Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:06 PM GMT

PDB ID	:	4NRL
Title	:	Structure of hemagglutinin with F95Y mutation of influenza virus B/Lee/40
Authors	:	Ni, F.; Mbawuike, I.N.; Kondrashkina, E.; Wang, Q.
Deposited on	:	2013-11-26
Resolution	:	2.72 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

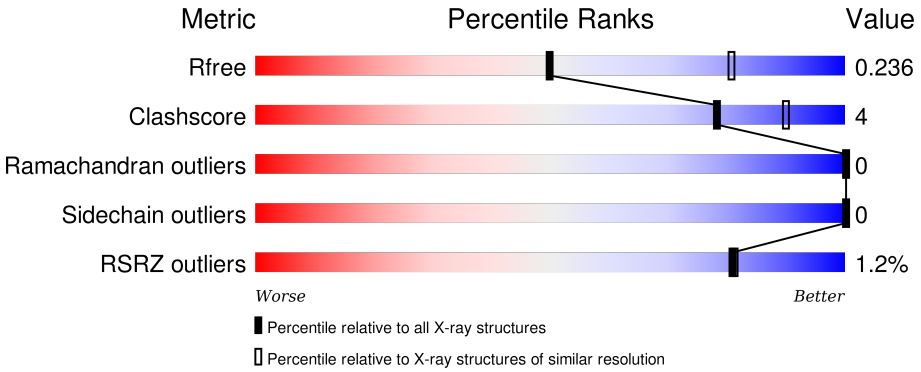
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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 <=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	346	88% 11%
1	C	346	90% 9%
1	E	346	90% 8%
2	B	182	88% 5% 7%
2	D	182	86% 7% 7%

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Mol	Chain	Length	Quality of chain
2	F	182	3% 87% 5% 7%

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
4	NAG	A	413	-	-	-	X
4	NAG	C	406	-	-	-	X
4	NAG	E	415	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12583 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2600	1631	461	492	16			
1	C	341	Total	C	N	O	S	0	0	0
			2600	1631	461	492	16			
1	E	341	Total	C	N	O	S	0	0	0
			2600	1631	461	492	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ARG	LYS	CONFLICT	UNP P03460
A	76	ILE	THR	CONFLICT	UNP P03460
A	90	VAL	ALA	CONFLICT	UNP P03460
A	95	TYR	PHE	ENGINEERED MUTATION	UNP P03460
A	147	THR	ALA	CONFLICT	UNP P03460
A	167	ILE	THR	CONFLICT	UNP P03460
C	38	ARG	LYS	CONFLICT	UNP P03460
C	76	ILE	THR	CONFLICT	UNP P03460
C	90	VAL	ALA	CONFLICT	UNP P03460
C	95	TYR	PHE	ENGINEERED MUTATION	UNP P03460
C	147	THR	ALA	CONFLICT	UNP P03460
C	167	ILE	THR	CONFLICT	UNP P03460
E	38	ARG	LYS	CONFLICT	UNP P03460
E	76	ILE	THR	CONFLICT	UNP P03460
E	90	VAL	ALA	CONFLICT	UNP P03460
E	95	TYR	PHE	ENGINEERED MUTATION	UNP P03460
E	147	THR	ALA	CONFLICT	UNP P03460
E	167	ILE	THR	CONFLICT	UNP P03460

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1289	806	220	257	6			
2	D	169	Total	C	N	O	S	0	0	0
			1281	800	219	256	6			
2	F	169	Total	C	N	O	S	0	0	0
			1281	800	219	256	6			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	54	SER	TYR	CONFLICT	UNP P03460
B	177	GLY	-	EXPRESSION TAG	UNP P03460
B	178	ALA	-	EXPRESSION TAG	UNP P03460
B	179	LEU	-	EXPRESSION TAG	UNP P03460
B	180	VAL	-	EXPRESSION TAG	UNP P03460
B	181	PRO	-	EXPRESSION TAG	UNP P03460
B	182	ARG	-	EXPRESSION TAG	UNP P03460
D	54	SER	TYR	CONFLICT	UNP P03460
D	177	GLY	-	EXPRESSION TAG	UNP P03460
D	178	ALA	-	EXPRESSION TAG	UNP P03460
D	179	LEU	-	EXPRESSION TAG	UNP P03460
D	180	VAL	-	EXPRESSION TAG	UNP P03460
D	181	PRO	-	EXPRESSION TAG	UNP P03460
D	182	ARG	-	EXPRESSION TAG	UNP P03460
F	54	SER	TYR	CONFLICT	UNP P03460
F	177	GLY	-	EXPRESSION TAG	UNP P03460
F	178	ALA	-	EXPRESSION TAG	UNP P03460
F	179	LEU	-	EXPRESSION TAG	UNP P03460
F	180	VAL	-	EXPRESSION TAG	UNP P03460
F	181	PRO	-	EXPRESSION TAG	UNP P03460
F	182	ARG	-	EXPRESSION TAG	UNP P03460

