



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:01 PM GMT

PDB ID : 4UO3
Title : Structure of the A_Equine_Richmond_07 H3 haemagglutinin mutant Ser30Thr
Authors : Vachieri, S.G.; Collins, P.J.; Haire, L.F.; Ogrodowicz, R.W.; Martin, S.R.; Walker, P.A.; Xiong, X.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2014-05-31
Resolution : 2.87 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

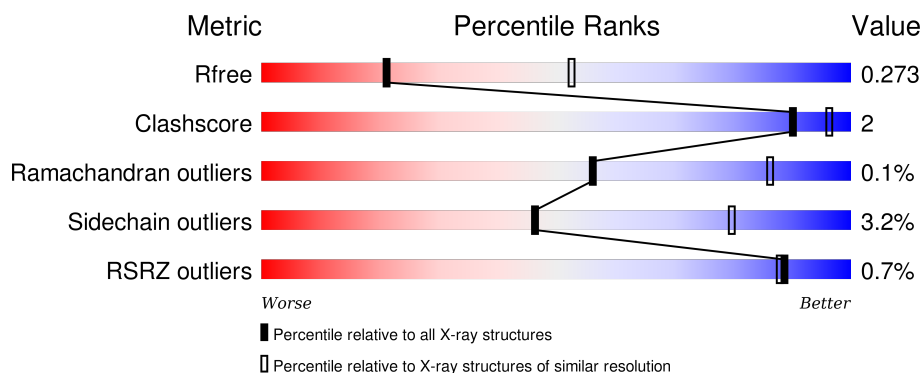
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	327	<div> <div>87%</div> <div>11%</div> <div>•</div> </div>
1	C	327	<div> <div>92%</div> <div>6%</div> <div>•</div> </div>
1	E	327	<div> <div>92%</div> <div>6%</div> <div>•</div> </div>
2	B	172	<div> <div>2%</div> <div>91%</div> <div>9%</div> </div>
2	D	172	<div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	172	<div> <div></div> <div>%</div> <div>87%</div> <div>12%</div> <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
3	FUC	A	400	X	-	-	-
7	FUC	C	410	X	-	-	-
7	NAG	C	411	-	-	-	X
7	NAG	C	412	X	-	-	-
8	FUC	D	200	X	-	-	-
8	FUC	F	200	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12508 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 H3 HAEMAGGLUTININ HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	6	0
			2542	1594	447	486	15			
1	C	320	Total	C	N	O	S	0	1	0
			2497	1561	441	480	15			
1	E	323	Total	C	N	O	S	0	2	0
			2524	1580	444	485	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	THR	SER	ENGINEERED MUTATION	UNP C3TUR9
C	30	THR	SER	ENGINEERED MUTATION	UNP C3TUR9
E	30	THR	SER	ENGINEERED MUTATION	UNP C3TUR9

- Molecule 2 is a protein called H3 HAEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	6	0
			1432	897	245	283	7			
2	D	172	Total	C	N	O	S	0	4	0
			1421	890	245	279	7			
2	F	171	Total	C	N	O	S	0	6	0
			1420	891	242	279	8			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	2	Total	C	N	O	0	0
			24	14	1	9		
8	F	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

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

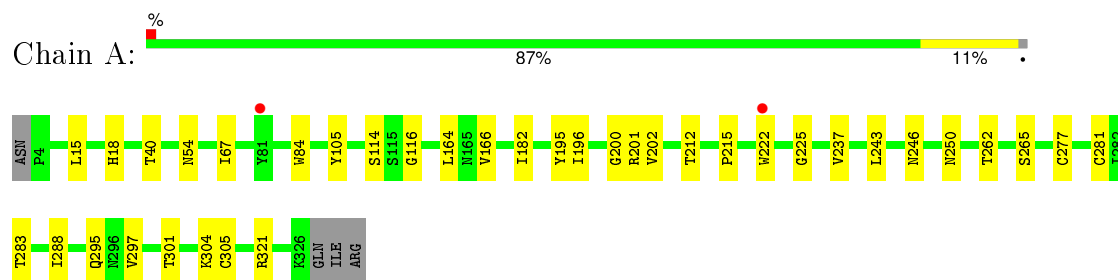
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	26	Total	O	0	0
			26	26		
11	B	27	Total	O	0	0
			27	27		
11	C	33	Total	O	0	0
			33	33		
11	D	13	Total	O	0	0
			13	13		
11	E	40	Total	O	0	0
			40	40		
11	F	19	Total	O	0	0
			19	19		

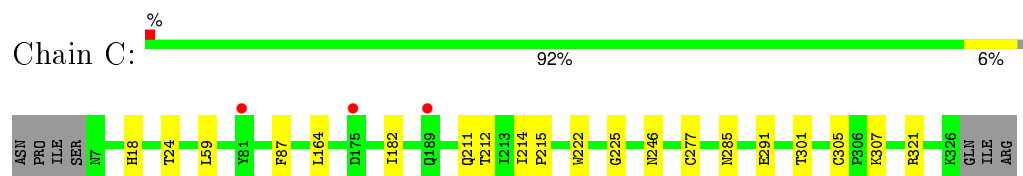
3 Residue-property plots [i](#)

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.

