



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:39 PM GMT

PDB ID : 4CZ0
Title : Structure of the A_mallard_Sweden_51_2002 H10 Avian Haemmagglutinin
in complex with avian receptor analog Su-3SLN
Authors : Vachieri, S.G.; Xiong, X.; Collins, P.J.; Walker, P.A.; Martin, S.R.; Haire,
L.F.; McCauley, J.W.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2014-04-16
Resolution : 3.20 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

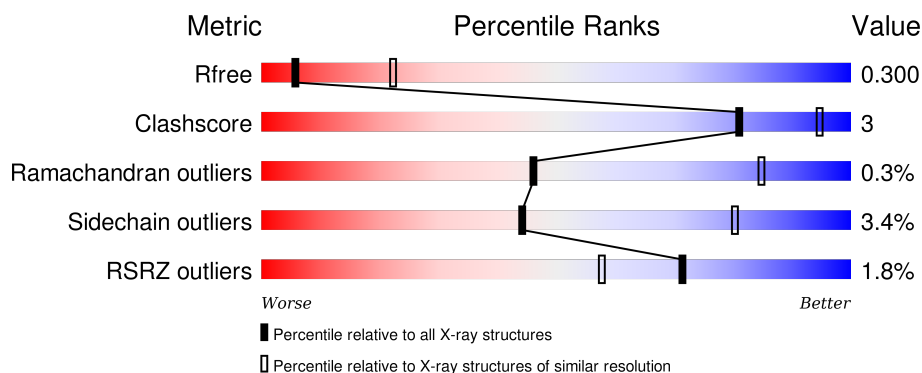
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	318	<div> <div>89%</div> <div>10% .</div> </div>
1	C	318	<div> <div>6%</div> <div>87%</div> <div>13%</div> </div>
1	E	318	<div> <div>6%</div> <div>88%</div> <div>12%</div> </div>
2	B	172	<div> <div>89%</div> <div>10% .</div> </div>
2	D	172	<div> <div>90%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	172	

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	420	X	-	-	-
3	NAG	C	401	X	-	-	-
3	NAG	C	420	X	-	-	-
3	NAG	E	401	X	-	-	X
3	NAG	E	420	X	-	-	-
3	NAG	F	211	X	-	-	-
4	GAL	A	702	X	-	-	-
4	GAL	C	702	X	-	-	-
4	GAL	E	702	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11837 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 HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2423	1498	436	473	16			
1	C	318	Total	C	N	O	S	0	0	0
			2421	1497	435	473	16			
1	E	318	Total	C	N	O	S	0	0	0
			2419	1495	435	473	16			

- Molecule 2 is a protein called HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1381	853	238	282	8			
2	D	172	Total	C	N	O	S	0	0	0
			1381	853	238	282	8			
2	F	172	Total	C	N	O	S	0	0	0
			1381	853	238	282	8			

- 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	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	3	Total	C	N	O	S	0	0
			50	25	2	22	1		
4	C	3	Total	C	N	O	S	0	0
			50	25	2	22	1		
4	E	3	Total	C	N	O	S	0	0
			50	25	2	22	1		

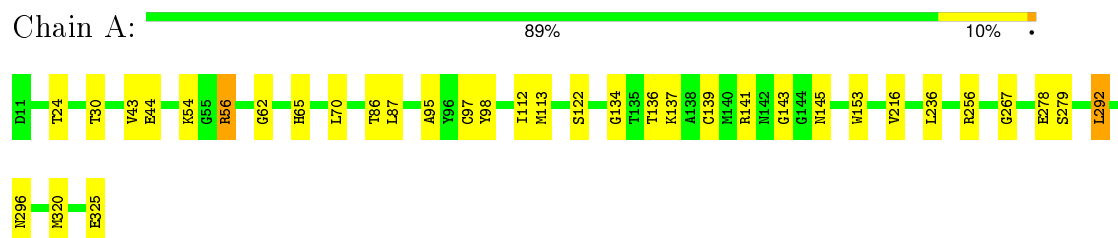
- Molecule 5 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	5	Total 61	C 34	N 2	O 25	0	0
5	D	5	Total 61	C 34	N 2	O 25	0	0
5	F	5	Total 61	C 34	N 2	O 25	0	0