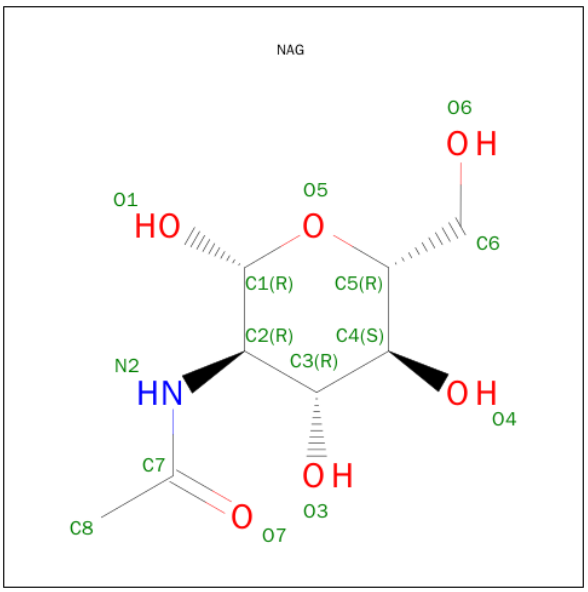
- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			68	37	2	29		
3	C	5	Total	C	N	O	0	0
			68	37	2	29		
3	E	5	Total	C	N	O	0	0
			68	37	2	29		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

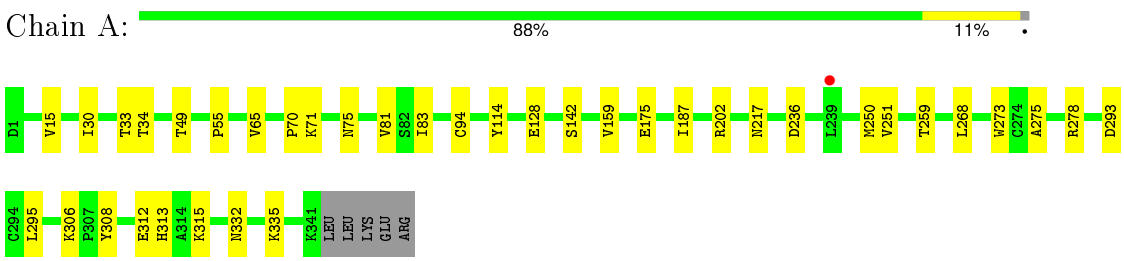
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	66	Total	O	0	0
			66	66		
7	B	13	Total	O	0	0
			13	13		
7	C	59	Total	O	0	0
			59	59		
7	D	29	Total	O	0	0
			29	29		
7	E	82	Total	O	0	0
			82	82		
7	F	20	Total	O	0	0
			20	20		

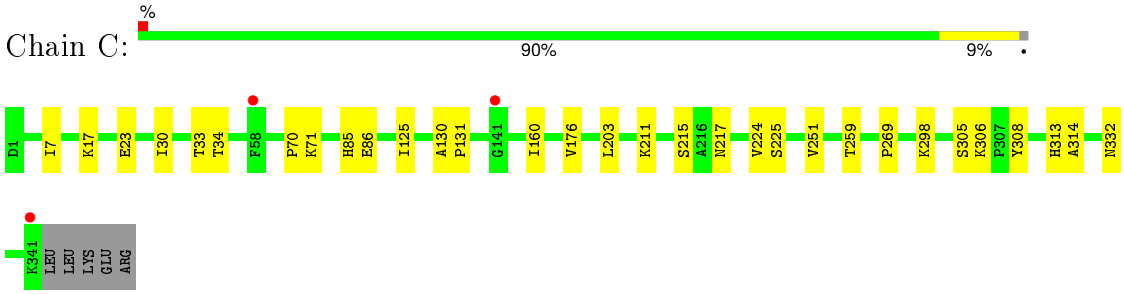
3 Residue-property plots (i)

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.

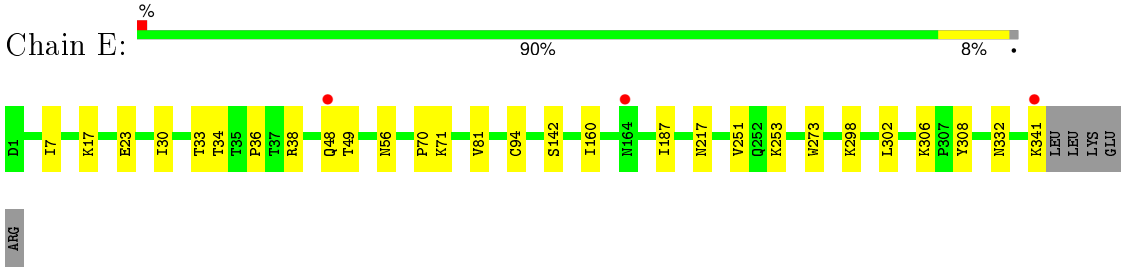
- Molecule 1: Hemagglutinin HA1 chain



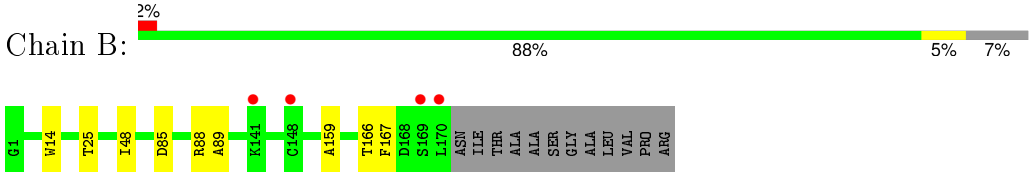
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

