



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:06 PM GMT

PDB ID : 4BH1
Title : H5 (tyTy) Influenza Virus Haemagglutinin in Complex with Avian Receptor Analogue 3'-SLN
Authors : Xiong, X.; Coombs, P.J.; Martin, S.R.; Liu, J.; Xiao, H.; McCauley, J.W.; Locher, K.; Walker, P.A.; Collins, P.J.; Kawaoka, Y.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2013-03-29
Resolution : 2.15 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

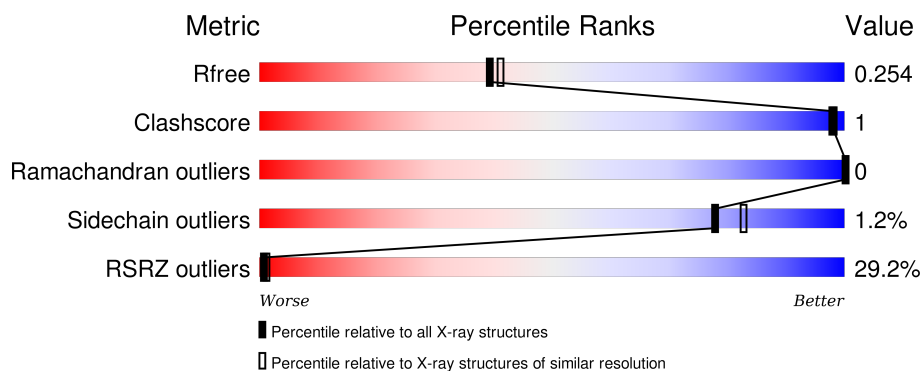
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	326	<div> <div>10%</div> <div>94%</div> <div>• •</div> </div>
1	C	326	<div> <div>18%</div> <div>94%</div> <div>• •</div> </div>
1	E	326	<div> <div>12%</div> <div>93%</div> <div>• •</div> </div>
2	B	166	<div> <div>55%</div> <div>86%</div> <div>• 13%</div> </div>
2	D	166	<div> <div>51%</div> <div>84%</div> <div>• 12%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	166	

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	GAL	A	1322	-	-	-	X
5	PO4	A	1325	-	-	-	X
5	PO4	C	1324	-	-	-	X
5	PO4	E	1324	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11980 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2526	1592	439	481	14			
1	C	319	Total	C	N	O	S	0	0	0
			2519	1587	439	479	14			
1	E	319	Total	C	N	O	S	0	0	0
			2519	1587	439	479	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	ARG	-	EXPRESSION TAG	UNP Q207Z6
A	324	GLU	-	EXPRESSION TAG	UNP Q207Z6
A	325	THR	-	EXPRESSION TAG	UNP Q207Z6
A	326	ARG	-	EXPRESSION TAG	UNP Q207Z6
C	323	ARG	-	EXPRESSION TAG	UNP Q207Z6
C	324	GLU	-	EXPRESSION TAG	UNP Q207Z6
C	325	THR	-	EXPRESSION TAG	UNP Q207Z6
C	326	ARG	-	EXPRESSION TAG	UNP Q207Z6
E	323	ARG	-	EXPRESSION TAG	UNP Q207Z6
E	324	GLU	-	EXPRESSION TAG	UNP Q207Z6
E	325	THR	-	EXPRESSION TAG	UNP Q207Z6
E	326	ARG	-	EXPRESSION TAG	UNP Q207Z6

- Molecule 2 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1129	697	200	224	8			
2	D	146	Total	C	N	O	S	0	0	0
			1130	698	201	223	8			
2	F	145	Total	C	N	O	S	0	0	0
			1129	697	200	224	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	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		

- 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	0	0
			46	25	2	19		
4	C	3	Total	C	N	O	0	0
			46	25	2	19		
4	E	3	Total	C	N	O	0	0
			46	25	2	19		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		