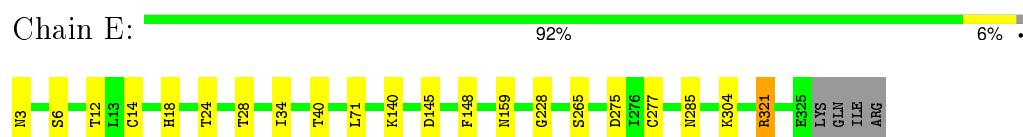
- Molecule 1: H3 HAEMAGGLUTININ HA1 CHAIN



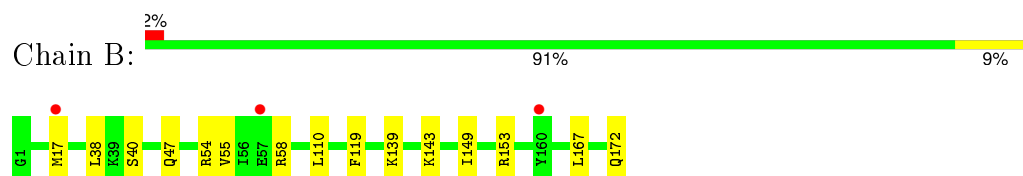
- Molecule 1: H3 HAEMAGGLUTININ HA1 CHAIN



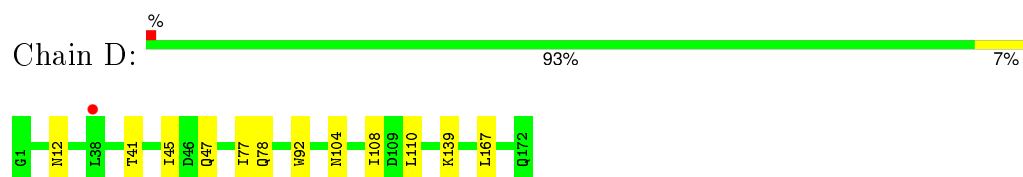
- Molecule 1: H3 HAEMAGGLUTININ HA1 CHAIN



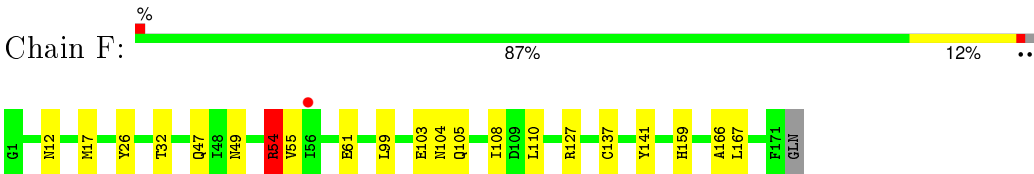
- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN



- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN



- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.82Å 129.62Å 195.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.89 – 2.87 64.81 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.7 (64.89-2.87) 98.7 (64.81-2.87)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.217 , 0.277 0.218 , 0.273	Depositor DCC
R_{free} test set	2353 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 46520 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12508	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: FUC, MAN, BMA, NAG, EDO

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	0.38	0/2614	0.58	0/3549
1	C	0.38	0/2553	0.59	0/3466
1	E	0.40	0/2584	0.60	0/3510
2	B	0.40	0/1475	0.60	0/1983
2	D	0.43	0/1458	0.60	0/1960
2	F	0.44	0/1463	0.66	1/1968 (0.1%)
All	All	0.40	0/12147	0.60	1/16436 (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
3	A	1	0
7	C	2	0
8	D	2	0
8	F	1	0
All	All	6	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	54	ARG	NE-CZ-NH1	5.56	123.08	120.30

