



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:48 AM GMT

PDB ID : 2UVO
Title : HIGH RESOLUTION CRYSTAL STRUCTURE OF WHEAT GERM AG-
GLUTININ IN COMPLEX WITH N-ACETYL-D-GLUCOSAMINE
Authors : Schwefel, D.; Wittmann, V.; Diederichs, K.; Welte, W.
Deposited on : 2007-03-13
Resolution : 1.40 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

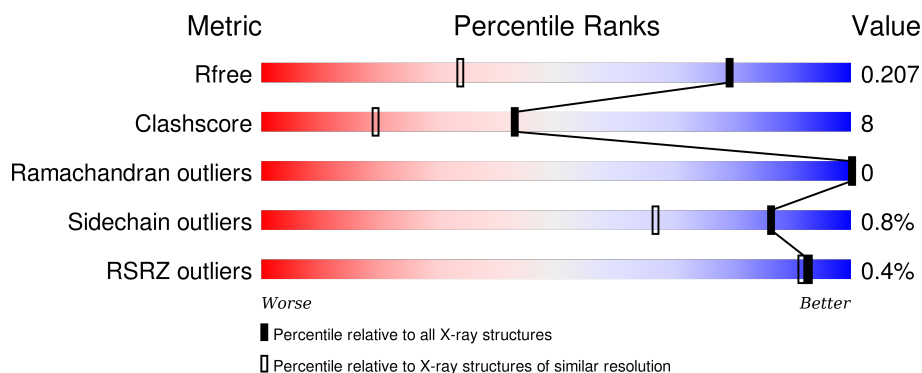
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1199 (1.40-1.40)
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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	171	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
1	B	171	<div> <div style="width: 96%;"></div> <div>96%</div> </div>
1	E	171	<div> <div style="width: 89%;"></div> <div>89%</div> <div style="width: 9%;"></div> <div>9%</div> </div>
1	F	171	<div> <div style="width: 91%;"></div> <div>91%</div> <div style="width: 8%;"></div> <div>8%</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
3	NAG	A	1176	X	-	-	X
3	NAG	B	1173	-	-	-	X
3	NAG	F	1174	-	-	-	X
4	GOL	A	1177[A]	-	-	-	X
4	GOL	A	1177[B]	-	-	-	X
4	GOL	E	1176	-	-	-	X
4	GOL	F	1178[A]	-	-	-	X
4	GOL	F	1178[B]	-	-	-	X

2 Entry composition [i](#)

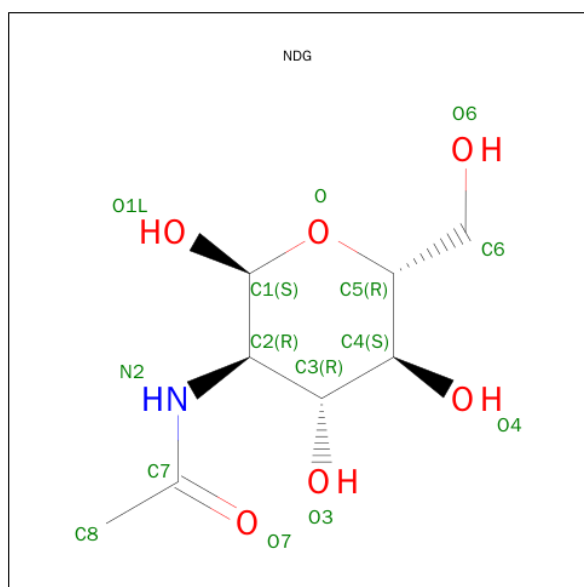
There are 5 unique types of molecules in this entry. The entry contains 5652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AGGLUTININ ISOLECTIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	3	0
			1177	691	215	237	34			
1	B	171	Total	C	N	O	S	0	1	0
			1172	685	214	238	35			
1	E	171	Total	C	N	O	S	2	3	0
			1183	695	215	238	35			
1	F	171	Total	C	N	O	S	0	5	0
			1191	698	217	240	36			

