



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:13 am GMT

PDB ID : 4Q7D
Title : Wild type Fc (wtFc)
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Deposited on : 2014-04-24
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

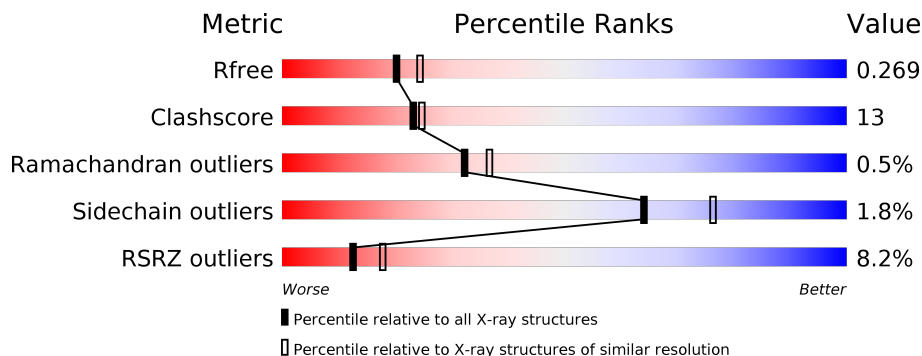
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	221	<div> <div>14%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>6%</div> </div> </div>
1	B	221	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	501	X	-	-	-
2	BMA	A	503	-	-	X	-
3	MAN	A	507	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3685 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

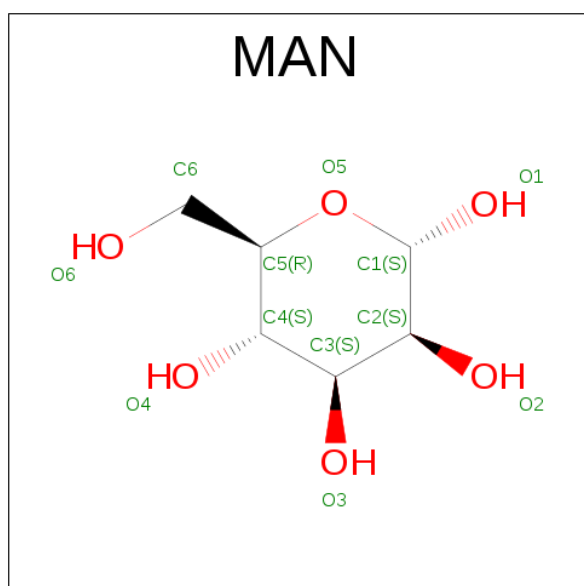
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	11	0	0
			1660	1057	279	318	6			
1	B	208	Total	C	N	O	S	11	0	0
			1662	1058	280	318	6			

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

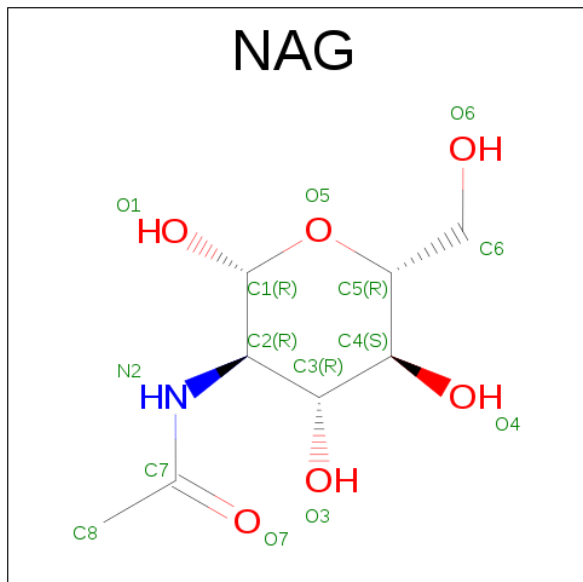
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	3	0
			74	42	3	29		

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

- 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 (8-MER).