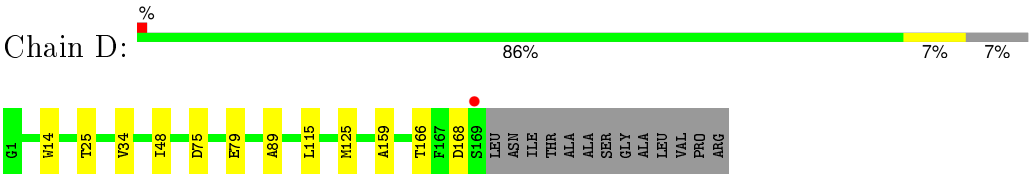


- Molecule 2: Hemagglutinin HA2 chain



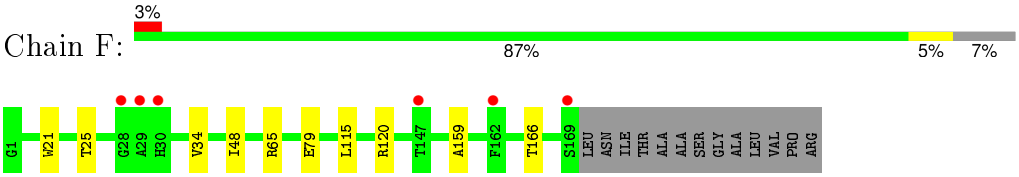
- Molecule 2: Hemagglutinin HA2 chain

Chain D:



- Molecule 2: Hemagglutinin HA2 chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	83.61Å 128.40Å 211.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 2.72 47.49 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.49-2.72) 95.5 (47.49-2.72)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1452)	Depositor
R, R_{free}	0.194 , 0.229 0.205 , 0.236	Depositor DCC
R_{free} test set	2946 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.800	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 59266 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12583	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GAL, SIA, BGC, BMA, NAG

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	0.23	0/2659	0.44	0/3614
1	C	0.23	0/2659	0.46	1/3614 (0.0%)
1	E	0.23	0/2659	0.45	0/3614
2	B	0.21	0/1308	0.37	0/1763
2	D	0.21	0/1300	0.36	0/1752
2	F	0.22	0/1300	0.37	0/1752
All	All	0.22	0/11885	0.42	1/16109 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	203	LEU	CB-CG-CD2	-5.90	100.96	111.00

There are no chirality outliers.

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	2600	0	2597	27	0
1	C	2600	0	2597	22	0
1	E	2600	0	2596	19	0
2	B	1289	0	1261	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1281	0	1251	10	0
2	F	1281	0	1251	8	0
3	A	68	0	58	1	0
3	C	68	0	58	1	0
3	E	68	0	58	2	0
4	A	112	0	100	0	0
4	C	84	0	75	4	0
4	E	140	0	125	2	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	1	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	C	39	0	34	0	0
7	A	66	0	0	8	0
7	B	13	0	0	2	0
7	C	59	0	0	9	0
7	D	29	0	0	2	0
7	E	82	0	0	2	0
7	F	20	0	0	2	0
All	All	12583	0	12139	89	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 4.