- Molecule 2 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



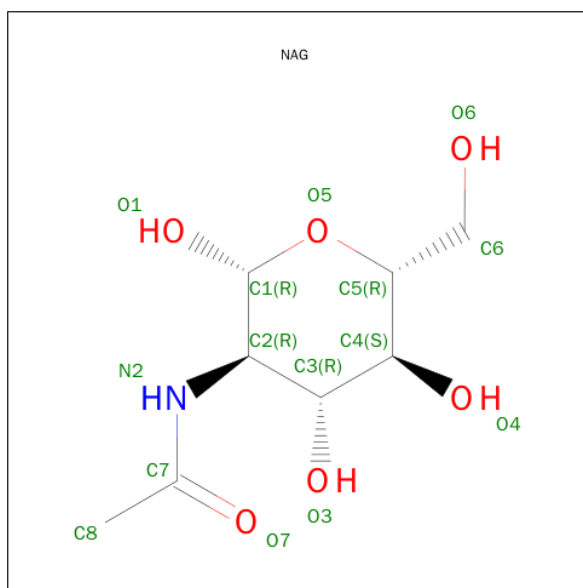
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	1
			15	8	1	6		
2	E	1	Total	C	N	O	0	1
			15	8	1	6		
2	E	1	Total	C	N	O	0	0
			15	8	1	6		
2	E	1	Total	C	N	O	0	0
			15	8	1	6		
2	F	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



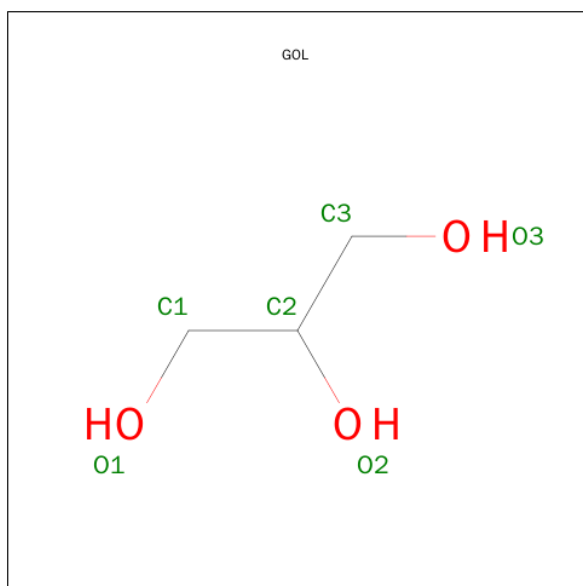
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			15	8	1	6		
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	1
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	1
			15	8	1	6		
3	E	1	Total	C	N	O	0	1
			15	8	1	6		
3	F	1	Total	C	N	O	0	0
			15	8	1	6		
3	F	1	Total	C	N	O	0	0
			15	8	1	6		
3	F	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		
4	B	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is water.

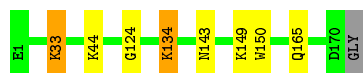
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total 182	O 182	0	0
5	B	177	Total 177	O 177	0	0
5	E	122	Total 122	O 122	0	0
5	F	142	Total 142	O 142	0	0

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: AGGLUTININ ISOLECTIN 1

Chain A:  95% ..




• Molecule 1: AGGLUTININ ISOLECTIN 1

Chain B:  96% ..




• Molecule 1: AGGLUTININ ISOLECTIN 1

Chain E:  89% 9% ..



• Molecule 1: AGGLUTININ ISOLECTIN 1

Chain F:  91% 8% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.39Å 91.51Å 94.50Å 90.00° 82.00° 90.00°	Depositor
Resolution (Å)	93.66 – 1.40 45.75 – 1.40	Depositor EDS
% Data completeness (in resolution range)	93.5 (93.66-1.40) 93.5 (45.75-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.3.0022	Depositor
R, R_{free}	0.181 , 0.204 0.182 , 0.207	Depositor DCC
R_{free} test set	6879 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 137253 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5652	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.08 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.2805e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, PCA, NAG, NDG

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	2.03	2/1200 (0.2%)	0.96	2/1605 (0.1%)
1	B	1.33	2/1189 (0.2%)	0.91	4/1590 (0.3%)
1	E	0.91	5/1206 (0.4%)	0.74	10/1612 (0.6%)
1	F	6.40	8/1220 (0.7%)	2.08	8/1630 (0.5%)
All	All	3.47	17/4815 (0.4%)	1.29	24/6437 (0.4%)