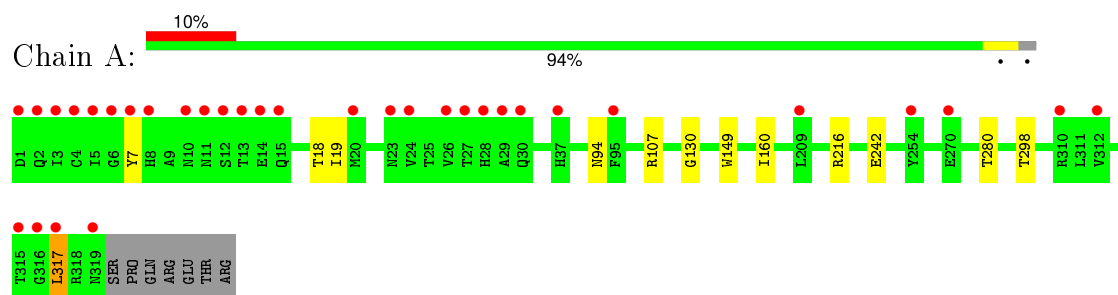
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	266	Total	O	0	0
			266	266		
6	B	36	Total	O	0	0
			36	36		
6	C	243	Total	O	0	0
			243	243		
6	D	35	Total	O	0	0
			35	35		
6	E	218	Total	O	0	0
			218	218		
6	F	30	Total	O	0	0
			30	30		

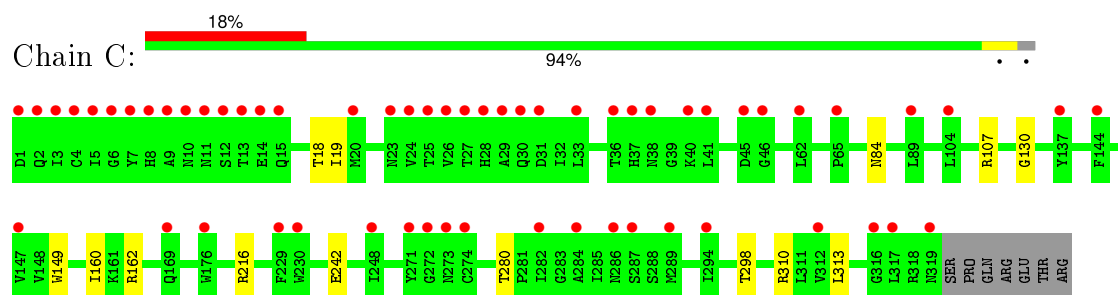
3 Residue-property plots [i](#)

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.

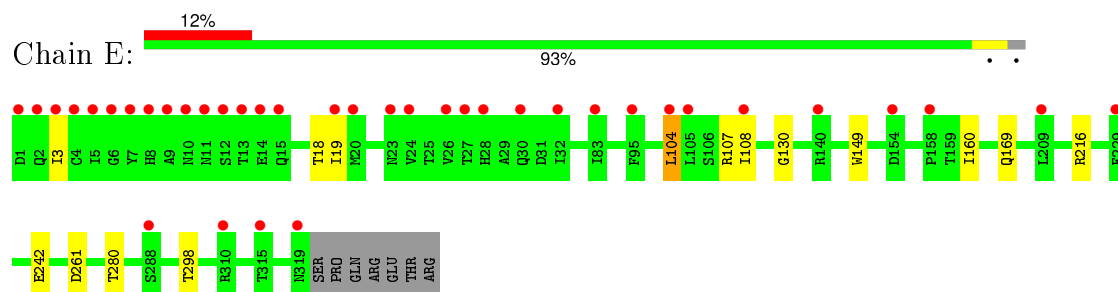
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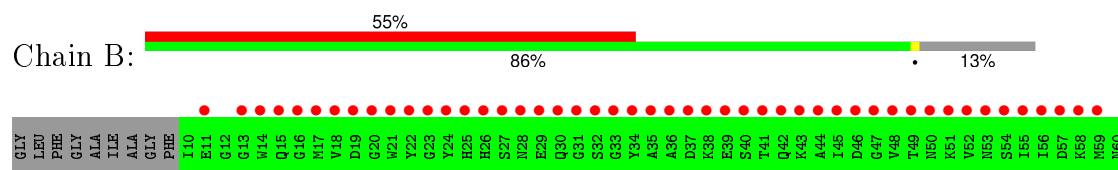
• Molecule 1: HEMAGGLUTININ

