



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:10 AM GMT

PDB ID : 2W59
Title : STRUCTURE OF AN AVIAN IGY-FC 3-4 FRAGMENT
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Deposited on : 2008-12-08
Resolution : 1.75 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

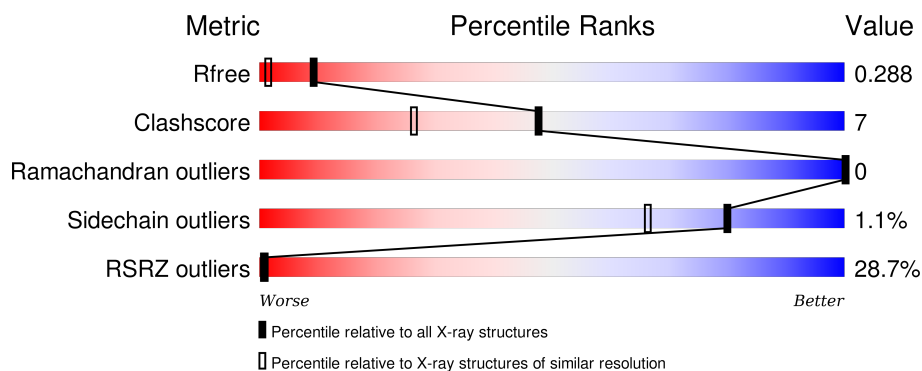
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	231	<div> <div>23%</div> <div>81%</div> <div>12%</div> <div>7%</div> </div>
1	B	231	<div> <div>31%</div> <div>79%</div> <div>13%</div> <div>7%</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	1567	X	-	-	-
2	MAN	A	1569	X	-	-	-
2	MAN	B	1569	X	-	-	-
3	GOL	B	1570	-	-	-	X
3	GOL	B	1572	-	-	-	X
3	GOL	B	1573	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4072 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 IGY FCU3-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	4	0
			1701	1082	293	315	11			
1	B	214	Total	C	N	O	S	0	5	0
			1701	1082	292	315	12			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

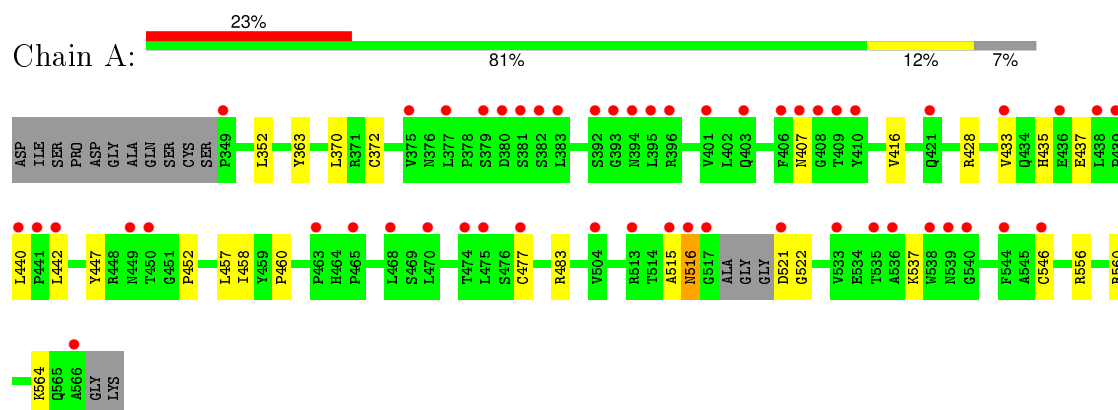
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	272	Total 272	O 272	0	0
4	B	284	Total 284	O 284	0	0