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	F	1	0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	139[A]	ARG	NE-CZ	155.39	3.35	1.33
1	F	139[B]	ARG	NE-CZ	155.39	3.35	1.33
1	A	33[A]	LYS	CE-NZ	48.00	2.69	1.49
1	A	33[B]	LYS	CE-NZ	48.00	2.69	1.49
1	B	26[A]	MET	SD-CE	-30.50	0.07	1.77
1	B	26[B]	MET	SD-CE	-30.50	0.07	1.77
1	F	139[A]	ARG	CD-NE	19.63	1.79	1.46
1	F	139[B]	ARG	CD-NE	19.63	1.79	1.46
1	E	16[A]	LEU	CB-CG	16.96	2.01	1.52
1	E	16[B]	LEU	CB-CG	16.96	2.01	1.52
1	F	91[A]	SER	CB-OG	-12.65	1.25	1.42
1	F	91[B]	SER	CB-OG	-12.65	1.25	1.42
1	F	26[A]	MET	SD-CE	11.60	2.42	1.77
1	F	26[B]	MET	SD-CE	11.60	2.42	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	171	GLY	C-OXT	7.12	1.36	1.23
1	E	10[A]	MET	CG-SD	5.46	1.95	1.81
1	E	10[B]	MET	CG-SD	5.46	1.95	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	139[A]	ARG	CD-NE-CZ	-55.24	46.27	123.60
1	F	139[B]	ARG	CD-NE-CZ	-55.24	46.27	123.60
1	A	33[A]	LYS	CD-CE-NZ	-21.35	62.59	111.70
1	A	33[B]	LYS	CD-CE-NZ	-21.35	62.59	111.70
1	B	26[A]	MET	CG-SD-CE	19.31	131.09	100.20
1	B	26[B]	MET	CG-SD-CE	19.31	131.09	100.20
1	F	139[A]	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	F	139[B]	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	F	139[A]	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	F	139[B]	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	E	16[A]	LEU	CB-CG-CD2	7.33	123.46	111.00
1	E	16[B]	LEU	CB-CG-CD2	7.33	123.46	111.00
1	F	26[A]	MET	CG-SD-CE	7.02	111.44	100.20
1	F	26[B]	MET	CG-SD-CE	7.02	111.44	100.20
1	E	16[A]	LEU	CA-CB-CG	-6.55	100.23	115.30
1	E	16[B]	LEU	CA-CB-CG	-6.55	100.23	115.30
1	E	10[A]	MET	CG-SD-CE	-5.81	90.91	100.20
1	E	10[B]	MET	CG-SD-CE	-5.81	90.91	100.20
1	E	16[A]	LEU	CB-CG-CD1	-5.50	101.66	111.00
1	E	16[B]	LEU	CB-CG-CD1	-5.50	101.66	111.00
1	B	26[A]	MET	CA-CB-CG	5.28	122.27	113.30
1	B	26[B]	MET	CA-CB-CG	5.28	122.27	113.30
1	E	33[A]	LYS	CG-CD-CE	-5.25	96.16	111.90
1	E	33[B]	LYS	CG-CD-CE	-5.25	96.16	111.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	128	THR	CB

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	1177	0	1027	12	0
1	B	1172	0	1008	17	0
1	E	1183	0	1032	21	1
1	F	1191	0	1040	34	0
2	A	30	0	28	0	0
2	B	45	0	44	0	0
2	E	45	0	43	2	1
2	F	15	0	15	0	0
3	A	30	0	29	0	0
3	B	45	0	45	0	0
3	E	15	0	15	0	0
3	F	45	0	45	2	0
4	A	12	0	15	0	0
4	B	6	0	8	0	0
4	E	6	0	7	0	0
4	F	12	0	14	0	0
5	A	182	0	0	1	0
5	B	177	0	0	0	0
5	E	122	0	0	1	0
5	F	142	0	0	1	0
All	All	5652	0	4415	77	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 8.