All (89) 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:E:48:GLN:NE2	7:E:559:HOH:O	1.96	0.98
1:A:128:GLU:OE1	7:A:565:HOH:O	1.92	0.88
1:E:56:ASN:OD1	7:E:546:HOH:O	1.91	0.86
1:C:215:SER:O	7:C:551:HOH:O	1.92	0.86
1:A:15:VAL:O	7:A:558:HOH:O	2.03	0.76
1:C:224:VAL:O	7:C:516:HOH:O	2.02	0.76
4:C:414:NAG:O7	7:C:504:HOH:O	2.07	0.73
1:A:335:LYS:O	7:A:541:HOH:O	2.06	0.72
2:D:159:ALA:HB3	2:D:166:THR:HG22	1.73	0.71
1:C:225:SER:O	7:C:508:HOH:O	2.09	0.70
1:A:65:VAL:O	7:A:511:HOH:O	2.09	0.70
2:B:159:ALA:HB3	2:B:166:THR:HG22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:HG22	1:C:308:TYR:HB2	1.75	0.69
2:D:125:MET:O	7:D:310:HOH:O	2.12	0.67
1:C:314:ALA:O	7:C:518:HOH:O	2.13	0.66
2:F:65:ARG:O	7:F:310:HOH:O	2.13	0.65
1:A:75:ASN:O	7:A:560:HOH:O	2.13	0.65
2:F:159:ALA:HB3	2:F:166:THR:HG22	1.78	0.65
1:A:293:ASP:O	7:A:534:HOH:O	2.15	0.64
1:A:312:GLU:OE2	7:A:566:HOH:O	2.16	0.63
4:E:411:NAG:H3	4:E:411:NAG:H83	1.82	0.62
1:E:217:ASN:ND2	1:E:251:VAL:O	2.33	0.61
2:D:79:GLU:OE1	7:D:304:HOH:O	2.17	0.61
2:D:14:TRP:CE2	2:D:25:THR:HG21	2.36	0.60
2:D:25:THR:HG22	2:D:34:VAL:HG22	1.83	0.58
4:C:414:NAG:H62	4:C:415:NAG:H82	1.85	0.58
2:F:25:THR:HG22	2:F:34:VAL:HG22	1.86	0.58
1:C:125:ILE:HD12	1:C:269:PRO:HG2	1.87	0.57
1:E:17:LYS:HG2	1:E:23:GLU:HG2	1.85	0.57
4:C:415:NAG:H83	4:C:415:NAG:H3	1.88	0.56
1:E:332:ASN:HA	2:F:48:ILE:HD13	1.88	0.56
1:E:160:ILE:HD11	3:E:401:SIA:H111	1.90	0.54
1:E:33:THR:HG22	1:E:308:TYR:HB2	1.89	0.53
1:E:34:THR:HG23	1:E:306:LYS:HG3	1.90	0.53
2:D:168:ASP:N	2:D:168:ASP:OD1	2.38	0.53
1:A:30:ILE:HG13	1:A:332:ASN:HB2	1.92	0.52
1:E:160:ILE:CD1	3:E:401:SIA:H111	2.39	0.52
1:A:49:THR:HG23	1:A:81:VAL:HG12	1.91	0.52
4:C:414:NAG:H2	7:C:504:HOH:O	2.11	0.51
2:B:14:TRP:CE2	2:B:25:THR:HG21	2.46	0.51
1:C:259:THR:N	7:C:551:HOH:O	2.43	0.50
1:C:217:ASN:ND2	1:C:251:VAL:O	2.45	0.50
1:C:17:LYS:HG2	1:C:23:GLU:HG2	1.94	0.50
2:B:88:ARG:HD3	7:B:303:HOH:O	2.13	0.49
1:E:7:ILE:HG13	2:F:115:LEU:HD21	1.94	0.49
2:F:120:ARG:O	7:F:312:HOH:O	2.19	0.48
1:A:187:ILE:HB	1:A:273:TRP:HB2	1.95	0.48
1:A:278:ARG:NH2	2:F:79:GLU:HG3	2.29	0.48
1:A:55:PRO:HD2	7:A:560:HOH:O	2.15	0.47
1:A:217:ASN:ND2	1:A:251:VAL:O	2.47	0.47
1:A:202:ARG:NH2	3:A:401:SIA:O7	2.47	0.47
1:C:332:ASN:HA	2:D:48:ILE:HD13	1.97	0.47
1:A:332:ASN:HA	2:B:48:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:HIS:CD2	1:C:86:GLU:HG3	2.51	0.46