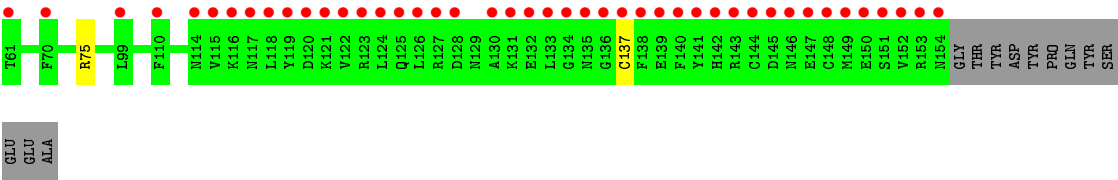


• Molecule 1: HEMAGGLUTININ

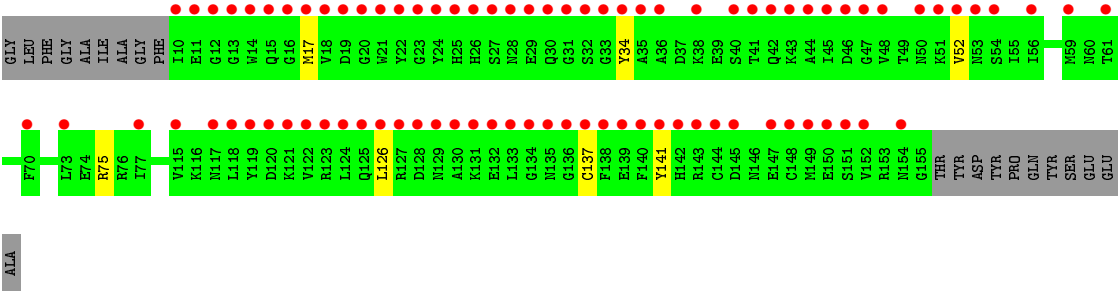
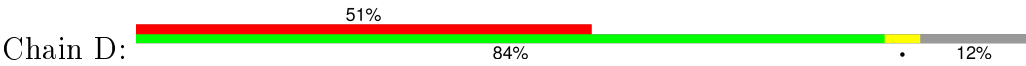


• Molecule 2: HEMAGGLUTININ

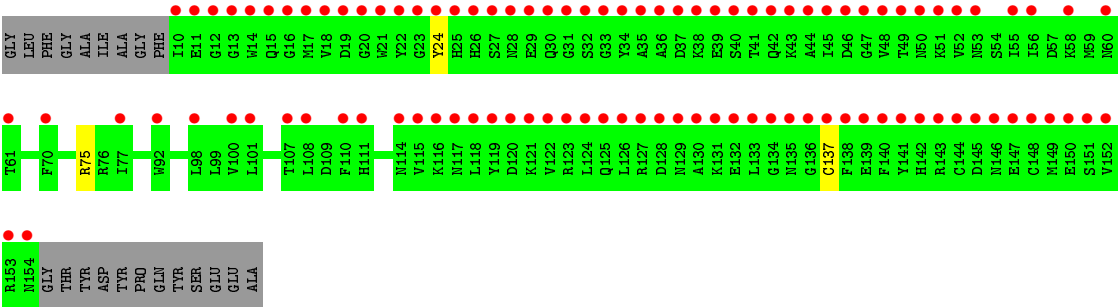
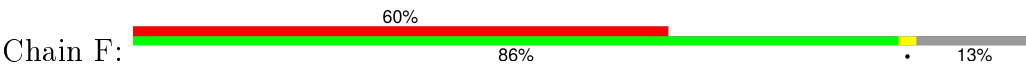




• Molecule 2: HEMAGGLUTININ



• Molecule 2: HEMAGGLUTININ



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.86Å 228.29Å 71.92Å 90.00° 113.71° 90.00°	Depositor
Resolution (Å)	62.48 – 2.15 43.13 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.0 (62.48-2.15) 97.8 (43.13-2.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.224 0.261 , 0.254	Depositor DCC
R_{free} test set	5489 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.9	EDS
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 109591 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11980	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GAL, NAG, SIA