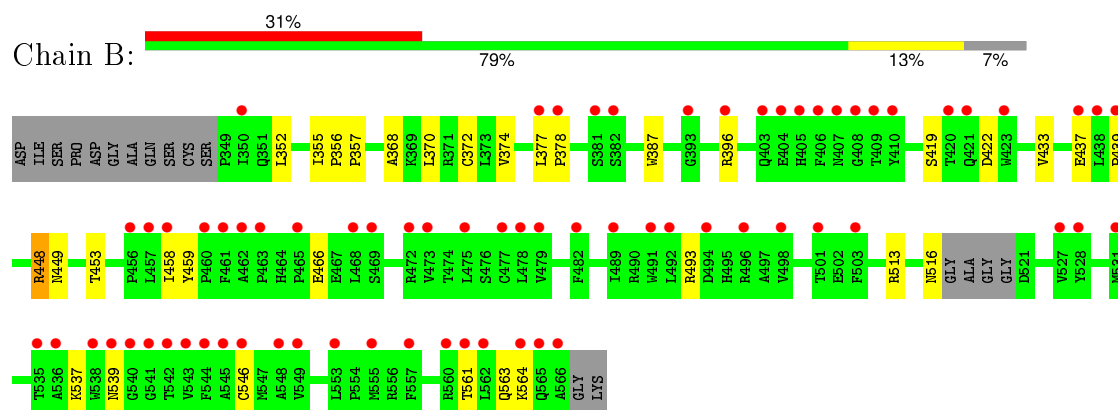
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: IGY FCU3-4



• Molecule 1: IGY FCU3-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.48Å 80.14Å 99.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 1.75 52.06 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.57-1.75) 96.9 (52.06-1.68)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.68Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.169 , 0.196 0.279 , 0.288	Depositor DCC
R_{free} test set	2764 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61160 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4072	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 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	0.33	0/1759	0.52	0/2400
1	B	0.34	0/1762	0.57	2/2404 (0.1%)
All	All	0.34	0/3521	0.55	2/4804 (0.0%)

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	2	0
2	B	1	0
All	All	3	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	B	448	ARG	NE-CZ-NH1	7.00	123.80	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1567	NAG	C1
2	A	1569	MAN	C1
2	B	1569	MAN	C1

There are no planarity outliers.

5.2 Too-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 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	1701	0	1684	20	0
1	B	1701	0	1682	31	0
2	A	39	0	34	0	0
2	B	39	0	34	0	0
3	A	6	0	8	2	0
3	B	30	0	40	8	0
4	A	272	0	0	4	2
4	B	284	0	0	6	2
All	All	4072	0	3482	52	2

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 7.