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

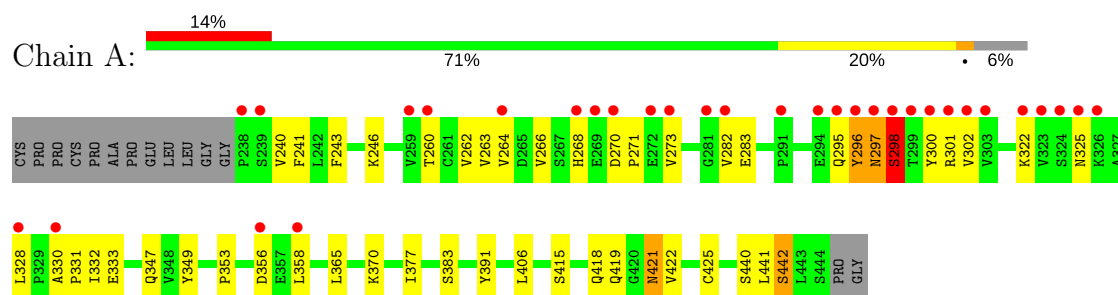
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total	O	0	0
			65	65		
6	B	100	Total	O	0	0
			100	100		

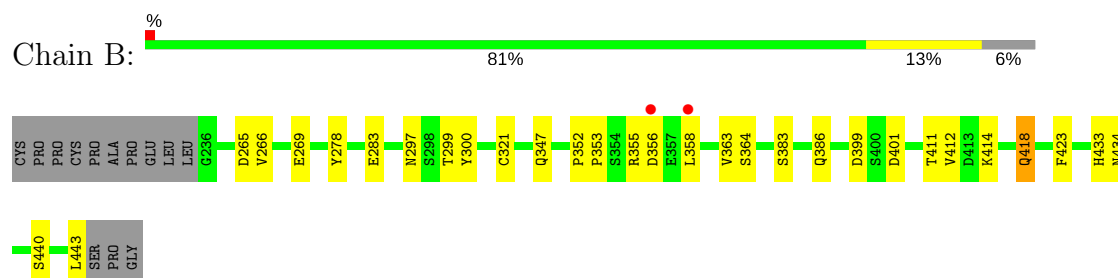
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Ig gamma-1 chain C region



• Molecule 1: Ig gamma-1 chain C region



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.52Å 79.48Å 137.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.09 – 2.35 52.09 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (52.09-2.35) 99.7 (52.09-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.34Å)	Xtriage
Refinement program	PHENIX REFINE	Depositor
R, R_{free}	0.211 , 0.264 0.216 , 0.269	Depositor DCC
R_{free} test set	3703 reflections (8.48%)	DCC
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3685	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, NAG, 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	1.04	4/1706 (0.2%)	0.95	8/2324 (0.3%)
1	B	0.85	2/1708 (0.1%)	0.83	1/2327 (0.0%)
All	All	0.95	6/3414 (0.2%)	0.89	9/4651 (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
2	A	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	ASN	C-N	-16.83	0.95	1.34
1	A	298	SER	C-N	-16.44	0.96	1.34
1	A	296	TYR	C-N	11.35	1.60	1.34
1	B	321	CYS	CB-SG	-6.15	1.71	1.82
1	A	425	CYS	CB-SG	-5.79	1.72	1.81
1	B	269	GLU	CG-CD	5.02	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	TYR	O-C-N	10.41	139.35	122.70
1	A	297	ASN	O-C-N	-9.82	106.99	122.70
1	A	296	TYR	CA-C-N	-9.46	96.39	117.20
1	A	297	ASN	C-N-CA	8.03	141.78	121.70
1	A	296	TYR	C-N-CA	-7.39	103.22	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASN	CA-C-N	7.04	132.69	117.20
1	A	298	SER	O-C-N	5.27	131.14	122.70
1	A	356	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	356	ASP	CB-CG-OD2	5.20	122.98	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	NAG	C1