1:E:49:THR:HG23	1:E:81:VAL:HG12	1.97	0.46
1:C:305:SER:O	7:C:524:HOH:O	2.21	0.46
1:C:34:THR:HG23	1:C:306:LYS:HG3	1.98	0.46
1:C:7:ILE:HG13	2:D:115:LEU:HD21	1.98	0.46
1:A:114:TYR:CG	1:A:275:ALA:HB1	2.52	0.45
1:C:30:ILE:HG13	1:C:332:ASN:HB2	1.99	0.45
1:A:34:THR:HG23	1:A:306:LYS:HG3	1.99	0.45
1:E:30:ILE:HG13	1:E:332:ASN:HB2	1.99	0.45
1:C:125:ILE:HD11	1:C:176:VAL:HG22	1.99	0.44
1:A:94:CYS:O	1:A:236:ASP:HB2	2.18	0.44
1:E:341:LYS:HB2	1:E:341:LYS:HE3	1.84	0.44
1:E:38:ARG:HG2	1:E:298:LYS:O	2.18	0.44
1:A:33:THR:HG22	1:A:308:TYR:HB2	2.01	0.43
1:A:159:VAL:HG11	1:A:268:LEU:HD12	2.00	0.43
1:C:211:LYS:HG2	1:C:224:VAL:HG22	2.01	0.43
1:E:36:PRO:HB3	1:E:302:LEU:HD22	2.01	0.42
1:C:160:ILE:HD11	3:C:401:SIA:H111	2.00	0.42
1:C:298:LYS:NZ	7:C:559:HOH:O	2.53	0.42
1:E:187:ILE:HB	1:E:273:TRP:HB2	2.00	0.42
1:A:313:HIS:CE1	2:B:89:ALA:HB2	2.54	0.42
1:A:70:PRO:O	1:A:71:LYS:HB2	2.19	0.42
1:C:70:PRO:O	1:C:71:LYS:HB2	2.20	0.42
1:A:83:ILE:HD11	1:A:295:LEU:HD13	2.02	0.42
1:C:130:ALA:HA	1:C:131:PRO:HD3	1.92	0.42
1:E:70:PRO:O	1:E:71:LYS:HB2	2.20	0.42
2:B:167:PHE:N	7:B:306:HOH:O	2.43	0.41
2:D:75:ASP:OD2	1:E:253:LYS:HE3	2.20	0.41
1:A:175:GLU:HG2	1:A:259:THR:HG22	2.02	0.41
1:C:313:HIS:CE1	2:D:89:ALA:HB2	2.56	0.41
5:D:201:NAG:H61	5:D:201:NAG:O3	2.19	0.41
4:E:415:NAG:HO6	2:F:21:TRP:HE1	1.69	0.41
1:A:94:CYS:HA	1:A:142:SER:O	2.21	0.40
1:A:315:LYS:NZ	2:B:85:ASP:OD2	2.39	0.40
1:A:250:MET:HE1	1:A:259:THR:O	2.22	0.40
1:E:94:CYS:HA	1:E:142:SER:O	2.22	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	339/346 (98%)	326 (96%)	13 (4%)	0	100	100
1	C	339/346 (98%)	326 (96%)	13 (4%)	0	100	100
1	E	339/346 (98%)	326 (96%)	13 (4%)	0	100	100
2	B	168/182 (92%)	167 (99%)	1 (1%)	0	100	100
2	D	167/182 (92%)	166 (99%)	1 (1%)	0	100	100
2	F	167/182 (92%)	166 (99%)	1 (1%)	0	100	100
All	All	1519/1584 (96%)	1477 (97%)	42 (3%)	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	293/298 (98%)	293 (100%)	0	100	100
1	C	293/298 (98%)	293 (100%)	0	100	100
1	E	293/298 (98%)	293 (100%)	0	100	100
2	B	137/145 (94%)	137 (100%)	0	100	100
2	D	136/145 (94%)	136 (100%)	0	100	100
2	F	136/145 (94%)	136 (100%)	0	100	100
All	All	1288/1329 (97%)	1288 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	114	HIS
1	C	85	HIS
1	C	154	ASN
2	D	27	HIS
1	E	154	ASN
1	E	217	ASN
1	E	241	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