All (77) 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:26[A]:MET:CG	1:B:26[A]:MET:CE	1.86	1.50
1:F:26[B]:MET:CG	1:F:26[B]:MET:CE	1.87	1.49
1:B:26[B]:MET:CE	1:B:26[B]:MET:CG	1.91	1.47
1:F:139[B]:ARG:CD	1:F:139[B]:ARG:NE	1.79	1.45
1:F:139[A]:ARG:CD	1:F:139[A]:ARG:NE	1.79	1.44
1:E:16[A]:LEU:CB	1:E:16[A]:LEU:CG	2.01	1.39
1:F:139[A]:ARG:HD3	1:F:139[A]:ARG:CZ	1.54	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33[A]:LYS:HD3	1:A:33[A]:LYS:NZ	1.63	1.12
1:F:26[A]:MET:SD	1:F:26[A]:MET:CE	2.42	1.07
1:F:139[B]:ARG:CZ	1:F:139[B]:ARG:CD	2.40	0.99
1:F:139[A]:ARG:CD	1:F:139[A]:ARG:CZ	2.47	0.91
1:E:2:ARG:O	1:F:10[B]:MET:SD	2.30	0.89
1:A:33[A]:LYS:CD	1:A:33[A]:LYS:NZ	2.40	0.85
1:F:139[A]:ARG:NH2	1:F:139[A]:ARG:HD3	1.97	0.80
1:E:100:ASN:HD22	1:F:14:ASN:HD22	1.31	0.79
1:A:124:GLY:H	1:A:143:ASN:HD21	1.32	0.78
1:F:128:THR:HG21	5:F:2084:HOH:O	1.83	0.78
1:F:139[B]:ARG:NE	1:F:139[B]:ARG:CG	2.47	0.77
1:B:26[A]:MET:CG	1:B:26[A]:MET:HE3	1.84	0.77
1:E:134:LYS:H	1:E:165:GLN:HE22	1.34	0.75
1:B:26[A]:MET:CE	1:B:26[A]:MET:CB	2.65	0.74
1:B:124:GLY:H	1:B:143:ASN:HD21	1.35	0.74
1:A:33[B]:LYS:NZ	1:A:33[B]:LYS:HD2	2.05	0.72
1:F:124:GLY:H	1:F:143:ASN:HD21	1.37	0.72
1:E:124:GLY:H	1:E:143:ASN:HD21	1.36	0.71
1:A:33[B]:LYS:CD	1:A:33[B]:LYS:NZ	2.53	0.71
1:A:134[A]:LYS:NZ	1:A:165:GLN:OE1	2.21	0.71
1:B:16:LEU:CD2	1:B:26[B]:MET:HG2	2.21	0.70
1:B:16:LEU:HD22	1:B:26[B]:MET:HG2	1.74	0.70
1:F:139[B]:ARG:CZ	1:F:139[B]:ARG:HD2	2.20	0.70
1:E:101:ASN:HB3	1:F:26[A]:MET:HE3	1.73	0.69
1:E:16[A]:LEU:CA	1:E:16[A]:LEU:CG	2.73	0.67
1:A:124:GLY:H	1:A:143:ASN:ND2	1.94	0.64
1:A:33[A]:LYS:HD3	1:A:33[A]:LYS:HZ3	1.62	0.63
1:E:16[A]:LEU:CD1	1:E:16[A]:LEU:CB	2.76	0.63
1:F:26[B]:MET:CG	1:F:26[B]:MET:HE2	1.82	0.62
1:B:124:GLY:H	1:B:143:ASN:ND2	1.97	0.61
1:E:10[B]:MET:CG	1:F:10[B]:MET:HG2	2.31	0.61
1:E:124:GLY:H	1:E:143:ASN:ND2	1.99	0.61
1:E:100:ASN:ND2	1:F:14:ASN:HD22	2.01	0.58
1:A:33[A]:LYS:CE	1:A:33[A]:LYS:NZ	2.69	0.56
1:E:10[A]:MET:HG2	1:F:10[A]:MET:CG	2.36	0.56
1:E:10[B]:MET:HG3	1:F:10[B]:MET:HG2	1.87	0.56
1:F:139[A]:ARG:NE	1:F:139[A]:ARG:CG	2.64	0.55
1:E:7:GLY:O	1:E:10[A]:MET:HB2	2.08	0.54
1:F:124:GLY:H	1:F:143:ASN:ND2	2.04	0.54
2:E:1175:NDG:H1	5:E:2110:HOH:O	2.08	0.54
1:E:10[A]:MET:HG2	1:F:10[A]:MET:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33[B]:LYS:NZ	1:A:33[B]:LYS:HD3	2.23	0.53
1:E:7:GLY:O	1:E:10[B]:MET:HB2	2.10	0.52
1:A:149:LYS:HE3	1:A:150:TRP:CZ2	2.44	0.52
1:F:2:ARG:O	1:F:7:GLY:HA3	2.13	0.49
1:E:28:GLY:HA3	3:F:1177:NAG:O4	2.15	0.47
1:E:12:CYS:HB3	1:E:16[A]:LEU:HB2	1.96	0.47
1:F:7:GLY:O	1:F:10[A]:MET:HB2	2.15	0.46
1:E:134:LYS:H	1:E:165:GLN:NE2	2.09	0.46
1:B:26[B]:MET:HE2	1:B:26[B]:MET:CG	2.02	0.45
1:B:2:ARG:O	1:B:7:GLY:HA3	2.17	0.44
1:F:7:GLY:O	1:F:10[B]:MET:HB2	2.17	0.43
1:F:26[B]:MET:HE1	1:F:26[B]:MET:SD	1.01	0.43
1:F:26[B]:MET:HE2	1:F:26[B]:MET:SD	1.01	0.43
1:F:66:TYR:CD2	3:F:1175:NAG:H2	2.54	0.43
1:F:26[B]:MET:HE3	1:F:26[B]:MET:SD	1.01	0.42
1:B:26[B]:MET:HE2	1:B:26[B]:MET:SD	1.00	0.42
1:B:26[B]:MET:HE3	1:B:26[B]:MET:SD	1.00	0.42
1:E:66:TYR:CD2	2:E:1172[A]:NDG:H2	2.55	0.42
1:B:16:LEU:CD2	1:B:26[B]:MET:CG	2.95	0.42
1:B:26[B]:MET:HE1	1:B:26[B]:MET:SD	1.00	0.42
1:B:26[A]:MET:SD	1:B:26[A]:MET:HE3	0.99	0.41
1:F:91[B]:SER:H	1:F:122:GLN:HE22	1.67	0.41
1:F:91[A]:SER:H	1:F:122:GLN:HE22	1.67	0.41
1:E:130:LYS:HA	1:E:131:PRO:HD3	1.93	0.41
1:B:26[A]:MET:SD	1:B:26[A]:MET:HE2	0.99	0.41
1:B:26[A]:MET:SD	1:B:26[A]:MET:HE1	0.99	0.41
1:A:44:LYS:HG3	5:A:2065:HOH:O	2.20	0.41
1:F:106:GLN:HB3	1:F:120:GLY:HA3	2.03	0.41
1:F:126:CYS:HB3	1:F:128:THR:HG22	2.03	0.41