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1660	0	1629	54	0
1	B	1662	0	1627	21	0
2	A	74	0	64	16	0
3	A	11	0	9	10	0
4	A	14	0	13	6	0
5	B	99	0	85	0	0
6	A	65	0	0	8	0
6	B	100	0	0	6	1
All	All	3685	0	3427	86	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:508:NAG:O3	6:A:642:HOH:O	1.61	1.17
1:A:353:PRO:HB2	1:A:358:LEU:CD2	1.77	1.15
1:A:353:PRO:HB2	1:A:358:LEU:HD21	1.13	1.09
1:A:260:THR:HG21	4:A:508:NAG:H61	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:HD22	2:A:501:NAG:C1	1.54	1.03
2:A:503:BMA:C6	3:A:507:MAN:C1	2.38	1.02
1:A:322:LYS:NZ	6:A:629:HOH:O	2.00	0.95
1:A:241:PHE:CE2	2:A:502:NAG:H4	2.05	0.91
1:A:297:ASN:HD21	2:A:501:NAG:C1	1.75	0.91
1:A:353:PRO:CB	1:A:358:LEU:HD21	2.02	0.90
1:A:301:ARG:NH1	2:A:502:NAG:O7	2.06	0.89
1:B:352:PRO:O	6:B:614:HOH:O	1.88	0.88
1:B:355:ARG:NH1	6:B:681:HOH:O	2.06	0.88
4:A:508:NAG:C4	6:A:642:HOH:O	2.22	0.86
1:A:241:PHE:HE2	2:A:502:NAG:H4	1.44	0.83
2:A:503:BMA:O6	3:A:507:MAN:C5	2.26	0.83
1:A:353:PRO:CB	1:A:358:LEU:CD2	2.55	0.82
2:A:503:BMA:O6	3:A:507:MAN:H5	1.82	0.79
1:B:353:PRO:HB2	1:B:358:LEU:CD2	2.14	0.77
2:A:503:BMA:C6	3:A:507:MAN:O5	2.34	0.76
1:B:347:GLN:OE1	6:B:633:HOH:O	2.05	0.73
2:A:503:BMA:O6	3:A:507:MAN:O5	2.06	0.71
1:A:260:THR:CG2	4:A:508:NAG:H61	2.19	0.71
2:A:503:BMA:H62	3:A:507:MAN:C1	2.24	0.68
1:A:370:LYS:NZ	6:A:640:HOH:O	2.28	0.66
1:A:377:ILE:O	6:A:661:HOH:O	2.13	0.65
1:A:353:PRO:CB	1:A:358:LEU:HD23	2.27	0.65
1:A:241:PHE:CE2	2:A:502:NAG:C4	2.80	0.64
1:B:353:PRO:HB2	1:B:358:LEU:HD23	1.80	0.63
1:A:391:TYR:OH	6:A:655:HOH:O	2.14	0.62
1:A:243:PHE:CE1	3:A:507:MAN:C1	2.83	0.62
1:A:260:THR:HG21	4:A:508:NAG:C6	2.25	0.60
1:A:325:ASN:O	1:A:328:LEU:HG	2.02	0.60
1:A:422:VAL:HG22	1:A:442:SER:OG	2.05	0.57
1:A:332:ILE:CG2	1:A:333:GLU:N	2.68	0.57
1:B:353:PRO:HB2	1:B:358:LEU:HD21	1.86	0.56
1:A:330:ALA:HB1	1:A:331:PRO:HD2	1.87	0.56
2:A:503:BMA:C6	3:A:507:MAN:C5	2.85	0.55
1:A:243:PHE:CZ	3:A:507:MAN:C1	2.91	0.54
1:B:399:ASP:O	1:B:401:ASP:N	2.41	0.54
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.90	0.53
1:A:260:THR:HG23	1:A:260:THR:O	2.10	0.51
1:A:282:VAL:HG23	1:A:283:GLU:O	2.11	0.51
1:A:262:VAL:CG1	1:A:301:ARG:NH1	2.74	0.51