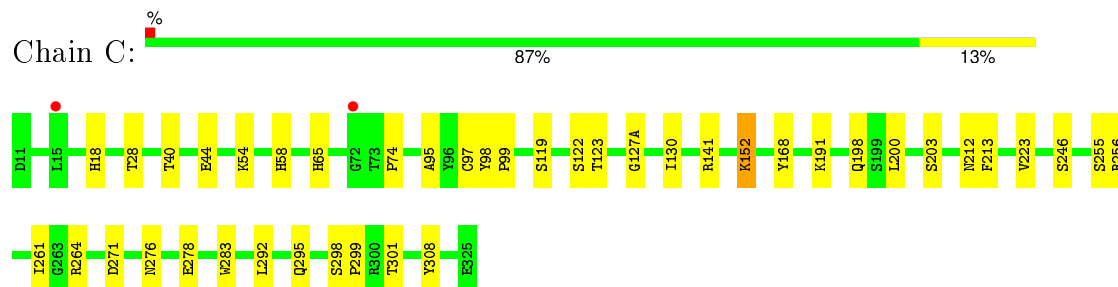
3 Residue-property plots [i](#)

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.

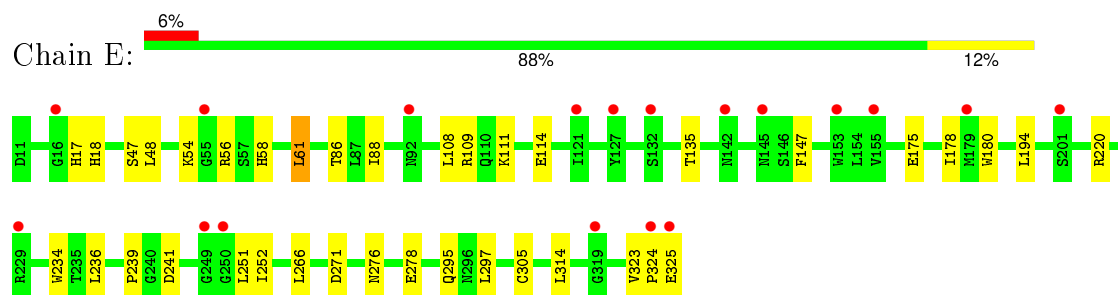
- Molecule 1: HAEMAGGLUTININ



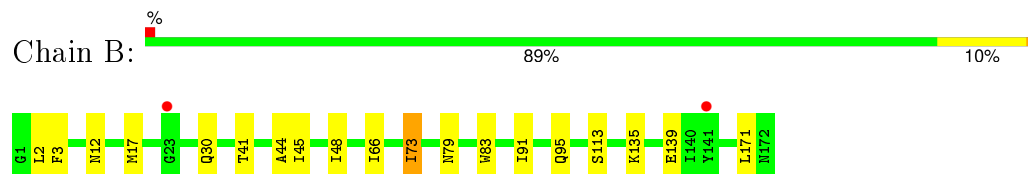
- Molecule 1: HAEMAGGLUTININ



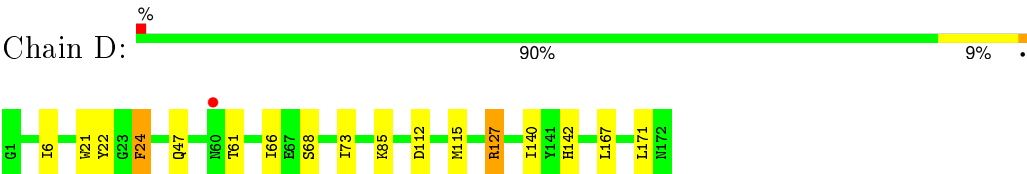
- Molecule 1: HAEMAGGLUTININ



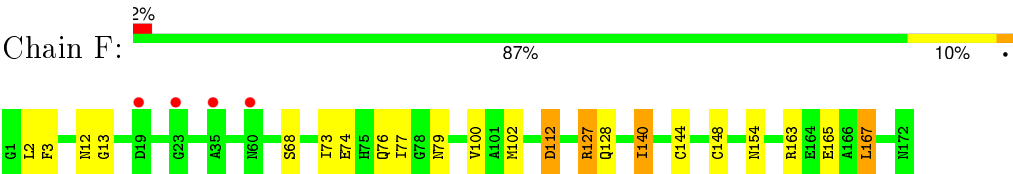
- Molecule 2: HAEMAGGLUTININ



- Molecule 2: HAEMAGGLUTININ



• Molecule 2: HAEMAGGLUTININ



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.11Å 216.09Å 81.49Å 90.00° 105.23° 90.00°	Depositor
Resolution (Å)	108.04 – 3.20 45.68 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (108.04-3.20) 98.9 (45.68-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.264 , 0.303 0.265 , 0.300	Depositor DCC
R_{free} test set	1875 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 5.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 37540 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11837	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: BMA, NAG, SIA, GAL, NGS, 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	0.27	0/2472	0.45	0/3350
1	C	0.32	1/2470 (0.0%)	0.46	0/3348
1	E	0.27	0/2468	0.46	0/3346
2	B	0.27	0/1406	0.43	0/1899
2	D	0.28	0/1406	0.45	0/1899
2	F	0.27	0/1406	0.43	0/1899
All	All	0.28	1/11628 (0.0%)	0.45	0/15741

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	A	1	0
4	C	1	0
4	E	1	0
All	All	3	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	168	TYR	C-N	-6.65	1.18	1.34

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	702	GAL	C1
4	C	702	GAL	C1

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Mol	Chain	Res	Type	Atom
4	E	702	GAL	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	2423	0	2356	17	0
1	C	2421	0	2348	17	0
1	E	2419	0	2345	17	0
2	B	1381	0	1268	13	0
2	D	1381	0	1268	11	0
2	F	1381	0	1267	14	0
3	A	28	0	26	0	0
3	C	28	0	26	1	0
3	E	28	0	26	1	0
3	F	14	0	13	0	0
4	A	50	0	40	0	0
4	C	50	0	40	0	0
4	E	50	0	40	0	0
5	B	61	0	52	0	0
5	D	61	0	52	0	0
5	F	61	0	52	1	0
All	All	11837	0	11219	75	0

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 3.