42 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	SIA	A	401	3	16,20,21	1.03	1 (6%)	18,28,31	1.53	5 (27%)
3	GAL	A	402	3	11,11,12	0.60	0	14,15,17	1.36	2 (14%)
3	NAG	A	403	3	14,14,15	0.20	0	15,19,21	0.31	0
3	GAL	A	404	3	11,11,12	0.89	0	14,15,17	1.92	2 (14%)
3	BGC	A	405	3	12,12,12	0.52	0	17,17,17	0.43	0
4	NAG	A	406	1,4	14,14,15	0.28	0	15,19,21	0.25	0
4	NAG	A	407	4	14,14,15	0.29	0	15,19,21	0.23	0
4	NAG	A	408	1,4	14,14,15	1.03	1 (7%)	15,19,21	2.23	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	409	4	14,14,15	0.28	0	15,19,21	0.25	0
4	NAG	A	411	1,4	14,14,15	0.95	1 (7%)	15,19,21	1.46	1 (6%)
4	NAG	A	412	4	14,14,15	0.40	0	15,19,21	0.46	0
4	NAG	A	413	1,4	14,14,15	0.87	1 (7%)	15,19,21	1.15	1 (6%)
4	NAG	A	414	4	14,14,15	0.27	0	15,19,21	0.35	0
3	SIA	C	401	3	16,20,21	1.34	1 (6%)	18,28,31	1.92	6 (33%)
3	GAL	C	402	3	11,11,12	0.67	0	14,15,17	1.21	2 (14%)
3	NAG	C	403	3	14,14,15	0.60	1 (7%)	15,19,21	1.13	1 (6%)
3	GAL	C	404	3	11,11,12	1.03	1 (9%)	14,15,17	1.22	2 (14%)
3	BGC	C	405	3	12,12,12	0.58	0	17,17,17	0.85	0
4	NAG	C	406	1,4	14,14,15	1.24	1 (7%)	15,19,21	2.05	1 (6%)
4	NAG	C	407	4	14,14,15	0.23	0	15,19,21	0.37	0
6	NAG	C	408	1,6	14,14,15	0.41	0	15,19,21	0.50	0
6	NAG	C	409	6	14,14,15	0.43	0	15,19,21	0.64	0
6	BMA	C	410	6	11,11,12	0.92	1 (9%)	14,15,17	1.12	1 (7%)
4	NAG	C	412	1,4	14,14,15	0.37	0	15,19,21	0.52	0
4	NAG	C	413	4	14,14,15	0.23	0	15,19,21	0.32	0
4	NAG	C	414	1,4	14,14,15	0.59	1 (7%)	15,19,21	0.52	0
4	NAG	C	415	4	14,14,15	0.34	0	15,19,21	1.30	1 (6%)
3	SIA	E	401	3	16,20,21	1.14	1 (6%)	18,28,31	1.62	7 (38%)
3	GAL	E	402	3	11,11,12	0.43	0	14,15,17	1.10	2 (14%)
3	NAG	E	403	3	14,14,15	0.24	0	15,19,21	0.43	0
3	GAL	E	404	3	11,11,12	0.76	0	14,15,17	1.09	1 (7%)
3	BGC	E	405	3	12,12,12	0.59	0	17,17,17	1.61	4 (23%)
4	NAG	E	406	1,4	14,14,15	0.36	0	15,19,21	0.29	0
4	NAG	E	407	4	14,14,15	0.22	0	15,19,21	0.21	0
4	NAG	E	409	1,4	14,14,15	1.21	1 (7%)	15,19,21	1.94	1 (6%)
4	NAG	E	410	4	14,14,15	0.30	0	15,19,21	0.51	0
4	NAG	E	411	1,4	14,14,15	1.52	2 (14%)	15,19,21	1.70	3 (20%)
4	NAG	E	412	4	14,14,15	0.42	0	15,19,21	0.67	1 (6%)
4	NAG	E	413	1,4	14,14,15	0.33	0	15,19,21	0.45	0
4	NAG	E	414	4	14,14,15	0.23	0	15,19,21	0.32	0
4	NAG	E	415	1,4	14,14,15	0.52	0	15,19,21	0.52	0
4	NAG	E	416	4	14,14,15	0.25	0	15,19,21	0.45	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	SIA	A	401	3	-	0/14/34/38	0/1/1/1
3	GAL	A	402	3	-	0/2/19/22	0/1/1/1
3	NAG	A	403	3	-	0/6/23/26	0/1/1/1
3	GAL	A	404	3	-	0/2/19/22	0/1/1/1
3	BGC	A	405	3	-	0/2/22/22	0/1/1/1
4	NAG	A	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	407	4	-	0/6/23/26	0/1/1/1
4	NAG	A	408	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	409	4	-	0/6/23/26	0/1/1/1
4	NAG	A	411	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	412	4	-	0/6/23/26	0/1/1/1
4	NAG	A	413	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	414	4	-	0/6/23/26	0/1/1/1
3	SIA	C	401	3	-	0/14/34/38	0/1/1/1
3	GAL	C	402	3	-	0/2/19/22	0/1/1/1
3	NAG	C	403	3	-	0/6/23/26	0/1/1/1
3	GAL	C	404	3	-	0/2/19/22	0/1/1/1
3	BGC	C	405	3	-	0/2/22/22	0/1/1/1
4	NAG	C	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	407	4	-	0/6/23/26	0/1/1/1
6	NAG	C	408	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	409	6	-	0/6/23/26	0/1/1/1
6	BMA	C	410	6	-	0/2/19/22	0/1/1/1
4	NAG	C	412	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	413	4	-	0/6/23/26	0/1/1/1