1:A:347:GLN:HG3	1:A:349:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:LEU:O	6:B:664:HOH:O	2.18	0.50
1:A:330:ALA:HB1	1:A:331:PRO:CD	2.41	0.50
4:A:508:NAG:H4	6:A:642:HOH:O	2.01	0.48
1:A:332:ILE:HG22	1:A:333:GLU:N	2.29	0.48
1:B:353:PRO:HB3	1:B:363:VAL:CG1	2.44	0.48
1:B:411:THR:HG22	6:B:660:HOH:O	2.14	0.48
1:A:246:LYS:NZ	6:A:642:HOH:O	2.46	0.47
1:A:365:LEU:HB3	1:A:441:LEU:HD23	1.96	0.47
1:A:264:VAL:HG11	2:A:501:NAG:O4	2.15	0.47
1:A:263:VAL:HB	1:A:302:VAL:HG13	1.97	0.46
1:A:262:VAL:HG11	1:A:301:ARG:HH12	1.80	0.46
1:A:264:VAL:HG11	2:A:502:NAG:O5	2.16	0.46
1:A:383:SER:OG	1:A:422:VAL:O	2.24	0.45
1:B:297:ASN:C	1:B:297:ASN:OD1	2.54	0.45
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.98	0.45
1:B:412:VAL:HG11	1:B:423:PHE:CE1	2.51	0.45
1:A:421:ASN:OD1	1:A:421:ASN:N	2.50	0.45
1:A:266:VAL:O	1:A:300:TYR:N	2.40	0.44
1:A:406:LEU:HD12	1:A:406:LEU:C	2.38	0.44
1:B:265:ASP:HA	1:B:299:THR:HB	1.99	0.44
1:B:411:THR:CG2	6:B:660:HOH:O	2.66	0.44
1:A:328:LEU:HD13	1:A:330:ALA:HA	2.00	0.43
1:B:353:PRO:CB	1:B:358:LEU:HD23	2.46	0.43
1:B:363:VAL:HG12	1:B:364:SER:N	2.34	0.43
2:A:503:BMA:C6	3:A:507:MAN:H5	2.48	0.42
1:A:296:TYR:O	1:A:296:TYR:CG	2.72	0.42
1:A:295:GLN:HB3	1:A:297:ASN:OD1	2.20	0.42
1:A:325:ASN:H	1:A:328:LEU:HD23	1.84	0.42
1:B:278:TYR:CE2	1:B:283:GLU:HB2	2.54	0.42
1:A:365:LEU:HB3	1:A:441:LEU:CD2	2.49	0.42
1:B:433:HIS:O	1:B:434:ASN:HB2	2.19	0.41
1:A:273:VAL:HG21	1:A:302:VAL:HG11	2.02	0.41
1:B:414:LYS:HG2	1:B:418:GLN:NE2	2.35	0.41
1:A:262:VAL:HG11	1:A:301:ARG:NH1	2.35	0.41
1:A:262:VAL:CG1	1:A:301:ARG:HH12	2.33	0.41
1:A:415:SER:O	1:A:418:GLN:N	2.53	0.41
1:B:353:PRO:HG3	1:B:363:VAL:HG12	2.03	0.41
1:A:240:VAL:HG21	1:A:332:ILE:HG21	2.02	0.41
1:A:297:ASN:O	1:A:298:SER:CB	2.67	0.40
1:A:270:ASP:N	1:A:271:PRO:HD3	2.36	0.40
1:A:268:HIS:ND1	1:A:300:TYR:HE1	2.19	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:669:HOH:O	6:B:680:HOH:O[4_555]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	205/221 (93%)	190 (93%)	13 (6%)	2 (1%)	18	18
1	B	206/221 (93%)	200 (97%)	6 (3%)	0	100	100
All	All	411/442 (93%)	390 (95%)	19 (5%)	2 (0%)	32	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	SER
1	A	419	GLN

