	1.81	0.45
2:D:25:GLU:HA	2:D:28:ARG:NH2	2.32	0.45
2:D:38:ASP:O	2:D:39:CYS:CB	2.65	0.45
2:C:28:ARG:HG2	2:C:32:ILE:HD12	1.99	0.45
1:B:358:LEU:HD22	1:B:418:GLN:NE2	2.32	0.45
1:A:368:LEU:HB2	1:A:407:TYR:CE1	2.52	0.44
1:B:253:ILE:HB	2:D:14:PHE:CG	2.53	0.44
1:B:350:THR:C	1:B:351:LEU:HD23	2.37	0.44
1:A:394:THR:HG23	1:A:407:TYR:O	2.18	0.44
1:A:264:VAL:O	1:A:265:ASP:HB2	2.18	0.44
1:B:369:VAL:O	1:B:405:PHE:HA	2.18	0.43
1:B:417:TRP:CE2	1:B:443:LEU:HD13	2.54	0.43
1:B:241:PHE:CZ	4:B:2:NAG:H61	2.53	0.43
1:B:430:GLU:HA	1:B:435:HIS:CD2	2.54	0.43
1:B:240:VAL:HG21	1:B:323:VAL:HG21	2.00	0.43
1:A:320:LYS:HG3	1:A:335:THR:OG1	2.19	0.43
1:B:325:ASN:O	1:B:328:LEU:HB2	2.19	0.43
1:A:294:GLU:HG2	1:A:300:TYR:CZ	2.54	0.43
2:C:8:MET:SD	2:C:12:ARG:NH2	2.78	0.43
1:A:278:TYR:CD2	1:A:283:GLU:HB2	2.53	0.43
1:B:364:SER:HB3	1:B:409:LYS:HD2	2.01	0.43
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.54	0.42
1:A:398:LEU:O	1:B:392:LYS:HD2	2.19	0.42
1:A:263:VAL:O	1:A:301:ARG:HA	2.19	0.42
1:A:318:GLU:HG3	1:A:337:SER:HB3	2.00	0.42
1:B:266:VAL:O	1:B:300:TYR:HB2	2.19	0.42
4:B:2:NAG:H82	4:B:8:FUC:C1	2.49	0.42
1:B:414:LYS:HB3	1:B:414:LYS:HE2	1.87	0.42
1:A:270:ASP:HA	1:A:326:LYS:NZ	2.34	0.42
1:A:311:GLN:O	1:A:315:ASN:N	2.52	0.42
1:A:278:TYR:HA	1:A:282:VAL:O	2.20	0.41
1:B:357:GLU:OE2	1:B:364:SER:OG	2.37	0.41
1:B:259:VAL:CG1	1:B:336:ILE:HD11	2.47	0.41
1:A:277:TRP:CD1	1:A:287:ALA:HB2	2.55	0.41
5:A:499:HOH:O	1:B:354:SER:HA	2.20	0.41
1:A:354:SER:HB2	1:B:349:TYR:HB3	2.02	0.41
1:B:246:LYS:O	1:B:249:ASP:HB2	2.20	0.41
1:B:365:LEU:HB3	1:B:441:LEU:HD23	2.03	0.41
1:B:434:ASN:HA	2:D:15:TYR:CG	2.56	0.41
2:C:24:ASN:OD1	2:C:27:GLN:HG3	2.21	0.40
1:A:255:ARG:CG	1:A:255:ARG:NH1	2.82	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:272:GLU:HB3	1:B:326:LYS:CE	2.51	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	206/212 (97%)	198 (96%)	6 (3%)	2 (1%)	22	23
1	B	206/212 (97%)	200 (97%)	6 (3%)	0	100	100
2	C	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
2	D	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	476/492 (97%)	460 (97%)	14 (3%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	A	296	TYR

### 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	194/196 (99%)	161 (83%)	33 (17%)	3	3
1	B	193/196 (98%)	165 (86%)	28 (14%)	5	4
2	C	32/32 (100%)	30 (94%)	2 (6%)	25	32
2	D	32/32 (100%)	28 (88%)	4 (12%)	7	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	451/456 (99%)	384 (85%)	67 (15%)	<b>4</b> <b>4</b>

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	254	SER
1	A	255	ARG
1	A	258	GLU
1	A	267	SER
1	A	268	HIS
1	A	269	GLU
1	A	270	ASP
1	A	272	GLU
1	A	274	LYS
1	A	286	ASN
1	A	288	LYS
1	A	290	LYS
1	A	293	GLU
1	A	296	TYR
1	A	307	THR
1	A	309	LEU
1	A	311	GLN
1	A	317	LYS
1	A	322	LYS
1	A	324	SER
1	A	326	LYS
1	A	328	LEU
1	A	342	GLN
1	A	347	GLN
1	A	360	LYS
1	A	368	LEU
1	A	390	ASN
1	A	392	LYS
1	A	409	LYS
1	A	419	GLN
1	A	424	SER
1	A	443	LEU
2	C	8	MET
2	C	34	SER
1	B	242	LEU
1	B	252	MET

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Mol	Chain	Res	Type
1	B	254	SER
1	B	255	ARG
1	B	267	SER
1	B	274	LYS
1	B	286	ASN
1	B	288	LYS
1	B	293	GLU
1	B	296	TYR
1	B	298	SER
1	B	309	LEU
1	B	311	GLN
1	B	317	LYS
1	B	318	GLU
1	B	322	LYS
1	B	324	SER
1	B	326	LYS
1	B	328	LEU
1	B	334	LYS
1	B	340	LYS
1	B	354	SER
1	B	360	LYS
1	B	364	SER
1	B	390	ASN
1	B	406	LEU
1	B	419	GLN
1	B	439	LYS
2	D	8	MET
2	D	13	ARG
2	D	28	ARG
2	D	39	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	ASN
1	A	390	ASN
1	A	429	HIS
1	A	434	ASN
2	C	19	HIS
1	B	361	ASN
1	B	362	GLN
1	B	384	ASN