All (52) 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)
1:B:419:SER:H	3:B:1571:GOL:H32	1.20	1.02
1:B:563:GLN:OE1	4:B:2271:HOH:O	1.88	0.89
1:A:564:LYS:NZ	4:A:2265:HOH:O	2.09	0.85
1:A:352:LEU:HD11	1:A:372:CYS:SG	2.24	0.78
1:B:422:ASP:OD1	3:B:1571:GOL:H31	1.87	0.74
1:A:515:ALA:N	1:A:516:ASN:HA	2.06	0.70
1:B:419:SER:N	3:B:1571:GOL:H32	2.02	0.70
1:B:513:ARG:HD3	4:B:2185:HOH:O	1.90	0.70
1:B:352:LEU:HD11	1:B:372[A]:CYS:SG	2.33	0.68
1:B:459:TYR:CE1	3:B:1572:GOL:H31	2.31	0.64
1:A:363:TYR:CD1	1:A:556:ARG:HD2	2.33	0.64
1:B:352:LEU:HD11	1:B:372[B]:CYS:SG	2.38	0.63
1:A:435:HIS:CE1	1:A:437:GLU:HG2	2.35	0.61
1:A:440:LEU:HG	4:A:2053:HOH:O	2.01	0.60
1:B:372[B]:CYS:HB2	1:B:387:TRP:CZ2	2.36	0.60
3:A:1570:GOL:H31	1:B:466:GLU:OE1	2.04	0.57
1:B:437:GLU:O	1:B:439:PRO:HD3	2.06	0.55
1:B:563:GLN:CD	4:B:2271:HOH:O	2.37	0.54
1:B:357:PRO:HB3	1:B:368:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ARG:CZ	1:A:521:ASP:HB3	2.39	0.53
1:B:372[A]:CYS:HB2	1:B:387:TRP:CZ2	2.44	0.53
4:A:2081:HOH:O	3:B:1574:GOL:H32	2.09	0.53
1:B:449:ASN:ND2	1:B:453:THR:HG22	2.23	0.53
1:A:433:VAL:CG1	1:A:442:LEU:HB3	2.40	0.52
1:B:561:THR:O	3:B:1574:GOL:H31	2.09	0.52
1:A:452:PRO:HG2	1:A:521:ASP:OD1	2.09	0.51
1:B:448:ARG:HD3	4:B:2253:HOH:O	2.10	0.51
1:B:449:ASN:HB2	3:B:1573:GOL:O2	2.11	0.51
1:A:521:ASP:CG	1:A:522:GLY:H	2.14	0.51
1:A:435:HIS:HE1	1:A:437:GLU:HG2	1.75	0.51
1:B:493:ARG:HD2	1:B:537:LYS:HE2	1.93	0.51
1:A:537:LYS:HD2	4:A:2237:HOH:O	2.11	0.50
1:A:460:PRO:HG3	1:A:560:ARG:HB3	1.92	0.49
1:A:516:ASN:ND2	1:A:516:ASN:C	2.66	0.49
1:B:396:ARG:HG3	4:B:2046:HOH:O	2.14	0.48
1:B:539:ASN:HA	1:B:564:LYS:HD2	1.95	0.48
1:A:352:LEU:HB3	1:A:442:LEU:HD22	1.96	0.47
1:A:516:ASN:HD22	1:A:516:ASN:C	2.18	0.47
1:B:352:LEU:HD13	1:B:433:VAL:HG21	1.96	0.47
1:B:448:ARG:HD2	1:B:449:ASN:O	2.15	0.47
1:B:458:ILE:O	3:B:1572:GOL:H2	2.17	0.45
1:A:428:ARG:HA	1:A:447:TYR:HB3	1.98	0.45
1:B:352:LEU:HD13	1:B:433:VAL:CG2	2.49	0.43
1:B:377:LEU:HA	1:B:378:PRO:HD3	1.88	0.42
1:B:352:LEU:HD13	1:B:374:VAL:HG22	2.02	0.42
1:B:355:ILE:HA	1:B:356:PRO:HD3	1.88	0.42
1:A:370:LEU:HB2	1:A:416:VAL:CG1	2.50	0.41
1:B:516:ASN:ND2	4:B:2194:HOH:O	2.52	0.41
1:B:374:VAL:HG22	1:B:433:VAL:HG21	2.03	0.41
1:B:357:PRO:HG3	1:B:370:LEU:HD23	2.02	0.41
1:A:458:ILE:HG23	1:A:477[A]:CYS:SG	2.61	0.41
1:A:457:LEU:HD22	3:A:1570:GOL:H11	2.04	0.40

All (2) 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)
4:A:2090:HOH:O	4:B:2016:HOH:O[3_455]	1.41	0.79
4:A:2245:HOH:O	4:B:2003:HOH:O[3_455]	1.87	0.33

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	215/231 (93%)	214 (100%)	1 (0%)	0	100	100
1	B	215/231 (93%)	211 (98%)	4 (2%)	0	100	100
All	All	430/462 (93%)	425 (99%)	5 (1%)	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	194/201 (96%)	190 (98%)	4 (2%)	61	37
1	B	195/201 (97%)	193 (99%)	2 (1%)	82	69
All	All	389/402 (97%)	383 (98%)	6 (2%)	80	55

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
1	A	516	ASN
1	A	546[A]	CYS
1	A	546[B]	CYS
1	B	546[A]	CYS
1	B	546[B]	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	GLN
1	A	516	ASN
1	B	449	ASN