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	400	FUC	C1

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Mol	Chain	Res	Type	Atom
7	C	410	FUC	C1
7	C	412	NAG	C1
8	D	200	FUC	C5,C1
8	F	200	FUC	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	2542	0	2513	20	0
1	C	2497	0	2445	9	0
1	E	2524	0	2477	10	0
2	B	1432	0	1370	5	0
2	D	1421	0	1360	5	0
2	F	1420	0	1358	12	0
3	A	49	0	43	1	0
4	A	42	0	39	0	0
4	B	14	0	13	0	0
4	C	14	0	13	2	0
4	E	14	0	13	1	0
5	A	61	0	52	1	0
5	C	122	0	104	1	0
6	A	4	0	6	0	0
6	E	4	0	6	0	0
6	F	4	0	6	0	0
7	C	71	0	61	0	0
8	D	24	0	22	0	0
8	F	24	0	22	0	0
9	E	28	0	25	0	0
10	E	39	0	34	1	0
11	A	26	0	0	0	0
11	B	27	0	0	0	0
11	C	33	0	0	0	0
11	D	13	0	0	0	0
11	E	40	0	0	1	0
11	F	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12508	0	11982	57	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 2.

All (57) 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:54:ARG:HG2	2:F:54:ARG:HH11	1.56	0.69
1:A:288[B]:ILE:HD11	1:A:297:VAL:HG11	1.76	0.68
2:B:47:GLN:NE2	2:B:110:LEU:HD13	2.14	0.62
1:E:34:ILE:HD11	1:E:321:ARG:NE	2.14	0.61
1:A:301:THR:HB	1:A:305:CYS:SG	2.43	0.58
1:E:28:THR:HB	2:F:105:GLN:OE1	2.05	0.56
1:C:307:LYS:HE2	2:D:92:TRP:CH2	2.40	0.56
1:A:202:VAL:O	1:A:212:THR:HA	2.07	0.54
1:E:285:ASN:ND2	4:E:451:NAG:H83	2.23	0.53
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.92	0.51
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.47	0.50
2:F:127:ARG:HG3	2:F:159:HIS:CD2	2.47	0.50
1:E:140:LYS:NZ	1:E:145:ASP:OD1	2.43	0.50
5:A:442:NAG:O3	5:A:443:BMA:O5	2.13	0.49
2:F:54:ARG:HH11	2:F:54:ARG:CG	2.24	0.49
1:C:222:TRP:CZ2	1:C:225:GLY:HA2	2.48	0.49
1:A:281:CYS:HB2	1:A:304:LYS:O	2.14	0.48
2:F:99:LEU:O	2:F:103:GLU:HG2	2.13	0.48
1:E:34:ILE:HD11	1:E:321:ARG:CD	2.44	0.48
1:E:304:LYS:HG3	2:F:61:GLU:HG2	1.96	0.48
2:F:104:ASN:O	2:F:108:ILE:HG12	2.14	0.48
1:C:285:ASN:HD22	4:C:451:NAG:H83	1.80	0.47
2:D:41:THR:HG22	2:D:45:ILE:HD12	1.96	0.47
3:A:400:FUC:H63	2:B:143:LYS:HE2	1.96	0.47
2:F:141:TYR:O	2:F:166:ALA:HA	2.15	0.47
1:C:285:ASN:ND2	4:C:451:NAG:H83	2.30	0.46
1:A:237:VAL:HG21	1:A:243:LEU:HB2	1.98	0.46
1:A:195:TYR:O	1:A:196:ILE:HB	2.15	0.45
2:F:47:GLN:NE2	2:F:110:LEU:HD13	2.31	0.45
1:E:71:LEU:O	1:E:148:PHE:HB3	2.17	0.44
1:A:182:ILE:HD11	1:A:215:PRO:HG3	1.99	0.44
1:A:201[B]:ARG:NH2	1:A:246:ASN:OD1	2.41	0.44
1:C:59:LEU:HD23	1:C:87:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:ASN:O	2:D:108:ILE:HG12	2.17	0.44
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.53	0.43
1:A:164:LEU:O	1:A:246:ASN:HA	2.18	0.43
2:D:77[B]:ILE:HG23	2:D:78:GLN:N	2.34	0.43
1:A:200:GLY:HA3	1:A:250:ASN:OD1	2.19	0.43
1:A:283:THR:CG2	1:A:288[B]:ILE:HD13	2.49	0.43
1:A:54:ASN:HB2	1:A:277:CYS:O	2.18	0.42
1:C:291:GLU:OE2	5:C:427:MAN:C4	2.67	0.42
1:E:12:THR:O	2:F:26:TYR:HA	2.19	0.42
1:A:15:LEU:HD12	1:A:15:LEU:N	2.35	0.42
2:B:149:ILE:HG22	2:B:153:ARG:HD3	2.00	0.42
1:A:67:ILE:HG13	1:A:105:TYR:CE1	2.55	0.41
1:C:164:LEU:O	1:C:246:ASN:HA	2.20	0.41
1:A:295:GLN:OE1	1:A:297:VAL:N	2.53	0.41
10:E:442:NAG:O3	10:E:443:BMA:O5	2.37	0.41
1:E:228:GLY:N	11:E:2015:HOH:O	2.50	0.41
1:C:301:THR:HB	1:C:305:CYS:SG	2.61	0.41
2:F:103:GLU:OE1	2:F:103:GLU:HA	2.21	0.41
1:E:14:CYS:HA	2:F:137:CYS:HA	2.03	0.41
1:C:182:ILE:HD11	1:C:215:PRO:HG3	2.03	0.40
2:D:47:GLN:NE2	2:D:110:LEU:HD13	2.37	0.40
1:A:201[B]:ARG:HB3	1:A:201[B]:ARG:HE	1.71	0.40