All (75) 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)
2:F:68:SER:H	2:F:73:ILE:HD11	1.60	0.66
1:E:17:HIS:O	2:F:13:GLY:HA3	1.96	0.65
1:C:65:HIS:HB3	1:C:95:ALA:HB2	1.78	0.65
2:B:139:GLU:HG3	2:D:127:ARG:HH22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:HG13	1:C:212:ASN:HB2	1.85	0.58
2:B:91:ILE:O	2:B:95:GLN:HB2	2.05	0.57
1:A:65:HIS:HB3	1:A:95:ALA:HB2	1.86	0.56
1:A:54:LYS:HB3	1:A:278:GLU:HB3	1.88	0.55
1:C:127(A):GLY:H	1:C:130:ILE:HD12	1.71	0.55
2:B:44:ALA:O	2:B:48:ILE:HG12	2.05	0.55
2:B:83:TRP:CH2	2:D:85:LYS:HG2	2.42	0.54
1:A:44:GLU:HB2	1:A:292:LEU:HD11	1.89	0.54
1:C:203:SER:HB2	1:C:246:SER:HB3	1.89	0.54
1:E:111:LYS:HE2	1:E:236:LEU:HD11	1.89	0.53
1:E:54:LYS:HB3	1:E:278:GLU:HB3	1.90	0.53
2:D:140:ILE:HG22	2:D:142:HIS:H	1.74	0.53
1:A:30:THR:HG21	2:D:47:GLN:HE21	1.74	0.52
1:A:122:SER:HA	1:A:256:ARG:HG2	1.91	0.52
2:F:163:ARG:O	2:F:167:LEU:HB2	2.10	0.51
1:E:56:ARG:HH11	1:E:86:THR:HG21	1.75	0.51
1:E:135:THR:HA	1:E:147:PHE:HB2	1.92	0.51
2:D:24:PHE:CD1	2:D:24:PHE:N	2.80	0.50
1:E:47:SER:HB2	1:E:297:LEU:HD22	1.93	0.50
1:A:136:THR:HG23	1:A:139:CYS:H	1.77	0.49
1:A:56:ARG:HD2	1:A:86:THR:OG1	2.12	0.49
1:A:43:VAL:HG12	1:A:296:ASN:HD22	1.78	0.48
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.96	0.48
1:C:40:THR:HB	3:C:420:NAG:H81	1.96	0.48
1:E:314:LEU:HB3	2:F:100:VAL:HG21	1.94	0.48
1:C:44:GLU:HG2	1:C:292:LEU:HD12	1.95	0.48
1:A:137:LYS:HE3	1:A:145:ASN:HD21	1.79	0.48
2:D:6:ILE:HG12	2:D:112:ASP:HA	1.95	0.47
1:C:54:LYS:HB3	1:C:278:GLU:HB3	1.95	0.47
2:F:140:ILE:H	2:F:140:ILE:HD13	1.79	0.47
2:D:68:SER:H	2:D:73:ILE:HD11	1.80	0.47
2:B:3:PHE:HZ	2:F:2:LEU:HB3	1.80	0.47
1:C:119:SER:HB2	1:C:261:ILE:HD11	1.98	0.46
2:F:144:CYS:HB3	2:F:148:CYS:HB3	1.92	0.46
1:C:122:SER:HA	1:C:256:ARG:HG2	1.97	0.45
2:B:79:ASN:HB3	2:D:66:ILE:HG22	1.99	0.45
1:A:113:MET:HB3	1:A:267:GLY:HA3	1.99	0.45
2:D:22:TYR:CD1	2:D:115:MET:HB3	2.51	0.45
2:F:3:PHE:HB2	2:F:112:ASP:HB3	1.98	0.45