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	0.32	0/2586	0.55	2/3515 (0.1%)
1	C	0.32	0/2579	0.55	2/3506 (0.1%)
1	E	0.31	0/2579	0.55	1/3506 (0.0%)
2	B	0.29	0/1149	0.44	0/1551
2	D	0.30	0/1150	0.44	0/1552
2	F	0.29	0/1149	0.43	0/1551
All	All	0.31	0/11192	0.52	5/15181 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	216	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	C	216	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	216	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	216	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2526	0	2460	7	0
1	C	2519	0	2447	7	0
1	E	2519	0	2447	6	1
2	B	1129	0	1007	1	0
2	D	1130	0	1008	2	0
2	F	1129	0	1007	1	0
3	A	14	0	13	0	0
3	C	14	0	13	0	0
3	E	14	0	13	0	0
4	A	46	0	40	0	0
4	C	46	0	40	0	0
4	E	46	0	40	0	0
5	A	10	0	0	0	0
5	C	5	0	0	0	0
5	E	5	0	0	0	0
6	A	266	0	0	2	1
6	B	36	0	0	0	0
6	C	243	0	0	3	0
6	D	35	0	0	0	0
6	E	218	0	0	0	0
6	F	30	0	0	0	0
All	All	11980	0	10535	22	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (22) 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:C:162:ARG:HD2	6:C:2149:HOH:O	2.03	0.58
1:C:84:ASN:ND2	6:C:2069:HOH:O	2.36	0.57
1:A:7:TYR:HB2	1:A:317:LEU:CD2	2.43	0.48
1:A:130:GLY:HA3	1:A:149:TRP:HB3	1.96	0.47
1:E:130:GLY:HA3	1:E:149:TRP:HB3	1.95	0.47
1:C:130:GLY:HA3	1:C:149:TRP:HB3	1.97	0.47
1:E:280:THR:HG22	1:E:298:THR:HG22	1.98	0.46
1:A:280:THR:HG22	1:A:298:THR:HG22	1.98	0.45
1:E:160:ILE:O	1:E:242:GLU:HA	2.17	0.45
1:C:313:LEU:HD13	2:D:52:VAL:HG12	1.98	0.45
1:A:94:ASN:ND2	6:A:2077:HOH:O	2.45	0.45
1:A:160:ILE:O	1:A:242:GLU:HA	2.17	0.44
1:C:160:ILE:O	1:C:242:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:MET:HG3	2:D:34:TYR:HB3	1.99	0.44
1:A:18:THR:HG22	1:A:19:ILE:N	2.33	0.43
1:C:280:THR:HG22	1:C:298:THR:HG22	1.98	0.43
1:E:18:THR:HG22	1:E:19:ILE:N	2.34	0.43
1:E:3:ILE:HD11	2:F:24:TYR:HB3	2.01	0.42
1:A:94:ASN:HB2	6:A:2078:HOH:O	2.20	0.41
1:C:18:THR:HG22	1:C:19:ILE:N	2.34	0.41
2:B:75:ARG:HG3	6:C:2090:HOH:O	2.20	0.41
1:E:104:LEU:HD13	1:E:108:ILE:HD12	2.02	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:GLN:NE2	6:A:2135:HOH:O[1_655]	2.09	0.11

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	317/326 (97%)	309 (98%)	8 (2%)	0	100	100
1	C	317/326 (97%)	309 (98%)	8 (2%)	0	100	100
1	E	317/326 (97%)	309 (98%)	8 (2%)	0	100	100
2	B	143/166 (86%)	137 (96%)	6 (4%)	0	100	100
2	D	144/166 (87%)	137 (95%)	7 (5%)	0	100	100
2	F	143/166 (86%)	137 (96%)	6 (4%)	0	100	100
All	All	1381/1476 (94%)	1338 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/292 (97%)	282 (99%)	2 (1%)	88	93
1	C	282/292 (97%)	280 (99%)	2 (1%)	88	93
1	E	282/292 (97%)	279 (99%)	3 (1%)	80	85
2	B	113/141 (80%)	112 (99%)	1 (1%)	84	89
2	D	112/141 (79%)	108 (96%)	4 (4%)	42	40
2	F	113/141 (80%)	111 (98%)	2 (2%)	66	71
All	All	1186/1299 (91%)	1172 (99%)	14 (1%)	78	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	317	LEU
2	B	137	CYS
1	C	107	ARG
1	C	310	ARG
2	D	75	ARG
2	D	126	LEU
2	D	137	CYS
2	D	141	TYR
1	E	104	LEU
1	E	107	ARG
1	E	261	ASP
2	F	75	ARG
2	F	137	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	C	2	GLN
2	D	15	GLN

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Mol	Chain	Res	Type
1	E	2	GLN
1	E	87	ASN
1	E	110	HIS

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 ⓘ

9 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	1321	4	16,20,21	0.46	0	18,28,31	1.01	1 (5%)
4	GAL	A	1322	4	11,11,12	0.41	0	14,15,17	1.00	1 (7%)
4	NAG	A	1323	4	15,15,15	0.36	0	17,21,21	0.84	1 (5%)
4	SIA	C	1321	4	16,20,21	0.55	0	18,28,31	1.06	1 (5%)
4	GAL	C	1322	4	11,11,12	0.33	0	14,15,17	1.25	2 (14%)
4	NAG	C	1323	4	15,15,15	0.42	0	17,21,21	0.70	0
4	SIA	E	1321	4	16,20,21	0.35	0	18,28,31	0.96	2 (11%)
4	GAL	E	1322	4	11,11,12	0.25	0	14,15,17	0.91	2 (14%)
4	NAG	E	1323	4	15,15,15	0.37	0	17,21,21	0.88	1 (5%)