There are no symmetry-related clashes.

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	327/327 (100%)	306 (94%)	21 (6%)	0	100	100
1	C	319/327 (98%)	304 (95%)	15 (5%)	0	100	100
1	E	323/327 (99%)	309 (96%)	13 (4%)	1 (0%)	46	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	176/172 (102%)	165 (94%)	11 (6%)	0	100	100
2	D	174/172 (101%)	161 (92%)	13 (8%)	0	100	100
2	F	175/172 (102%)	165 (94%)	10 (6%)	0	100	100
All	All	1494/1497 (100%)	1410 (94%)	83 (6%)	1 (0%)	56	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	277	CYS

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	291/290 (100%)	284 (98%)	7 (2%)	57	85
1	C	283/290 (98%)	276 (98%)	7 (2%)	55	84
1	E	287/290 (99%)	278 (97%)	9 (3%)	47	80
2	B	152/146 (104%)	142 (93%)	10 (7%)	21	49
2	D	150/146 (103%)	147 (98%)	3 (2%)	63	88
2	F	150/146 (103%)	141 (94%)	9 (6%)	24	55
All	All	1313/1308 (100%)	1268 (97%)	45 (3%)	46	78

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	40	THR
1	A	114	SER
1	A	166	VAL
1	A	262	THR
1	A	265	SER
1	A	321	ARG

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Mol	Chain	Res	Type
2	B	17[A]	MET
2	B	17[B]	MET
2	B	40[A]	SER
2	B	40[B]	SER
2	B	54	ARG
2	B	55	VAL
2	B	58	ARG
2	B	139	LYS
2	B	167	LEU
2	B	172	GLN
1	C	18	HIS
1	C	24	THR
1	C	211	GLN
1	C	212	THR
1	C	214	ILE
1	C	277	CYS
1	C	321	ARG
2	D	12	ASN
2	D	139	LYS
2	D	167	LEU
1	E	3	ASN
1	E	6	SER
1	E	18	HIS
1	E	24	THR
1	E	40	THR
1	E	159	ASN
1	E	265	SER
1	E	275	ASP
1	E	321	ARG
2	F	12	ASN
2	F	17[A]	MET
2	F	17[B]	MET
2	F	32[A]	THR
2	F	32[B]	THR
2	F	49	ASN
2	F	54	ARG
2	F	55	VAL
2	F	167	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	54	ASN
2	B	42	GLN
2	B	47	GLN
2	B	49	ASN
1	C	33	GLN
2	D	47	GLN
2	D	49	ASN
2	D	53	ASN
2	F	12	ASN
2	F	47	GLN
2	F	53	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 ⓘ