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Mol	Chain	Res	Type
1	B	390	ASN
1	B	418	GLN
1	B	429	HIS
1	B	434	ASN
2	D	19	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

16 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	$\# Z  > 2$
3	NAG	A	1	1,3	12,14,15	0.62	0	15,19,21	0.79	1 (6%)
3	NAG	A	2	3	12,14,15	0.63	0	15,19,21	0.51	0
3	BMA	A	3	3	10,11,12	0.51	0	11,15,17	0.72	0
3	MAN	A	4	3	10,11,12	0.42	0	11,15,17	0.69	0
3	NAG	A	5	3	12,14,15	0.57	0	15,19,21	0.81	1 (6%)
3	MAN	A	6	3	10,11,12	0.43	0	11,15,17	0.59	0
3	FUL	A	8	3	9,10,11	0.45	0	10,14,16	0.54	0
3	NAG	A	9	3	12,14,15	0.55	0	15,19,21	0.77	0
4	NAG	B	1	1,4	12,14,15	0.55	0	15,19,21	0.82	0
4	NAG	B	2	4	12,14,15	0.43	0	15,19,21	0.81	0
4	BMA	B	3	4	10,11,12	0.48	0	11,15,17	1.36	2 (18%)
4	MAN	B	4	4	10,11,12	0.41	0	11,15,17	0.53	0
4	NAG	B	5	4	12,14,15	0.55	0	15,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	B	6	4	10,11,12	0.70	0	11,15,17	1.17	2 (18%)
4	FUC	B	8	4	9,10,11	0.58	0	10,14,16	0.55	0
4	NDG	B	9	4	12,14,15	0.49	0	15,19,21	0.91	1 (6%)

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	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	MAN	A	4	3	-	0/2/19/22	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1
3	MAN	A	6	3	-	0/2/19/22	0/1/1/1
3	FUL	A	8	3	-	0/0/17/20	1/1/1/1
3	NAG	A	9	3	-	0/6/23/26	0/1/1/1
4	NAG	B	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	NAG	B	5	4	-	0/6/23/26	0/1/1/1
4	MAN	B	6	4	-	0/2/19/22	0/1/1/1
4	FUC	B	8	4	1/1/4/5	0/0/17/20	1/1/1/1
4	NDG	B	9	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3	BMA	C4-C3-C2	3.00	114.54	110.50
4	B	6	MAN	C4-C3-C2	2.51	113.88	110.50
4	B	3	BMA	O3-C3-C4	-2.32	105.14	110.35
4	B	9	NDG	C3-C2-N2	-2.27	108.30	111.76
3	A	5	NAG	C2-N2-C7	-2.20	119.40	123.09
4	B	6	MAN	O2-C2-C3	2.10	114.71	110.18
3	A	1	NAG	C2-N2-C7	-2.05	119.64	123.09

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
4	B	8	FUC	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	8	FUC	C1-C2-C3-C4-C5-O5
3	A	8	FUL	C1-C2-C3-C4-C5-O5

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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	208/212 (98%)	-0.07	10 (4%)	29 39	19, 36, 72, 96	0
1	B	208/212 (98%)	0.00	6 (2%)	49 59	21, 36, 72, 92	0
2	C	34/34 (100%)	-0.02	1 (2%)	49 59	25, 42, 71, 99	0
2	D	34/34 (100%)	0.33	2 (5%)	22 30	29, 48, 73, 88	0
All	All	484/492 (98%)	-0.01	19 (3%)	38 48	19, 38, 73, 99	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	6	PHE	9.8
1	A	296	TYR	7.2
1	B	296	TYR	5.7
2	D	6	PHE	4.7
1	A	299	THR	3.2
1	B	366	THR	3.1
1	A	300	TYR	2.7
1	B	368	LEU	2.6
1	A	368	LEU	2.5
1	B	367	CYS	2.4
1	B	407	TYR	2.3
1	A	294	GLU	2.2
1	A	366	THR	2.1
1	A	268	HIS	2.1
1	A	298	SER	2.1
2	D	23	LEU	2.1
1	A	367	CYS	2.1
1	B	269	GLU	2.0
1	A	351	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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	NDG	B	9	14/15	0.21	17.18	75,84,90,93	0
3	NAG	A	9	14/15	0.22	6.28	84,91,95,99	0
3	NAG	A	5	14/15	0.13	0.41	60,65,68,75	0
3	MAN	A	4	11/12	0.14	0.22	49,56,65,66	0
3	FUL	A	8	10/11	0.26	-0.01	80,85,91,97	0
3	NAG	A	2	14/15	0.13	-0.08	52,57,62,62	0
3	BMA	A	3	11/12	0.10	-0.29	37,46,51,52	0
4	FUC	B	8	10/11	0.23	-0.32	66,71,75,90	0
4	NAG	B	1	14/15	0.14	-0.49	49,56,66,71	0
4	NAG	B	2	14/15	0.12	-0.54	38,47,50,60	0
3	NAG	A	1	14/15	0.15	-0.73	62,75,83,87	0
4	NAG	B	5	14/15	0.10	-0.92	33,36,41,42	0
4	MAN	B	4	11/12	0.08	-1.21	33,41,48,50	0
4	BMA	B	3	11/12	0.07	-7.67	44,46,55,57	0
3	MAN	A	6	11/12	0.13	-	59,67,76,78	0
4	MAN	B	6	11/12	0.12	-	49,57,62,71	0

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.