1:A:70:LEU:HD11	1:A:112:ILE:HD11	1.98	0.45
2:B:3:PHE:CZ	2:F:2:LEU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:SER:HB2	2:F:2:LEU:O	2.17	0.44
1:A:97:CYS:SG	1:A:98:TYR:N	2.90	0.44
1:E:58:HIS:HE1	1:E:276:ASN:HD21	1.65	0.44
1:E:241:ASP:HA	3:E:401:NAG:H82	2.00	0.44
2:B:73:ILE:HD13	2:B:73:ILE:H	1.82	0.44
1:E:61:LEU:HB2	1:E:88:ILE:O	2.18	0.44
2:B:41:THR:O	2:B:45:ILE:HG12	2.18	0.43
1:E:175:GLU:HB3	1:E:239:PRO:HD3	2.01	0.43
1:C:152:LYS:HD3	1:C:255:SER:HB3	2.00	0.43
2:F:74:GLU:HB3	2:F:77:ILE:HG22	2.01	0.43
1:A:325:GLU:HG2	2:B:12:ASN:HD22	1.83	0.43
1:E:295:GLN:HB2	1:E:297:LEU:HD12	2.01	0.42
1:C:283:TRP:HB3	1:C:301:THR:HG22	2.01	0.42
5:F:201:NAG:H61	5:F:202:NAG:HN2	1.84	0.42
1:E:56:ARG:NH1	1:E:86:THR:HG21	2.34	0.42
1:E:108:LEU:HD23	1:E:234:TRP:CD2	2.55	0.42
1:E:180:TRP:HB2	1:E:251:LEU:HD11	2.02	0.42
1:C:99:PRO:HB3	1:C:223:VAL:HB	2.02	0.42
1:A:141:ARG:C	1:A:143:GLY:H	2.23	0.42
2:B:171:LEU:HD23	2:D:167:LEU:HD23	2.01	0.42
1:C:58:HIS:HE1	1:C:276:ASN:HD21	1.68	0.42
2:B:66:ILE:HG22	2:F:79:ASN:HB3	2.02	0.41
1:E:325:GLU:HG3	2:F:12:ASN:HB2	2.02	0.41
1:C:295:GLN:HG3	1:C:308:TYR:HA	2.01	0.41
2:F:127:ARG:HG2	2:F:128:GLN:HG2	2.01	0.41
1:C:298:SER:HA	1:C:299:PRO:HD3	1.94	0.41
1:C:18:HIS:CD2	2:D:21:TRP:HA	2.56	0.40
1:E:323:VAL:HA	1:E:324:PRO:HD3	1.95	0.40
1:A:56:ARG:NH2	1:A:279:SER:O	2.54	0.40
1:C:97:CYS:SG	1:C:98:TYR:N	2.95	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	316/318 (99%)	299 (95%)	16 (5%)	1 (0%)	46	85
1	C	316/318 (99%)	300 (95%)	15 (5%)	1 (0%)	46	85
1	E	316/318 (99%)	309 (98%)	7 (2%)	0	100	100
2	B	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
2	D	170/172 (99%)	160 (94%)	8 (5%)	2 (1%)	16	60
2	F	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	30	75
All	All	1458/1470 (99%)	1391 (95%)	62 (4%)	5 (0%)	46	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	61	THR
2	F	127	ARG
2	D	127	ARG
1	A	62	GLY
1	C	74	PRO