34 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FUC	A	400	3	10,10,11	1.10	1 (10%)	14,14,16	3.06	5 (35%)
3	NAG	A	401	1,3	14,14,15	0.50	0	15,19,21	1.56	3 (20%)
3	NAG	A	402	3	14,14,15	0.50	0	15,19,21	1.00	1 (6%)
3	BMA	A	403	3	11,11,12	0.38	0	14,15,17	0.94	0
5	NAG	A	441	1,5	14,14,15	0.63	0	15,19,21	0.91	0
5	NAG	A	442	5	14,14,15	0.64	0	15,19,21	0.99	0
5	BMA	A	443	5	11,11,12	0.39	0	14,15,17	2.71	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	444	5	11,11,12	0.61	0	14,15,17	1.35	2 (14%)
5	MAN	A	447	5	11,11,12	0.84	0	14,15,17	2.64	5 (35%)
7	FUC	C	410	7	10,10,11	0.77	0	14,14,16	1.54	2 (14%)
7	NAG	C	411	1,7	14,14,15	0.96	1 (7%)	15,19,21	1.36	3 (20%)
7	NAG	C	412	7	14,14,15	0.51	0	15,19,21	1.23	2 (13%)
7	BMA	C	413	7	11,11,12	0.25	0	14,15,17	1.16	1 (7%)
7	MAN	C	414	7	11,11,12	0.55	0	14,15,17	1.13	1 (7%)
7	MAN	C	417	7	11,11,12	0.70	0	14,15,17	1.61	3 (21%)
5	NAG	C	421	1,5	14,14,15	0.60	0	15,19,21	1.12	1 (6%)
5	NAG	C	422	5	14,14,15	0.54	0	15,19,21	1.13	1 (6%)
5	BMA	C	423	5	11,11,12	0.44	0	14,15,17	1.24	1 (7%)
5	MAN	C	424	5	11,11,12	0.49	0	14,15,17	1.88	4 (28%)
5	MAN	C	427	5	11,11,12	0.47	0	14,15,17	1.07	2 (14%)
5	NAG	C	441	1,5	14,14,15	0.54	0	15,19,21	1.55	2 (13%)
5	NAG	C	442	5	14,14,15	0.58	0	15,19,21	0.99	0
5	BMA	C	443	5	11,11,12	0.26	0	14,15,17	1.28	1 (7%)
5	MAN	C	444	5	11,11,12	0.57	0	14,15,17	1.87	4 (28%)
5	MAN	C	447	5	11,11,12	0.54	0	14,15,17	1.05	1 (7%)
8	FUC	D	200	8	10,10,11	0.49	0	14,14,16	2.77	4 (28%)
8	NAG	D	201	8,2	14,14,15	0.46	0	15,19,21	1.17	2 (13%)
9	NAG	E	421	1,9	14,14,15	0.53	0	15,19,21	1.93	5 (33%)
9	NAG	E	422	9	14,14,15	0.59	0	15,19,21	0.95	1 (6%)
10	NAG	E	441	1,10	14,14,15	0.61	0	15,19,21	1.13	1 (6%)
10	NAG	E	442	10	14,14,15	0.58	0	15,19,21	1.03	1 (6%)
10	BMA	E	443	10	11,11,12	0.35	0	14,15,17	0.86	1 (7%)
8	FUC	F	200	8	10,10,11	0.86	0	14,14,16	2.20	4 (28%)
8	NAG	F	201	8,2	14,14,15	0.53	0	15,19,21	1.42	2 (13%)