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 ⓘ

6 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	1567	1,2	14,14,15	0.48	0	15,19,21	1.10	1 (6%)
2	NAG	A	1568	2	14,14,15	0.45	0	15,19,21	1.28	1 (6%)
2	MAN	A	1569	2	11,11,12	0.71	0	14,15,17	1.34	1 (7%)
2	NAG	B	1567	1,2	14,14,15	0.45	0	15,19,21	1.35	1 (6%)
2	NAG	B	1568	2	14,14,15	0.49	0	15,19,21	1.26	2 (13%)
2	MAN	B	1569	2	11,11,12	0.70	0	14,15,17	1.70	2 (14%)

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	1567	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1568	2	-	0/6/23/26	0/1/1/1
2	MAN	A	1569	2	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	B	1567	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1568	2	-	0/6/23/26	0/1/1/1
2	MAN	B	1569	2	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1568	NAG	C4-C3-C2	-3.62	105.60	111.23
2	B	1568	NAG	C2-N2-C7	-2.51	119.81	123.04
2	B	1569	MAN	C2-C3-C4	2.39	115.11	111.04
2	A	1567	NAG	C1-O5-C5	2.79	115.78	112.25
2	B	1568	NAG	C1-O5-C5	3.48	116.66	112.25
2	B	1567	NAG	C1-O5-C5	4.11	117.47	112.25
2	A	1569	MAN	C1-C2-C3	4.29	114.62	109.54
2	B	1569	MAN	C1-C2-C3	5.21	115.70	109.54

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1569	MAN	C1
2	A	1569	MAN	C1
2	A	1567	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

6 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	GOL	A	1570	-	5,5,5	0.31	0	5,5,5	0.31	0
3	GOL	B	1570	-	5,5,5	0.37	0	5,5,5	0.52	0
3	GOL	B	1571	-	5,5,5	0.42	0	5,5,5	0.47	0
3	GOL	B	1572	-	5,5,5	0.35	0	5,5,5	0.48	0
3	GOL	B	1573	-	5,5,5	0.26	0	5,5,5	0.30	0
3	GOL	B	1574	-	5,5,5	0.34	0	5,5,5	0.16	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
3	GOL	A	1570	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1570	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1571	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1572	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1573	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1574	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1570	GOL	2	0
3	B	1571	GOL	3	0
3	B	1572	GOL	2	0
3	B	1573	GOL	1	0
3	B	1574	GOL	2	0