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	269/270 (100%)	263 (98%)	6 (2%)	60	87
1	C	268/270 (99%)	258 (96%)	10 (4%)	41	79
1	E	268/270 (99%)	256 (96%)	12 (4%)	34	74
2	B	144/146 (99%)	139 (96%)	5 (4%)	43	80
2	D	144/146 (99%)	142 (99%)	2 (1%)	74	92
2	F	144/146 (99%)	137 (95%)	7 (5%)	31	72
All	All	1237/1248 (99%)	1195 (97%)	42 (3%)	44	80

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	56	ARG
1	A	87	LEU
1	A	236	LEU
1	A	292	LEU
1	A	320	MET
2	B	2	LEU
2	B	17	MET
2	B	30	GLN
2	B	73	ILE
2	B	135	LYS
1	C	28	THR
1	C	123	THR
1	C	141	ARG
1	C	152	LYS
1	C	191	LYS
1	C	198	GLN
1	C	200	LEU
1	C	213	PHE
1	C	264	ARG
1	C	271	ASP
2	D	24	PHE
2	D	171	LEU
1	E	18	HIS
1	E	48	LEU
1	E	61	LEU
1	E	109	ARG
1	E	114	GLU
1	E	178	ILE
1	E	194	LEU
1	E	220	ARG
1	E	252	ILE
1	E	266	LEU
1	E	271	ASP
1	E	305	CYS
2	F	76	GLN
2	F	102	MET
2	F	112	ASP
2	F	140	ILE
2	F	154	ASN
2	F	165	GLU
2	F	167	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	110	GLN
1	A	198	GLN
1	A	212	ASN
1	A	296	ASN
1	C	18	HIS
1	C	198	GLN
1	C	276	ASN
2	D	30	GLN
2	D	47	GLN
2	D	169	ASN
1	E	18	HIS
1	E	33	GLN
1	E	212	ASN
1	E	276	ASN
2	F	76	GLN
2	F	125	GLN
2	F	169	ASN
2	F	172	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 ⓘ