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	FUC	A	400	3	1/1/4/5	0/0/17/20	0/1/1/1
3	NAG	A	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	A	403	3	-	0/2/19/22	0/1/1/1
5	NAG	A	441	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	442	5	-	0/6/23/26	0/1/1/1
5	BMA	A	443	5	-	0/2/19/22	0/1/1/1
5	MAN	A	444	5	-	0/2/19/22	0/1/1/1
5	MAN	A	447	5	-	0/2/19/22	0/1/1/1
7	FUC	C	410	7	1/1/4/5	0/0/17/20	0/1/1/1
7	NAG	C	411	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	412	7	1/1/5/7	0/6/23/26	0/1/1/1
7	BMA	C	413	7	-	0/2/19/22	0/1/1/1
7	MAN	C	414	7	-	0/2/19/22	0/1/1/1
7	MAN	C	417	7	-	0/2/19/22	0/1/1/1
5	NAG	C	421	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	422	5	-	0/6/23/26	0/1/1/1
5	BMA	C	423	5	-	0/2/19/22	0/1/1/1
5	MAN	C	424	5	-	0/2/19/22	1/1/1/1
5	MAN	C	427	5	-	0/2/19/22	0/1/1/1
5	NAG	C	441	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	442	5	-	0/6/23/26	0/1/1/1
5	BMA	C	443	5	-	0/2/19/22	0/1/1/1
5	MAN	C	444	5	-	0/2/19/22	0/1/1/1
5	MAN	C	447	5	-	0/2/19/22	0/1/1/1
8	FUC	D	200	8	2/2/4/5	0/0/17/20	0/1/1/1
8	NAG	D	201	8,2	-	0/6/23/26	0/1/1/1
9	NAG	E	421	1,9	-	0/6/23/26	0/1/1/1
9	NAG	E	422	9	-	0/6/23/26	0/1/1/1
10	NAG	E	441	1,10	-	0/6/23/26	0/1/1/1
10	NAG	E	442	10	-	0/6/23/26	0/1/1/1
10	BMA	E	443	10	-	0/2/19/22	0/1/1/1
8	FUC	F	200	8	1/1/4/5	0/0/17/20	0/1/1/1
8	NAG	F	201	8,2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	411	NAG	O5-C1	-2.29	1.39	1.43
3	A	400	FUC	O5-C1	-2.10	1.40	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	FUC	C1-C2-C3	-9.14	98.73	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	200	FUC	C1-C2-C3	-5.87	102.60	109.54
7	C	411	NAG	O4-C4-C5	-3.30	100.51	109.24
9	E	421	NAG	O4-C4-C3	-3.24	103.05	110.34
7	C	414	MAN	O4-C4-C3	-2.84	103.94	110.34
3	A	401	NAG	O4-C4-C3	-2.74	104.17	110.34
5	A	447	MAN	C3-C4-C5	-2.57	105.72	110.20
3	A	400	FUC	C1-O5-C5	-2.51	108.50	112.38
5	C	441	NAG	O7-C7-C8	-2.51	117.46	122.06
5	A	443	BMA	O3-C3-C4	-2.44	104.84	110.34
7	C	412	NAG	C3-C4-C5	-2.42	105.98	110.20
7	C	411	NAG	O7-C7-C8	-2.21	118.00	122.06
10	E	442	NAG	C2-N2-C7	-2.17	120.25	123.04
9	E	421	NAG	O7-C7-C8	-2.11	118.18	122.06
8	F	201	NAG	C3-C4-C5	-2.07	106.59	110.20
5	C	444	MAN	C6-C5-C4	-2.07	107.92	113.02
5	C	424	MAN	O5-C5-C6	2.02	111.72	107.35
10	E	443	BMA	C1-C2-C3	2.03	111.94	109.54
7	C	411	NAG	O7-C7-N2	2.08	126.11	121.86
9	E	422	NAG	C3-C4-C5	2.09	113.83	110.20
7	C	410	FUC	O5-C1-C2	2.16	114.37	110.86
3	A	401	NAG	O6-C6-C5	2.17	118.51	111.33
9	E	421	NAG	O3-C3-C2	2.19	113.44	109.11
5	C	421	NAG	C3-C4-C5	2.20	114.04	110.20
5	C	424	MAN	O5-C1-C2	2.21	114.45	110.86
5	A	447	MAN	O5-C1-C2	2.26	114.52	110.86
5	C	444	MAN	C3-C4-C5	2.26	114.14	110.20
3	A	400	FUC	O2-C2-C3	2.31	114.77	110.12
8	D	201	NAG	O5-C5-C6	2.31	112.35	107.35
3	A	402	NAG	C3-C4-C5	2.31	114.23	110.20
8	F	200	FUC	C3-C4-C5	2.37	113.72	109.72
8	D	201	NAG	C1-O5-C5	2.47	115.38	112.25
5	C	424	MAN	C1-C2-C3	2.49	112.48	109.54
8	F	200	FUC	O5-C1-C2	2.51	114.92	110.86
5	C	443	BMA	C1-C2-C3	2.52	112.52	109.54
5	C	427	MAN	C1-O5-C5	2.53	115.46	112.25
7	C	417	MAN	C3-C4-C5	2.56	114.67	110.20
5	A	444	MAN	O5-C5-C6	2.57	112.92	107.35
5	C	427	MAN	C3-C4-C5	2.59	114.71	110.20
5	C	444	MAN	O5-C5-C6	2.60	112.98	107.35
8	D	200	FUC	O5-C5-C4	2.61	114.05	109.53
7	C	413	BMA	C1-O5-C5	2.63	115.59	112.25
5	A	447	MAN	O5-C5-C6	2.71	113.21	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	417	MAN	C1-O5-C5	2.77	115.76	112.25
5	C	447	MAN	C1-O5-C5	2.83	115.83	112.25
5	C	422	NAG	C1-O5-C5	2.83	115.84	112.25
5	A	444	MAN	C1-O5-C5	2.87	115.89	112.25
8	F	200	FUC	O5-C5-C4	2.98	114.69	109.53
7	C	412	NAG	C1-O5-C5	3.01	116.07	112.25
10	E	441	NAG	C1-O5-C5	3.02	116.09	112.25
5	C	423	BMA	C1-C2-C3	3.04	113.14	109.54
9	E	421	NAG	C2-N2-C7	3.18	127.12	123.04
3	A	401	NAG	C1-O5-C5	3.29	116.42	112.25
3	A	400	FUC	O5-C5-C4	3.58	115.73	109.53
3	A	400	FUC	C3-C4-C5	3.62	115.82	109.72
7	C	410	FUC	O5-C5-C6	3.72	112.28	106.13
9	E	421	NAG	C8-C7-N2	3.74	123.27	116.11
7	C	417	MAN	C1-C2-C3	4.03	114.31	109.54
8	F	201	NAG	C1-O5-C5	4.22	117.61	112.25
5	C	441	NAG	C1-O5-C5	4.36	117.78	112.25
8	D	200	FUC	C1-C2-C3	4.49	114.85	109.54
5	A	443	BMA	C3-C4-C5	4.71	118.40	110.20
5	C	444	MAN	C1-O5-C5	5.02	118.62	112.25
8	D	200	FUC	C1-O5-C5	5.04	120.17	112.38
5	A	447	MAN	C1-O5-C5	5.10	118.72	112.25
5	C	424	MAN	C1-O5-C5	5.49	119.22	112.25
8	D	200	FUC	O5-C1-C2	6.65	121.65	110.86
5	A	447	MAN	C1-C2-C3	6.79	117.58	109.54
5	A	443	BMA	C1-O5-C5	7.79	122.13	112.25