5.3.2 Protein sidechains [i](#)

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	194/204 (95%)	191 (98%)	3 (2%)	70	81
1	B	193/204 (95%)	189 (98%)	4 (2%)	59	72
All	All	387/408 (95%)	380 (98%)	7 (2%)	64	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	421	ASN
1	A	440	SER
1	A	442	SER
1	B	383	SER
1	B	386	GLN
1	B	418	GLN
1	B	440	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	501	1,2	14,14,15	0.74	0	15,19,21	1.20	1 (6%)
2	NAG	A	502	2	14,14,15	0.73	0	15,19,21	1.03	1 (6%)
2	BMA	A	503	3,2	11,11,12	0.62	0	13,15,17	1.66	3 (23%)
2	MAN	A	504	2	11,11,12	0.61	0	13,15,17	1.43	1 (7%)
2	NAG	A	505	2	14,14,15	0.47	0	15,19,21	1.13	2 (13%)
2	FUC	A	506	2	9,10,11	0.60	0	13,14,16	1.22	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	501	1,5	14,14,15	0.55	0	15,19,21	1.75	4 (26%)
5	NAG	B	502	5	14,14,15	0.65	0	15,19,21	0.96	0
5	BMA	B	503	5	11,11,12	0.39	0	13,15,17	1.31	1 (7%)
5	MAN	B	504	5	11,11,12	0.64	0	13,15,17	1.21	2 (15%)
5	NAG	B	505	5	14,14,15	0.70	0	15,19,21	1.53	4 (26%)
5	MAN	B	506	5	11,11,12	0.41	0	13,15,17	1.42	1 (7%)
5	NAG	B	507	5	14,14,15	0.67	0	15,19,21	1.03	0
5	FUC	B	508	5	9,10,11	0.69	0	13,14,16	0.60	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
2	NAG	A	501	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	BMA	A	503	3,2	-	0/2/19/22	0/1/1/1
2	MAN	A	504	2	-	0/2/19/22	0/1/1/1
2	NAG	A	505	2	-	0/6/23/26	0/1/1/1
2	FUC	A	506	2	-	0/0/17/20	0/1/1/1
5	NAG	B	501	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	502	5	-	0/6/23/26	0/1/1/1
5	BMA	B	503	5	-	0/2/19/22	0/1/1/1
5	MAN	B	504	5	-	0/2/19/22	0/1/1/1
5	NAG	B	505	5	-	0/6/23/26	0/1/1/1
5	MAN	B	506	5	-	0/2/19/22	0/1/1/1
5	NAG	B	507	5	-	0/6/23/26	0/1/1/1
5	FUC	B	508	5	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	BMA	O3-C3-C4	-3.54	102.66	110.36
2	A	503	BMA	O6-C6-C5	-2.75	102.09	111.34
2	A	502	NAG	C8-C7-N2	-2.04	112.42	116.11
2	A	501	NAG	C1-O5-C5	2.11	115.07	112.17
5	B	505	NAG	C2-N2-C7	2.13	126.05	122.94
5	B	501	NAG	C1-C2-N2	2.14	114.15	110.49
2	A	505	NAG	O5-C1-C2	2.16	114.48	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	NAG	O5-C1-C2	2.23	114.58	111.47
2	A	506	FUC	O2-C2-C1	2.37	113.99	109.18
5	B	505	NAG	C3-C4-C5	2.37	114.39	110.22
5	B	504	MAN	O4-C4-C5	2.41	115.36	109.28
5	B	504	MAN	C1-O5-C5	2.46	115.56	112.17
5	B	501	NAG	C8-C7-N2	2.46	120.55	116.11
5	B	501	NAG	C2-N2-C7	2.77	126.98	122.94
2	A	503	BMA	C1-O5-C5	2.90	116.16	112.17
5	B	505	NAG	C4-C3-C2	3.00	115.41	111.02
2	A	505	NAG	C1-O5-C5	3.15	116.51	112.17
5	B	506	MAN	C1-O5-C5	3.59	117.12	112.17
2	A	504	MAN	C1-O5-C5	3.68	117.24	112.17
5	B	503	BMA	C1-O5-C5	3.78	117.37	112.17
5	B	501	NAG	C1-O5-C5	4.06	117.77	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	3	0
2	A	502	NAG	5	0
2	A	503	BMA	8	0