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, 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	215/231 (93%)	1.40	52 (24%)	1 1	12, 32, 76, 95	0
1	B	214/231 (92%)	1.64	71 (33%)	0 1	12, 27, 69, 103	0
All	All	429/462 (92%)	1.52	123 (28%)	1 1	12, 29, 76, 103	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	ASN	8.1
1	B	406	PHE	6.4
1	A	566	ALA	5.8
1	A	410	TYR	5.3
1	B	404	GLU	5.2
1	B	382	SER	5.1
1	B	538	TRP	5.0
1	A	438	LEU	4.8
1	A	381	SER	4.5
1	A	406	PHE	4.5
1	B	378	PRO	4.5
1	B	405	HIS	4.2
1	A	521	ASP	4.1
1	A	379	SER	4.0
1	B	350	ILE	4.0
1	B	409	THR	3.9
1	A	517	GLY	3.8
1	B	566	ALA	3.8
1	A	375	VAL	3.7
1	B	544	PHE	3.7
1	A	407	ASN	3.7
1	B	565	GLN	3.6
1	B	496	ARG	3.6
1	B	541	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	3.5
1	A	468	LEU	3.5
1	A	392	SER	3.5
1	A	515	ALA	3.4
1	A	383	LEU	3.4
1	B	403	GLN	3.4
1	B	408	GLY	3.4
1	B	438	LEU	3.3
1	B	562	LEU	3.3
1	A	440	LEU	3.1
1	A	450	THR	3.1
1	A	380	ASP	3.1
1	A	442	LEU	3.1
1	B	477[A]	CYS	3.1
1	B	553	LEU	3.0
1	B	460	PRO	3.0
1	B	475	LEU	3.0
1	B	473	VAL	3.0
1	B	543	VAL	3.0
1	B	377	LEU	2.9
1	B	462	ALA	2.9
1	B	557	PHE	2.9
1	A	441	PRO	2.9
1	A	394	ASN	2.8
1	A	408	GLY	2.8
1	B	540	GLY	2.8
1	A	538	TRP	2.8
1	B	461	PHE	2.8
1	B	381	SER	2.8
1	A	449	ASN	2.8
1	B	494	ASP	2.8
1	A	477[A]	CYS	2.8
1	B	491	TRP	2.7
1	B	546[A]	CYS	2.7
1	A	395	LEU	2.7
1	B	457	LEU	2.7
1	B	527	VAL	2.7
1	A	504	VAL	2.6
1	A	540	GLY	2.6
1	B	531	MET	2.6
1	B	456	PRO	2.6
1	B	465	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	458	ILE	2.6
1	A	470	LEU	2.5
1	B	492	LEU	2.5
1	B	410	TYR	2.5
1	B	393	GLY	2.5
1	B	561	THR	2.5
1	A	377	LEU	2.5
1	B	548	ALA	2.5
1	B	555	MET	2.5
1	B	535	THR	2.4
1	A	465	PRO	2.4
1	B	437	GLU	2.4
1	B	439	PRO	2.4
1	B	503	PHE	2.4
1	B	564	LYS	2.4
1	A	546[A]	CYS	2.3
1	A	475	LEU	2.3
1	B	536	ALA	2.3
1	B	479	VAL	2.3
1	B	498	VAL	2.3
1	B	463	PRO	2.3
1	B	407	ASN	2.3
1	B	396	ARG	2.3
1	A	433	VAL	2.3
1	A	409	THR	2.2
1	A	513	ARG	2.2
1	A	401	VAL	2.2
1	A	533	VAL	2.2
1	B	482	PHE	2.2
1	A	463	PRO	2.2
1	B	478	LEU	2.2
1	B	542	THR	2.2
1	B	539	ASN	2.2
1	A	393	GLY	2.2
1	B	560	ARG	2.2
1	B	549	VAL	2.2
1	A	544	PHE	2.1
1	B	472	ARG	2.1
1	B	545	ALA	2.1
1	B	528	TYR	2.1
1	A	349	PRO	2.1
1	B	501	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	536	ALA	2.1
1	B	468	LEU	2.1
1	B	489	ILE	2.1
1	B	423	TRP	2.1
1	A	421	GLN	2.0
1	A	474	THR	2.0
1	B	420	THR	2.0
1	B	469	SER	2.0
1	A	436	GLU	2.0
1	B	421	GLN	2.0
1	A	439	PRO	2.0
1	A	539	ASN	2.0
1	A	382	SER	2.0
1	A	535	THR	2.0
1	A	403	GLN	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	1568	14/15	0.75	0.24	1.21	71,74,90,93	0
2	NAG	B	1568	14/15	0.80	0.15	-0.54	61,67,76,80	0
2	MAN	B	1569	11/12	0.56	0.20	-	77,79,81,82	11
2	MAN	A	1569	11/12	0.32	0.27	-	71,77,81,82	11
2	NAG	B	1567	14/15	0.73	0.23	-	66,73,81,85	0
2	NAG	A	1567	14/15	0.91	0.21	-	70,75,78,81	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
3	GOL	B	1570	6/6	0.84	0.27	3.35	24,45,51,62	0
3	GOL	B	1572	6/6	0.56	0.28	2.87	34,43,48,58	0
3	GOL	B	1573	6/6	0.83	0.18	2.62	23,57,58,67	0
3	GOL	A	1570	6/6	0.82	0.22	1.38	39,56,65,71	0
3	GOL	B	1574	6/6	0.69	0.27	0.92	32,59,64,69	0
3	GOL	B	1571	6/6	0.73	0.22	0.91	20,38,46,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.