4	NAG	C	414	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	415	4	-	0/6/23/26	0/1/1/1
3	SIA	E	401	3	-	0/14/34/38	0/1/1/1
3	GAL	E	402	3	-	0/2/19/22	0/1/1/1
3	NAG	E	403	3	-	0/6/23/26	0/1/1/1
3	GAL	E	404	3	-	0/2/19/22	0/1/1/1
3	BGC	E	405	3	-	0/2/22/22	0/1/1/1
4	NAG	E	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	407	4	-	0/6/23/26	0/1/1/1
4	NAG	E	409	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	410	4	-	0/6/23/26	0/1/1/1
4	NAG	E	411	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	412	4	-	0/6/23/26	0/1/1/1
4	NAG	E	413	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	414	4	-	0/6/23/26	0/1/1/1
4	NAG	E	415	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	416	4	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	411	NAG	O5-C1	-5.02	1.35	1.43
3	E	401	SIA	C5-N5	-2.80	1.41	1.45
3	C	401	SIA	C5-N5	-2.32	1.42	1.45
4	C	414	NAG	O5-C1	-2.01	1.40	1.43
3	A	401	SIA	C10-N5	2.10	1.42	1.34
3	C	403	NAG	O5-C1	2.10	1.47	1.43
4	E	411	NAG	C1-C2	2.13	1.55	1.52
6	C	410	BMA	C1-C2	2.42	1.58	1.52
3	C	404	GAL	C2-C3	2.70	1.56	1.52
4	A	413	NAG	O5-C1	2.97	1.48	1.43
4	A	411	NAG	O5-C1	3.49	1.49	1.43
4	A	408	NAG	O5-C1	3.67	1.49	1.43
4	E	409	NAG	O5-C1	4.43	1.51	1.43
4	C	406	NAG	O5-C1	4.52	1.51	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	SIA	O6-C2-C3	-5.00	100.25	109.86
3	A	401	SIA	O6-C2-C3	-3.71	102.73	109.86
3	E	401	SIA	O6-C2-C3	-3.41	103.29	109.86
4	E	411	NAG	C1-O5-C5	-3.20	108.19	112.25
3	C	401	SIA	C7-C6-C5	-2.96	109.84	114.32
6	C	410	BMA	O2-C2-C3	-2.93	104.22	110.12
3	C	404	GAL	O3-C3-C4	-2.87	103.87	110.34
3	E	401	SIA	C7-C6-C5	-2.77	110.12	114.32
3	A	404	GAL	O3-C3-C4	-2.58	104.54	110.34
3	C	401	SIA	C6-C5-N5	-2.55	106.63	111.07
3	E	401	SIA	C3-C4-C5	-2.51	108.67	111.47
3	E	405	BGC	O5-C1-C2	-2.46	105.88	109.80
3	A	401	SIA	C8-C7-C6	-2.34	108.30	113.01
3	E	401	SIA	C6-C5-N5	-2.26	107.13	111.07
3	C	401	SIA	C9-C8-C7	-2.22	107.27	112.48
3	A	401	SIA	C7-C6-C5	-2.21	110.97	114.32
3	C	401	SIA	C4-C5-N5	-2.18	105.67	110.41
3	E	401	SIA	C8-C7-C6	-2.17	108.64	113.01
3	A	401	SIA	C3-C4-C5	-2.12	109.11	111.47
3	E	404	GAL	O3-C3-C4	-2.10	105.62	110.34
3	E	401	SIA	C4-C5-N5	-2.09	105.87	110.41
3	E	401	SIA	O6-C6-C5	2.02	111.79	108.48
3	C	401	SIA	O8-C8-C7	2.03	114.12	109.02
3	E	402	GAL	C1-C2-C3	2.06	111.98	109.54
4	E	411	NAG	C4-C3-C2	2.20	114.65	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	SIA	C11-C10-N5	2.20	120.32	116.11
3	C	402	GAL	C1-O5-C5	2.27	115.13	112.25
4	E	412	NAG	C1-O5-C5	2.43	115.33	112.25
3	A	402	GAL	C1-C2-C3	2.43	112.42	109.54
3	E	405	BGC	C4-C3-C2	2.45	115.36	110.79
3	E	402	GAL	C1-O5-C5	2.47	115.39	112.25
3	C	404	GAL	C1-C2-C3	2.60	112.62	109.54
3	C	402	GAL	C1-C2-C3	2.65	112.67	109.54
3	E	405	BGC	O5-C5-C4	2.83	115.00	109.68
3	A	402	GAL	C1-O5-C5	3.16	116.26	112.25
4	A	413	NAG	C1-O5-C5	3.95	117.25	112.25
3	C	403	NAG	C1-O5-C5	4.15	117.52	112.25
3	E	405	BGC	C3-C4-C5	4.32	117.74	110.20
4	E	411	NAG	C2-N2-C7	4.63	128.98	123.04
4	C	415	NAG	C2-N2-C7	4.75	129.15	123.04
4	A	408	NAG	C2-N2-C7	4.95	129.40	123.04
4	A	411	NAG	C1-O5-C5	5.46	119.17	112.25
3	A	404	GAL	C1-O5-C5	5.86	119.68	112.25
4	A	408	NAG	C1-O5-C5	6.68	120.72	112.25
4	E	409	NAG	C1-O5-C5	7.39	121.63	112.25
4	C	406	NAG	C1-O5-C5	7.80	122.15	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	SIA	1	0
3	C	401	SIA	1	0
4	C	414	NAG	3	0
4	C	415	NAG	2	0
3	E	401	SIA	2	0
4	E	411	NAG	1	0
4	E	415	NAG	1	0