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)
1:E:33[A]:LYS:NZ	2:E:1175:NDG:O1L[2_856]	1.86	0.34

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	171/171 (100%)	166 (97%)	5 (3%)	0	100	100
1	B	170/171 (99%)	167 (98%)	3 (2%)	0	100	100
1	E	172/171 (101%)	168 (98%)	4 (2%)	0	100	100
1	F	174/171 (102%)	171 (98%)	3 (2%)	0	100	100
All	All	687/684 (100%)	672 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	122/119 (102%)	120 (98%)	2 (2%)	70	38
1	B	120/119 (101%)	120 (100%)	0	100	100
1	E	122/119 (102%)	119 (98%)	3 (2%)	55	17
1	F	124/119 (104%)	123 (99%)	1 (1%)	86	67
All	All	488/476 (102%)	482 (99%)	6 (1%)	86	52

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

Mol	Chain	Res	Type
1	A	134[A]	LYS
1	A	134[B]	LYS

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Mol	Chain	Res	Type
1	E	10[A]	MET
1	E	10[B]	MET
1	E	37	ASN
1	F	92	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	B	58	ASN
1	B	143	ASN
1	E	37	ASN
1	E	59	GLN
1	E	100	ASN
1	E	143	ASN
1	E	165	GLN
1	F	92	GLN
1	F	122	GLN
1	F	143	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	1.40	1 (14%)	9,10,12	1.86	3 (33%)
1	PCA	B	1	1	7,8,9	1.40	1 (14%)	9,10,12	1.54	2 (22%)
1	PCA	E	1	1	7,8,9	1.49	1 (14%)	9,10,12	1.80	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PCA	F	1	1	7,8,9	1.54	1 (14%)	9,10,12	1.74	3 (33%)