24 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SIA	A	701	4	16,20,21	0.33	0	18,28,31	0.82	1 (5%)
4	GAL	A	702	4	11,11,12	0.49	0	14,15,17	1.40	3 (21%)
4	NGS	A	703	4	19,19,19	0.62	0	22,28,28	1.52	2 (9%)
5	NAG	B	201	2,5	14,14,15	0.49	0	15,19,21	1.06	1 (6%)
5	NAG	B	202	5	14,14,15	0.46	0	15,19,21	0.64	0
5	BMA	B	203	5	11,11,12	0.47	0	14,15,17	0.70	0
5	MAN	B	204	5	11,11,12	0.59	0	14,15,17	1.08	2 (14%)
5	MAN	B	207	5	11,11,12	0.54	0	14,15,17	1.43	2 (14%)
4	SIA	C	701	4	16,20,21	0.38	0	18,28,31	1.17	2 (11%)
4	GAL	C	702	4	11,11,12	0.54	0	14,15,17	1.70	3 (21%)
4	NGS	C	703	4	19,19,19	0.62	0	22,28,28	1.28	2 (9%)
5	NAG	D	201	2,5	14,14,15	0.48	0	15,19,21	0.93	0
5	NAG	D	202	5	14,14,15	0.62	0	15,19,21	1.41	2 (13%)
5	BMA	D	203	5	11,11,12	0.45	0	14,15,17	1.11	1 (7%)
5	MAN	D	204	5	11,11,12	0.63	0	14,15,17	1.20	1 (7%)
5	MAN	D	207	5	11,11,12	0.57	0	14,15,17	0.98	1 (7%)
4	SIA	E	701	4	16,20,21	0.36	0	18,28,31	0.75	1 (5%)
4	GAL	E	702	4	11,11,12	0.60	0	14,15,17	1.99	3 (21%)
4	NGS	E	703	4	19,19,19	0.58	0	22,28,28	1.04	2 (9%)
5	NAG	F	201	2,5	14,14,15	0.42	0	15,19,21	1.09	1 (6%)
5	NAG	F	202	5	14,14,15	0.51	0	15,19,21	0.90	0
5	BMA	F	203	5	11,11,12	0.45	0	14,15,17	0.58	0
5	MAN	F	204	5	11,11,12	0.63	0	14,15,17	1.36	1 (7%)
5	MAN	F	207	5	11,11,12	0.57	0	14,15,17	0.97	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
4	SIA	A	701	4	-	0/14/34/38	0/1/1/1
4	GAL	A	702	4	1/1/4/5	0/2/19/22	0/1/1/1
4	NGS	A	703	4	-	0/10/30/30	0/1/1/1
5	NAG	B	201	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	202	5	-	0/6/23/26	0/1/1/1
5	BMA	B	203	5	-	0/2/19/22	0/1/1/1
5	MAN	B	204	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	B	207	5	-	0/2/19/22	0/1/1/1
4	SIA	C	701	4	-	0/14/34/38	0/1/1/1
4	GAL	C	702	4	1/1/4/5	0/2/19/22	0/1/1/1
4	NGS	C	703	4	-	0/10/30/30	0/1/1/1
5	NAG	D	201	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	202	5	-	0/6/23/26	0/1/1/1