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	410	1	14,14,15	0.52	0	15,19,21	0.93	1 (6%)
5	NAG	B	201	2	14,14,15	1.55	1 (7%)	15,19,21	1.25	1 (6%)
5	NAG	C	411	1	14,14,15	0.79	1 (7%)	15,19,21	0.62	0
5	NAG	D	201	2	14,14,15	1.95	2 (14%)	15,19,21	2.64	1 (6%)
5	NAG	E	408	1	14,14,15	0.79	1 (7%)	15,19,21	0.57	0
5	NAG	F	201	2	14,14,15	0.33	0	15,19,21	0.87	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	410	1	-	0/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	C	411	1	-	0/6/23/26	0/1/1/1
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	NAG	E	408	1	-	0/6/23/26	0/1/1/1
5	NAG	F	201	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	NAG	O5-C1	-5.68	1.34	1.43
5	E	408	NAG	O5-C1	-2.76	1.39	1.43
5	C	411	NAG	O5-C1	-2.70	1.39	1.43
5	D	201	NAG	C1-C2	3.37	1.57	1.52
5	D	201	NAG	O5-C1	6.43	1.54	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	201	NAG	C1-O5-C5	-4.30	106.79	112.25
5	F	201	NAG	C1-O5-C5	2.29	115.16	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	410	NAG	C1-O5-C5	3.37	116.53	112.25
5	D	201	NAG	C1-O5-C5	9.88	124.79	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	201	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, 95^{th} 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	341/346 (98%)	-0.17	1 (0%)	94	95	14, 27, 46, 77	0
1	C	341/346 (98%)	-0.12	3 (0%)	85	86	18, 32, 50, 69	0
1	E	341/346 (98%)	-0.25	3 (0%)	85	86	15, 27, 44, 78	0
2	B	170/182 (93%)	-0.01	4 (2%)	62	62	15, 41, 70, 85	0
2	D	169/182 (92%)	-0.22	1 (0%)	90	91	15, 33, 45, 77	0
2	F	169/182 (92%)	0.02	6 (3%)	46	47	13, 37, 57, 83	0
All	All	1531/1584 (96%)	-0.14	18 (1%)	81	81	13, 31, 53, 85	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	169	SER	5.0
1	C	141	GLY	3.2
1	E	164	ASN	3.0
1	A	239	LEU	2.9
1	C	58	PHE	2.7
2	F	29	ALA	2.7
2	F	28	GLY	2.5
2	B	170	LEU	2.5
2	B	141	LYS	2.4
2	F	162	PHE	2.4
2	B	148	CYS	2.4
2	B	169	SER	2.4
2	F	30	HIS	2.2
2	F	147	THR	2.2
2	D	169	SER	2.2
1	E	341	LYS	2.1
1	C	341	LYS	2.1
1	E	48	GLN	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	C	406	14/15	0.89	0.29	4.99	41,54,65,69	0
4	NAG	E	415	14/15	0.90	0.19	2.78	43,49,57,63	0
4	NAG	A	413	14/15	0.87	0.21	2.53	48,59,72,81	0
4	NAG	C	414	14/15	0.95	0.20	1.92	34,45,59,64	0
4	NAG	A	406	14/15	0.93	0.24	1.76	42,51,63,70	0
4	NAG	A	411	14/15	0.92	0.27	1.45	41,53,64,66	0
3	SIA	A	401	20/21	0.95	0.18	0.89	20,28,36,38	0
3	SIA	C	401	20/21	0.91	0.24	0.66	35,46,52,53	0
6	NAG	C	408	14/15	0.87	0.21	0.57	38,45,54,63	0
4	NAG	C	412	14/15	0.93	0.21	0.44	45,53,62,73	0
4	NAG	E	406	14/15	0.90	0.21	0.17	44,57,65,71	0
4	NAG	E	409	14/15	0.94	0.14	-0.20	33,41,46,51	0
4	NAG	E	413	14/15	0.93	0.18	-0.51	34,45,68,70	0
3	SIA	E	401	20/21	0.96	0.15	-0.55	24,27,31,32	0
4	NAG	A	414	14/15	0.82	0.25	-	60,83,87,87	0
4	NAG	E	407	14/15	0.84	0.36	-	70,77,88,89	0
3	GAL	A	404	11/12	0.78	0.45	-	76,86,96,99	0
4	NAG	C	407	14/15	0.88	0.33	-	68,76,83,85	0
4	NAG	A	409	14/15	0.88	0.37	-	65,75,81,85	0
6	NAG	C	409	14/15	0.88	0.21	-	33,46,59,60	0
3	BGC	C	405	12/12	0.54	0.67	-	83,98,102,102	0
4	NAG	C	415	14/15	0.78	0.25	-	55,70,85,86	0
3	GAL	C	404	11/12	0.72	0.48	-	87,97,104,105	0
3	NAG	C	403	14/15	0.83	0.44	-	69,89,97,100	0
4	NAG	E	410	14/15	0.86	0.18	-	44,58,66,73	0
3	GAL	E	404	11/12	0.84	0.45	-	83,99,104,106	0
3	BGC	A	405	12/12	0.72	0.44	-	71,85,93,96	0
4	NAG	E	416	14/15	0.74	0.30	-	67,75,81,81	0
3	GAL	C	402	11/12	0.94	0.24	-	52,55,63,65	0
4	NAG	E	414	14/15	0.85	0.28	-	64,80,83,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	A	407	14/15	0.86	0.36	-	63,80,86,87	0
4	NAG	A	408	14/15	0.90	0.24	-	40,59,67,67	0
3	BGC	E	405	12/12	0.67	0.53	-	63,91,101,101	0
4	NAG	C	413	14/15	0.91	0.27	-	60,76,90,93	0
3	NAG	A	403	14/15	0.88	0.33	-	61,72,78,79	0
3	NAG	E	403	14/15	0.87	0.29	-	57,74,80,81	0
4	NAG	A	412	14/15	0.74	0.41	-	74,83,93,99	0
6	BMA	C	410	11/12	0.86	0.18	-	39,53,60,63	0
4	NAG	E	411	14/15	0.59	0.32	-	57,67,78,80	0
3	GAL	A	402	11/12	0.93	0.18	-	36,40,49,51	0
3	GAL	E	402	11/12	0.97	0.17	-	31,34,42,42	0
4	NAG	E	412	14/15	0.74	0.42	-	74,84,89,91	0

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, 95^{th} 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	E	408	14/15	0.63	0.31	-	51,82,88,92	0
5	NAG	A	410	14/15	0.87	0.20	-	65,72,82,87	0
5	NAG	B	201	14/15	0.72	0.34	-	91,104,114,115	0
5	NAG	D	201	14/15	0.77	0.33	-	55,67,74,74	0
5	NAG	F	201	14/15	0.86	0.29	-	61,68,74,76	0
5	NAG	C	411	14/15	0.73	0.41	-	77,89,106,108	0

6.5 Other polymers

There are no such residues in this entry.