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
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1
1	PCA	F	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	PCA	CD-N	3.55	1.45	1.33
1	A	1	PCA	CD-N	3.58	1.45	1.33
1	E	1	PCA	CD-N	3.74	1.46	1.33
1	F	1	PCA	CD-N	3.86	1.46	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CA-N-CD	-3.15	103.26	113.81
1	E	1	PCA	CA-N-CD	-2.96	103.90	113.81
1	F	1	PCA	CA-N-CD	-2.88	104.15	113.81
1	B	1	PCA	CA-N-CD	-2.59	105.12	113.81
1	E	1	PCA	O-C-CA	-2.25	119.50	125.44
1	F	1	PCA	OE-CD-CG	-2.17	121.96	126.81
1	A	1	PCA	O-C-CA	-2.06	120.00	125.44
1	B	1	PCA	CB-CA-N	2.08	109.28	103.20
1	F	1	PCA	CB-CA-N	2.41	110.23	103.20
1	E	1	PCA	CB-CA-N	2.46	110.38	103.20
1	A	1	PCA	CB-CA-N	2.88	111.61	103.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 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$
2	NDG	A	1173[A]	-	15,15,15	1.40	3 (20%)	17,21,21	1.42	2 (11%)
3	NAG	A	1174[B]	-	15,15,15	1.30	3 (20%)	17,21,21	1.37	3 (17%)
2	NDG	A	1175	-	15,15,15	1.13	2 (13%)	17,21,21	1.31	1 (5%)
3	NAG	A	1176	-	15,15,15	1.45	3 (20%)	17,21,21	1.56	3 (17%)
4	GOL	A	1177[A]	-	5,5,5	0.96	0	5,5,5	1.31	1 (20%)
4	GOL	A	1177[B]	-	5,5,5	0.85	0	5,5,5	0.51	0
3	NAG	B	1173	-	15,15,15	1.24	3 (20%)	17,21,21	1.57	4 (23%)
2	NDG	B	1174[A]	-	15,15,15	1.33	2 (13%)	17,21,21	1.29	2 (11%)
3	NAG	B	1175[B]	-	15,15,15	1.24	2 (13%)	17,21,21	1.32	3 (17%)
2	NDG	B	1176	-	15,15,15	0.40	0	17,21,21	0.75	0
2	NDG	B	1177[A]	-	15,15,15	1.13	3 (20%)	17,21,21	1.40	3 (17%)
3	NAG	B	1178[B]	-	15,15,15	1.18	3 (20%)	17,21,21	1.17	2 (11%)
4	GOL	B	1179	-	5,5,5	0.31	0	5,5,5	0.17	0
2	NDG	E	1172[A]	-	15,15,15	1.26	2 (13%)	17,21,21	1.00	1 (5%)
3	NAG	E	1173[B]	-	15,15,15	1.20	1 (6%)	17,21,21	0.99	1 (5%)
2	NDG	E	1174	-	15,15,15	0.41	0	17,21,21	0.62	0
2	NDG	E	1175	-	15,15,15	1.19	2 (13%)	17,21,21	1.56	4 (23%)
4	GOL	E	1176	-	5,5,5	1.07	0	5,5,5	0.46	0
3	NAG	F	1174	-	15,15,15	1.36	2 (13%)	17,21,21	1.77	3 (17%)
3	NAG	F	1175	-	15,15,15	1.29	2 (13%)	17,21,21	1.47	2 (11%)
2	NDG	F	1176	-	15,15,15	0.40	0	17,21,21	0.76	1 (5%)
3	NAG	F	1177	-	15,15,15	0.47	0	17,21,21	0.93	1 (5%)
4	GOL	F	1178[A]	-	5,5,5	1.04	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	F	1178[B]	-	5,5,5	1.02	0	5,5,5	0.96	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	NDG	A	1173[A]	-	-	0/6/26/26	0/1/1/1
3	NAG	A	1174[B]	-	-	0/6/26/26	0/1/1/1
2	NDG	A	1175	-	-	0/6/26/26	0/1/1/1
3	NAG	A	1176	-	1/1/6/7	0/6/26/26	0/1/1/1
4	GOL	A	1177[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1177[B]	-	-	0/4/4/4	0/0/0/0
3	NAG	B	1173	-	-	0/6/26/26	0/1/1/1
2	NDG	B	1174[A]	-	-	0/6/26/26	0/1/1/1
3	NAG	B	1175[B]	-	-	0/6/26/26	0/1/1/1
2	NDG	B	1176	-	-	0/6/26/26	0/1/1/1
2	NDG	B	1177[A]	-	-	0/6/26/26	0/1/1/1
3	NAG	B	1178[B]	-	-	0/6/26/26	0/1/1/1
4	GOL	B	1179	-	-	0/4/4/4	0/0/0/0
2	NDG	E	1172[A]	-	-	0/6/26/26	0/1/1/1
3	NAG	E	1173[B]	-	-	0/6/26/26	0/1/1/1
2	NDG	E	1174	-	-	0/6/26/26	0/1/1/1
2	NDG	E	1175	-	-	0/6/26/26	0/1/1/1
4	GOL	E	1176	-	-	0/4/4/4	0/0/0/0
3	NAG	F	1174	-	-	0/6/26/26	0/1/1/1
3	NAG	F	1175	-	-	0/6/26/26	0/1/1/1
2	NDG	F	1176	-	-	0/6/26/26	0/1/1/1
3	NAG	F	1177	-	-	0/6/26/26	0/1/1/1
4	GOL	F	1178[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	F	1178[B]	-	-	0/4/4/4	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1176	NAG	O3-C3	-3.74	1.34	1.43
2	A	1173[A]	NDG	O-C1	-3.18	1.37	1.43
3	B	1175[B]	NAG	O7-C7	-3.08	1.16	1.23
2	B	1174[A]	NDG	O7-C7	-3.03	1.16	1.23
3	F	1174	NAG	O5-C1	-2.71	1.37	1.43
2	E	1175	NDG	O3-C3	-2.71	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1175	NAG	O5-C1	-2.68	1.38	1.43