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	A	507	2,4	11,11,12	0.78	0	13,15,17	1.48	1 (7%)
4	NAG	A	508	3	14,14,15	0.95	1 (7%)	15,19,21	1.28	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	MAN	A	507	2,4	-	0/2/19/22	0/1/1/1
4	NAG	A	508	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	508	NAG	O5-C5	-2.04	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	508	NAG	O4-C4-C3	3.44	117.84	110.36
3	A	507	MAN	C1-O5-C5	4.55	118.44	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	MAN	10	0
4	A	508	NAG	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th 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 ²)	Q<0.9
1	A	207/221 (93%)	0.84	32 (15%) 2 3	26, 52, 96, 122	4 (1%)
1	B	208/221 (94%)	0.12	2 (0%) 82 90	27, 43, 68, 81	4 (1%)
All	All	415/442 (93%)	0.48	34 (8%) 12 18	26, 46, 89, 122	8 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	TYR	11.6
1	A	300	TYR	6.6
1	A	291	PRO	6.3
1	A	299	THR	5.8
1	A	358	LEU	5.0
1	A	273	VAL	4.7
1	A	295	GLN	4.7
1	A	298	SER	4.3
1	A	238	PRO	4.0
1	A	269	GLU	4.0
1	A	268	HIS	3.9
1	A	297	ASN	3.9
1	A	302	VAL	3.8
1	A	323	VAL	3.5
1	A	239	SER	3.4
1	A	301	ARG	3.2
1	A	326	LYS	3.2
1	A	303	VAL	3.0
1	A	325	ASN	2.9
1	A	264	VAL	2.8
1	A	328	LEU	2.6
1	A	356	ASP	2.5
1	A	260	THR	2.5
1	B	356	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	324	SER	2.4
1	A	270	ASP	2.2
1	A	322	LYS	2.2
1	A	282	VAL	2.2
1	A	294	GLU	2.2
1	A	272	GLU	2.2
1	A	281	GLY	2.2
1	A	259	VAL	2.1
1	B	358	LEU	2.1
1	A	330	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	502	14/15	0.65	0.21	-0.93	37,40,44,46	14
5	NAG	B	507	14/15	0.87	0.12	-1.45	43,47,56,56	0
5	MAN	B	506	11/12	0.85	0.16	-	48,54,57,58	0
2	BMA	A	503	11/12	0.64	0.25	-	40,42,43,45	0
5	NAG	B	505	14/15	0.67	0.21	-	82,90,92,96	0
5	NAG	B	502	14/15	0.91	0.19	-	56,63,67,67	0
5	BMA	B	503	11/12	0.89	0.16	-	51,52,53,57	0
2	FUC	A	506	10/11	0.72	0.24	-	47,49,56,56	3
2	NAG	A	501	14/15	0.73	0.25	-	41,42,45,47	14
2	MAN	A	504	11/12	0.88	0.14	-	50,53,59,68	0
5	MAN	B	504	11/12	0.80	0.16	-	52,59,63,74	0
2	NAG	A	505	14/15	0.79	0.22	-	76,81,85,86	0
5	NAG	B	501	14/15	0.77	0.20	-	74,88,93,96	0
5	FUC	B	508	10/11	0.60	0.40	-	99,103,108,109	0

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	A	508	14/15	0.78	0.25	0.33	37,43,50,52	0
3	MAN	A	507	11/12	0.71	0.20	-	44,46,51,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.