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	400	FUC	C1
7	C	412	NAG	C1
8	F	200	FUC	C1
7	C	410	FUC	C1
8	D	200	FUC	C5
8	D	200	FUC	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	424	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	FUC	1	0
5	A	442	NAG	1	0
5	A	443	BMA	1	0
5	C	427	MAN	1	0
10	E	442	NAG	1	0
10	E	443	BMA	1	0

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
6	EDO	A	1201	-	3,3,3	0.55	0	2,2,2	0.29	0
4	NAG	A	421	1	14,14,15	0.65	0	15,19,21	1.13	1 (6%)
4	NAG	A	431	1	14,14,15	0.53	0	15,19,21	1.26	1 (6%)
4	NAG	A	451	1	14,14,15	0.60	0	15,19,21	1.79	5 (33%)
4	NAG	B	201	2	14,14,15	0.87	1 (7%)	15,19,21	1.52	2 (13%)
4	NAG	C	451	1	14,14,15	0.62	0	15,19,21	1.97	3 (20%)
6	EDO	E	1201	-	3,3,3	0.59	0	2,2,2	0.21	0
4	NAG	E	451	1	14,14,15	0.69	0	15,19,21	1.97	5 (33%)
6	EDO	F	1201	-	3,3,3	0.50	0	2,2,2	0.38	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
6	EDO	A	1201	-	-	0/1/1/1	0/0/0/0
4	NAG	A	421	1	-	0/6/23/26	0/1/1/1
4	NAG	A	431	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	451	1	-	0/6/23/26	0/1/1/1
4	NAG	B	201	2	-	0/6/23/26	0/1/1/1
4	NAG	C	451	1	-	0/6/23/26	0/1/1/1
6	EDO	E	1201	-	-	0/1/1/1	0/0/0/0
4	NAG	E	451	1	-	0/6/23/26	0/1/1/1
6	EDO	F	1201	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	201	NAG	C1-C2	2.25	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	451	NAG	O7-C7-C8	-3.17	116.25	122.06
4	C	451	NAG	C3-C2-N2	-2.69	104.12	110.56
4	A	451	NAG	C4-C3-C2	-2.53	107.30	111.23
4	A	451	NAG	O7-C7-C8	-2.13	118.16	122.06
4	A	451	NAG	O5-C5-C6	2.27	112.27	107.35
4	E	451	NAG	C4-C3-C2	2.29	114.78	111.23
4	A	451	NAG	C8-C7-N2	2.39	120.68	116.11
4	B	201	NAG	C1-O5-C5	2.49	115.41	112.25
4	E	451	NAG	C2-N2-C7	2.96	126.84	123.04
4	A	421	NAG	C4-C3-C2	3.00	115.89	111.23
4	E	451	NAG	C1-O5-C5	3.04	116.10	112.25
4	C	451	NAG	C8-C7-N2	3.11	122.06	116.11
4	B	201	NAG	C4-C3-C2	3.67	116.94	111.23
4	A	431	NAG	C1-O5-C5	4.02	117.35	112.25
4	A	451	NAG	C1-O5-C5	4.36	117.79	112.25
4	E	451	NAG	C8-C7-N2	4.47	124.66	116.11
4	C	451	NAG	C2-N2-C7	4.57	128.91	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	451	NAG	2	0
4	E	451	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	323/327 (98%)	0.38	2 (0%) 90 89	42, 59, 80, 95	0
1	C	320/327 (97%)	0.31	3 (0%) 85 84	36, 60, 80, 98	0
1	E	323/327 (98%)	0.19	0 100 100	37, 54, 73, 91	0
2	B	172/172 (100%)	0.30	3 (1%) 73 71	35, 55, 70, 76	0
2	D	172/172 (100%)	0.28	1 (0%) 90 89	36, 55, 72, 94	0
2	F	171/172 (99%)	0.17	1 (0%) 90 89	36, 49, 67, 85	0
All	All	1481/1497 (98%)	0.28	10 (0%) 89 88	35, 56, 76, 98	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	TRP	3.6
1	C	81	TYR	3.0
2	F	56	ILE	2.7
1	C	175	ASP	2.4
1	C	189	GLN	2.4
2	B	160	TYR	2.3
2	D	38[A]	LEU	2.3
1	A	81	TYR	2.2
2	B	57	GLU	2.2
2	B	17[A]	MET	2.1