3	A	1174[B]	NAG	O5-C1	-2.61	1.38	1.43
3	F	1174	NAG	O4-C4	-2.54	1.36	1.43
3	B	1173	NAG	O7-C7	-2.53	1.17	1.23
2	B	1174[A]	NDG	O-C1	-2.53	1.38	1.43
3	B	1173	NAG	C2-N2	-2.52	1.41	1.45
3	B	1178[B]	NAG	O3-C3	-2.48	1.37	1.43
3	A	1174[B]	NAG	O7-C7	-2.46	1.17	1.23
2	A	1173[A]	NDG	O7-C7	-2.45	1.17	1.23
2	A	1175	NDG	O7-C7	-2.40	1.17	1.23
3	E	1173[B]	NAG	O7-C7	-2.39	1.17	1.23
2	E	1172[A]	NDG	O7-C7	-2.36	1.17	1.23
2	E	1175	NDG	O-C1	-2.35	1.38	1.43
2	B	1177[A]	NDG	O3-C3	-2.34	1.37	1.43
3	F	1175	NAG	O5-C5	-2.33	1.38	1.44
3	B	1178[B]	NAG	O5-C1	-2.27	1.38	1.43
2	E	1172[A]	NDG	O-C1	-2.15	1.39	1.43
3	B	1175[B]	NAG	O5-C1	-2.12	1.39	1.43
2	B	1177[A]	NDG	O-C1	-2.12	1.39	1.43
3	B	1173	NAG	O3-C3	-2.11	1.37	1.43
2	A	1175	NDG	O3-C3	-2.05	1.38	1.43
3	A	1176	NAG	O7-C7	-2.05	1.18	1.23
2	A	1173[A]	NDG	C2-N2	-2.02	1.42	1.45
2	B	1177[A]	NDG	O7-C7	-2.01	1.18	1.23
3	B	1178[B]	NAG	O7-C7	-2.01	1.18	1.23
3	A	1174[B]	NAG	C2-N2	-2.00	1.42	1.45
3	A	1176	NAG	C1-C2	2.31	1.55	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1174	NAG	C1-O5-C5	-4.13	105.84	113.47
3	B	1173	NAG	O3-C3-C2	-3.80	101.91	109.66
2	B	1177[A]	NDG	C6-C5-C4	-3.76	103.74	113.02
3	B	1178[B]	NAG	C6-C5-C4	-3.48	104.43	113.02
3	F	1174	NAG	C4-C3-C2	-3.42	105.69	110.43
2	A	1173[A]	NDG	C3-C4-C5	-3.35	104.36	110.20
2	A	1173[A]	NDG	O1L-C1-O	-3.12	101.72	110.25
3	A	1174[B]	NAG	C3-C4-C5	-2.97	105.02	110.20
4	A	1177[A]	GOL	C3-C2-C1	-2.82	100.05	111.12
2	E	1172[A]	NDG	C6-C5-C4	-2.80	106.11	113.02
3	B	1175[B]	NAG	O1-C1-O5	-2.80	102.59	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1174[A]	NDG	C6-C5-C4	-2.50	106.84	113.02
3	E	1173[B]	NAG	C6-C5-C4	-2.48	106.89	113.02
3	B	1173	NAG	C3-C2-N2	-2.42	105.65	110.66
2	E	1175	NDG	O3-C3-C2	-2.41	104.74	109.66
3	B	1175[B]	NAG	O5-C5-C4	-2.39	105.20	109.68
2	B	1177[A]	NDG	C3-C4-C5	-2.36	106.09	110.20
3	B	1175[B]	NAG	C6-C5-C4	-2.27	107.41	113.02
3	B	1173	NAG	C4-C3-C2	-2.19	107.40	110.43
2	E	1175	NDG	C4-C3-C2	-2.13	107.48	110.43
2	B	1174[A]	NDG	O-C5-C4	-2.12	105.70	109.68
3	A	1174[B]	NAG	C1-O5-C5	-2.11	109.56	113.47
3	F	1177	NAG	C3-C4-C5	-2.02	106.67	110.20
3	F	1175	NAG	O1-C1-O5	-2.02	104.72	110.25
3	B	1178[B]	NAG	C3-C4-C5	-2.01	106.70	110.20
2	F	1176	NDG	C1-O-C5	2.00	117.17	113.47
3	A	1174[B]	NAG	C6-C5-C4	2.06	118.09	113.02
3	B	1173	NAG	O4-C4-C3	2.24	115.38	110.34
2	E	1175	NDG	O-C5-C4	2.36	114.11	109.68
3	A	1176	NAG	C3-C2-N2	2.52	115.88	110.66
2	A	1175	NDG	O-C5-C4	2.67	114.69	109.68
3	A	1176	NAG	O6-C6-C5	2.68	120.20	111.33
2	B	1177[A]	NDG	C1-O-C5	2.72	118.50	113.47
3	F	1174	NAG	C3-C4-C5	3.39	116.11	110.20
3	A	1176	NAG	C1-O5-C5	3.60	120.12	113.47
3	F	1175	NAG	C1-O5-C5	3.89	120.66	113.47
2	E	1175	NDG	C1-O-C5	4.21	121.27	113.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1176	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1172[A]	NDG	1	0
2	E	1175	NDG	1	1
3	F	1175	NAG	1	0
3	F	1177	NAG	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	169/171 (98%)	-0.48	0 100 100	10, 13, 20, 27	1 (0%)
1	B	170/171 (99%)	-0.40	1 (0%) 90 89	10, 14, 21, 28	1 (0%)
1	E	170/171 (99%)	-0.28	1 (0%) 90 89	10, 17, 26, 32	2 (1%)
1	F	170/171 (99%)	-0.22	1 (0%) 90 89	10, 18, 29, 35	1 (0%)
All	All	679/684 (99%)	-0.34	3 (0%) 93 91	10, 15, 25, 35	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	171	GLY	3.1
1	F	51	GLY	2.6
1	B	171	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	F	1	8/9	0.92	0.10	-	25,26,27,27	0
1	PCA	A	1	8/9	0.95	0.10	-	16,17,18,19	0
1	PCA	B	1	8/9	0.95	0.09	-	17,18,18,19	0
1	PCA	E	1	8/9	0.91	0.21	-	22,23,23,24	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