5	BMA	D	203	5	-	0/2/19/22	0/1/1/1
5	MAN	D	204	5	-	0/2/19/22	0/1/1/1
5	MAN	D	207	5	-	0/2/19/22	0/1/1/1
4	SIA	E	701	4	-	0/14/34/38	0/1/1/1
4	GAL	E	702	4	1/1/4/5	0/2/19/22	0/1/1/1
4	NGS	E	703	4	-	0/10/30/30	0/1/1/1
5	NAG	F	201	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	202	5	-	0/6/23/26	0/1/1/1
5	BMA	F	203	5	-	0/2/19/22	0/1/1/1
5	MAN	F	204	5	-	0/2/19/22	0/1/1/1
5	MAN	F	207	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	SIA	C7-C6-C5	-2.46	110.60	114.32
4	C	702	GAL	O3-C3-C2	-2.16	106.10	110.00
4	A	702	GAL	O3-C3-C2	-2.12	106.16	110.00
5	F	207	MAN	C1-C2-C3	2.00	111.91	109.54
4	C	702	GAL	C1-O5-C5	2.12	114.94	112.25
4	E	702	GAL	O5-C1-C2	2.25	114.50	110.86
5	B	204	MAN	C1-O5-C5	2.26	115.12	112.25
4	E	701	SIA	O6-C6-C5	2.28	112.22	108.48
4	E	703	NGS	C3-C4-C5	2.39	114.36	110.20
5	B	201	NAG	C1-O5-C5	2.41	115.31	112.25
4	A	701	SIA	O6-C6-C5	2.46	112.52	108.48
4	E	703	NGS	O5-C5-C4	2.49	114.36	109.68
5	F	207	MAN	C1-O5-C5	2.54	115.47	112.25
5	D	207	MAN	C1-O5-C5	2.60	115.55	112.25
5	D	203	BMA	C3-C4-C5	2.64	114.80	110.20
4	A	702	GAL	C1-O5-C5	2.67	115.64	112.25
5	B	204	MAN	C1-C2-C3	2.85	112.91	109.54
5	B	207	MAN	C1-C2-C3	2.86	112.92	109.54
5	F	201	NAG	C1-O5-C5	2.95	115.99	112.25
5	D	202	NAG	C3-C4-C5	2.98	115.39	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	703	NGS	C3-C4-C5	3.04	115.49	110.20
4	A	702	GAL	C1-C2-C3	3.19	113.31	109.54
5	D	204	MAN	C1-C2-C3	3.36	113.51	109.54
4	C	701	SIA	O6-C6-C5	3.44	114.12	108.48
4	E	702	GAL	C1-O5-C5	3.48	116.67	112.25
4	C	703	NGS	C4-C3-C2	3.82	115.73	110.43
4	A	703	NGS	C3-C4-C5	3.84	116.89	110.20
5	B	207	MAN	C1-O5-C5	3.86	117.15	112.25
5	D	202	NAG	C4-C3-C2	3.88	117.27	111.23
5	F	204	MAN	C1-C2-C3	3.90	114.16	109.54
4	A	703	NGS	C4-C3-C2	4.99	117.35	110.43
4	C	702	GAL	C1-C2-C3	5.04	115.50	109.54
4	E	702	GAL	C1-C2-C3	5.70	116.29	109.54