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
7	NAG	C	411	14/15	0.94	0.23	2.19	53,56,66,71	0
5	NAG	C	421	14/15	0.94	0.24	0.99	63,70,75,75	0
3	NAG	A	402	14/15	0.87	0.21	0.55	82,89,94,97	0
3	NAG	A	401	14/15	0.88	0.20	0.12	77,80,86,90	0
5	NAG	A	442	14/15	0.93	0.21	0.03	63,66,71,74	0
5	NAG	C	442	14/15	0.90	0.26	-0.13	77,82,87,91	0
10	NAG	E	442	14/15	0.94	0.18	-2.68	57,62,67,68	0
9	NAG	E	422	14/15	0.78	0.21	-	86,95,105,107	0
10	BMA	E	443	11/12	0.85	0.17	-	70,73,77,77	0
7	MAN	C	414	11/12	0.88	0.17	-	64,68,70,70	0
5	NAG	C	422	14/15	0.82	0.22	-	79,83,90,96	0
9	NAG	E	421	14/15	0.82	0.26	-	67,73,78,87	0
5	MAN	A	447	11/12	0.78	0.19	-	91,95,97,100	0
3	BMA	A	403	11/12	0.71	0.29	-	100,104,109,109	0
3	FUC	A	400	10/11	0.92	0.22	-	92,94,96,97	0
5	NAG	A	441	14/15	0.95	0.18	-	60,61,64,67	0
5	MAN	C	444	11/12	0.78	0.20	-	109,114,117,120	0
5	BMA	C	423	11/12	0.69	0.26	-	102,108,112,116	0
5	MAN	C	424	11/12	0.40	0.29	-	118,121,124,125	0
5	BMA	C	443	11/12	0.83	0.14	-	95,99,104,107	0
7	BMA	C	413	11/12	0.90	0.15	-	72,73,84,88	0
8	NAG	D	201	14/15	0.64	0.28	-	94,100,103,105	0
5	MAN	C	447	11/12	0.65	0.29	-	97,99,104,104	0
5	MAN	C	427	11/12	0.00	0.62	-	113,120,123,123	0
7	NAG	C	412	14/15	0.93	0.22	-	61,66,70,73	0
5	NAG	C	441	14/15	0.94	0.19	-	72,75,78,79	0
5	BMA	A	443	11/12	0.82	0.15	-	78,81,87,88	0
5	MAN	A	444	11/12	0.77	0.17	-	90,93,95,95	0
10	NAG	E	441	14/15	0.93	0.19	-	59,62,70,73	0
7	FUC	C	410	10/11	0.92	0.26	-	77,80,82,85	0
8	NAG	F	201	14/15	0.90	0.17	-	71,76,79,79	0
8	FUC	D	200	10/11	0.64	0.36	-	106,110,114,116	0
7	MAN	C	417	11/12	0.76	0.37	-	89,91,93,93	0
8	FUC	F	200	10/11	0.71	0.27	-	79,83,85,87	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
6	EDO	A	1201	4/4	0.68	0.32	1.50	74,77,78,78	0
4	NAG	A	451	14/15	0.74	0.26	1.22	79,86,89,89	0
4	NAG	E	451	14/15	0.82	0.23	1.14	62,67,68,70	0
6	EDO	E	1201	4/4	0.92	0.23	0.90	59,60,65,66	0
4	NAG	C	451	14/15	0.84	0.19	-0.11	67,70,75,77	0
6	EDO	F	1201	4/4	0.84	0.22	-0.47	74,76,77,78	0
4	NAG	B	201	14/15	0.74	0.33	-	77,86,89,90	0
4	NAG	A	431	14/15	0.73	0.24	-	79,84,90,92	0
4	NAG	A	421	14/15	0.86	0.24	-	67,71,74,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.