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, 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	NAG	A	1176	15/15	0.87	0.13	6.15	17,26,30,31	0
4	GOL	F	1178[A]	6/6	0.86	0.14	5.97	20,20,22,23	6
4	GOL	F	1178[B]	6/6	0.86	0.14	5.83	20,24,26,29	6
3	NAG	B	1173	15/15	0.75	0.20	5.20	37,49,51,52	0
3	NAG	F	1174	15/15	0.85	0.12	3.86	33,40,41,45	0
4	GOL	A	1177[B]	6/6	0.85	0.16	3.14	30,33,34,34	6
4	GOL	A	1177[A]	6/6	0.85	0.16	3.03	16,17,18,19	6
4	GOL	E	1176	6/6	0.92	0.13	2.11	31,32,33,35	0
3	NAG	B	1178[B]	15/15	0.91	0.12	1.50	18,20,22,23	15
2	NDG	E	1175	15/15	0.89	0.11	1.49	26,28,31,32	0
2	NDG	B	1177[A]	15/15	0.91	0.12	1.22	22,24,26,28	15
4	GOL	B	1179	6/6	0.94	0.08	1.03	20,21,22,23	0
2	NDG	E	1174	15/15	0.93	0.07	0.98	18,20,24,26	0
3	NAG	F	1175	15/15	0.88	0.10	0.85	25,28,32,34	0
3	NAG	B	1175[B]	15/15	0.95	0.08	0.73	9,12,14,17	15
3	NAG	A	1174[B]	15/15	0.93	0.10	0.65	15,19,22,23	15
2	NDG	B	1174[A]	15/15	0.95	0.08	0.61	14,16,18,19	15
2	NDG	A	1173[A]	15/15	0.94	0.09	0.46	14,20,23,25	15
2	NDG	A	1175	15/15	0.97	0.06	0.31	11,15,19,22	0
2	NDG	B	1176	15/15	0.97	0.06	-0.06	11,15,17,20	0
2	NDG	F	1176	15/15	0.95	0.07	-0.14	17,20,24,25	0
2	NDG	E	1172[A]	15/15	0.96	0.06	-0.26	12,18,21,23	15
3	NAG	E	1173[B]	15/15	0.96	0.06	-0.32	18,26,27,28	15
3	NAG	F	1177	15/15	0.96	0.06	-0.48	12,14,19,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.