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	702	GAL	C1
4	E	702	GAL	C1
4	A	702	GAL	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	201	NAG	1	0
5	F	202	NAG	1	0

5.6 Ligand geometry

7 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	NAG	A	401	1	14,14,15	0.48	0	15,19,21	0.78	0
3	NAG	A	420	1	14,14,15	0.45	0	15,19,21	0.88	0
3	NAG	C	401	1	14,14,15	0.51	0	15,19,21	0.83	0
3	NAG	C	420	1	14,14,15	0.48	0	15,19,21	0.65	0
3	NAG	E	401	1	14,14,15	0.49	0	15,19,21	1.74	2 (13%)
3	NAG	E	420	1	14,14,15	0.44	0	15,19,21	0.86	0
3	NAG	F	211	2	14,14,15	0.45	0	15,19,21	0.72	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	NAG	A	401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	420	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	420	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	420	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	211	2	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	NAG	C3-C4-C5	3.85	116.91	110.20
3	E	401	NAG	C1-O5-C5	4.81	118.35	112.25

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	401	NAG	C1
3	A	420	NAG	C1
3	C	401	NAG	C1
3	E	420	NAG	C1
3	F	211	NAG	C1
3	C	420	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	420	NAG	1	0
3	E	401	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

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	318/318 (100%)	-0.06	0 100 100	67, 87, 114, 122	0
1	C	318/318 (100%)	-0.05	2 (0%) 90 84	67, 86, 121, 147	0
1	E	318/318 (100%)	0.34	18 (5%) 27 15	90, 124, 149, 160	0
2	B	172/172 (100%)	0.03	2 (1%) 81 69	61, 78, 92, 98	0
2	D	172/172 (100%)	0.12	1 (0%) 90 84	68, 90, 111, 125	0
2	F	172/172 (100%)	0.13	4 (2%) 64 49	73, 103, 130, 137	0
All	All	1470/1470 (100%)	0.08	27 (1%) 71 58	61, 93, 136, 160	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	250	GLY	6.5
2	F	60	ASN	4.9
1	E	249	GLY	4.3
1	E	92	ASN	3.7
1	E	155	VAL	3.6
1	E	324	PRO	3.6
2	F	35	ALA	3.2
2	D	60	ASN	3.2
1	E	325	GLU	3.1
1	E	153	TRP	2.9
1	E	127	TYR	2.8
1	C	72	GLY	2.4
2	B	23	GLY	2.4
1	E	319	GLY	2.4
1	E	132	SER	2.4
1	E	121	ILE	2.4
1	E	142	ASN	2.3
1	E	16	GLY	2.3
1	E	179	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	141	TYR	2.2
1	C	15	LEU	2.2
2	F	23	GLY	2.2
1	E	145	ASN	2.1
1	E	229	ARG	2.1
1	E	201	SER	2.0
2	F	19	ASP	2.0
1	E	55	GLY	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
5	NAG	D	201	14/15	0.76	0.23	0.58	98,101,104,105	0
4	SIA	A	701	20/21	0.92	0.21	0.10	84,86,90,90	0
5	NAG	F	201	14/15	0.84	0.24	-0.34	99,102,108,113	0
4	SIA	C	701	20/21	0.81	0.25	-0.54	129,144,147,147	0
4	SIA	E	701	20/21	0.90	0.16	-0.85	83,87,91,92	0
5	NAG	B	201	14/15	0.87	0.15	-2.70	86,89,92,94	0
4	GAL	E	702	11/12	0.88	0.23	-	95,101,104,106	0
5	BMA	D	203	11/12	0.88	0.14	-	123,128,135,135	0
4	NGS	C	703	19/19	0.65	0.49	-	162,167,170,171	0
5	MAN	D	207	11/12	0.82	0.25	-	121,128,136,138	0
5	NAG	B	202	14/15	0.87	0.19	-	96,101,107,111	0
5	MAN	F	207	11/12	0.74	0.50	-	144,147,151,153	0
5	MAN	B	207	11/12	0.67	0.40	-	115,119,121,121	0
5	NAG	D	202	14/15	0.88	0.27	-	105,110,116,119	0
4	NGS	E	703	19/19	0.86	0.28	-	113,124,135,137	0
5	MAN	F	204	11/12	0.43	0.49	-	140,143,148,152	0
5	MAN	D	204	11/12	0.80	0.35	-	131,137,144,144	0
5	MAN	B	204	11/12	0.49	0.43	-	127,131,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GAL	A	702	11/12	0.90	0.14	-	91,94,97,97	0
5	BMA	F	203	11/12	0.73	0.35	-	133,140,146,148	0
4	NGS	A	703	19/19	0.87	0.15	-	98,100,108,108	0
4	GAL	C	702	11/12	0.75	0.28	-	148,152,155,156	0
5	BMA	B	203	11/12	0.68	0.33	-	115,120,126,126	0
5	NAG	F	202	14/15	0.86	0.19	-	117,121,128,128	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(\AA^2)	Q<0.9
3	NAG	E	401	14/15	0.70	0.35	2.49	130,134,138,140	0
3	NAG	C	401	14/15	0.78	0.25	1.08	102,105,108,108	0
3	NAG	A	401	14/15	0.80	0.28	0.65	129,133,139,142	0
3	NAG	A	420	14/15	0.84	0.30	-	89,91,93,94	0
3	NAG	E	420	14/15	0.74	0.28	-	126,129,135,137	0
3	NAG	F	211	14/15	0.75	0.36	-	136,139,143,144	0
3	NAG	C	420	14/15	0.84	0.23	-	92,97,101,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.