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	1321	4	-	0/14/34/38	0/1/1/1
4	GAL	A	1322	4	-	0/2/19/22	0/1/1/1
4	NAG	A	1323	4	-	0/6/26/26	0/1/1/1
4	SIA	C	1321	4	-	0/14/34/38	0/1/1/1
4	GAL	C	1322	4	-	0/2/19/22	0/1/1/1
4	NAG	C	1323	4	-	0/6/26/26	0/1/1/1
4	SIA	E	1321	4	-	0/14/34/38	0/1/1/1
4	GAL	E	1322	4	-	0/2/19/22	0/1/1/1
4	NAG	E	1323	4	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1321	SIA	C6-C5-N5	-2.63	106.48	111.07
4	C	1321	SIA	C6-C5-N5	-2.48	106.75	111.07
4	A	1323	NAG	C3-C2-N2	-2.38	105.74	110.66
4	E	1323	NAG	C3-C2-N2	-2.33	105.83	110.66
4	E	1321	SIA	C6-C5-N5	-2.24	107.16	111.07
4	E	1321	SIA	C4-C5-N5	-2.23	105.56	110.41
4	E	1322	GAL	O3-C3-C2	-2.10	106.20	110.00
4	A	1322	GAL	C1-C2-C3	2.00	111.91	109.54
4	E	1322	GAL	C1-C2-C3	2.04	111.96	109.54
4	C	1322	GAL	C1-O5-C5	2.16	114.99	112.25
4	C	1322	GAL	C1-C2-C3	2.90	112.97	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1320	1	14,14,15	0.45	0	15,19,21	1.37	2 (13%)
5	PO4	A	1324	-	4,4,4	0.41	0	6,6,6	0.27	0
5	PO4	A	1325	-	4,4,4	0.36	0	6,6,6	0.28	0
3	NAG	C	1320	1	14,14,15	0.52	0	15,19,21	1.42	2 (13%)
5	PO4	C	1324	-	4,4,4	0.40	0	6,6,6	0.26	0
3	NAG	E	1320	1	14,14,15	0.36	0	15,19,21	1.07	1 (6%)
5	PO4	E	1324	-	4,4,4	0.49	0	6,6,6	0.27	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	1320	1	-	0/6/23/26	0/1/1/1
5	PO4	A	1324	-	-	0/0/0/0	0/0/0/0
5	PO4	A	1325	-	-	0/0/0/0	0/0/0/0
3	NAG	C	1320	1	-	0/6/23/26	0/1/1/1
5	PO4	C	1324	-	-	0/0/0/0	0/0/0/0
3	NAG	E	1320	1	-	0/6/23/26	0/1/1/1
5	PO4	E	1324	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1320	NAG	C3-C4-C5	-2.15	106.44	110.20
3	C	1320	NAG	C3-C4-C5	-2.09	106.55	110.20
3	E	1320	NAG	C1-O5-C5	2.70	115.68	112.25
3	A	1320	NAG	C1-O5-C5	3.69	116.93	112.25
3	C	1320	NAG	C1-O5-C5	3.86	117.14	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	319/326 (97%)	1.27	33 (10%) 9 14	23, 38, 124, 285	0
1	C	319/326 (97%)	1.29	59 (18%) 2 3	22, 40, 101, 147	0
1	E	319/326 (97%)	1.13	38 (11%) 6 10	24, 41, 129, 233	0
2	B	145/166 (87%)	6.05	92 (63%) 0 0	25, 172, 220, 245	0
2	D	146/166 (87%)	3.73	85 (58%) 0 0	29, 126, 188, 208	0
2	F	145/166 (87%)	5.77	100 (68%) 0 0	24, 166, 204, 226	0
All	All	1393/1476 (94%)	2.47	407 (29%) 1 1	22, 47, 193, 285	0

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	23	GLY	34.5
2	D	138	PHE	34.3
2	B	138	PHE	33.3
2	F	138	PHE	25.0
1	A	3	ILE	24.1
2	D	140	PHE	22.4
2	F	122	VAL	22.3
1	A	4	CYS	21.6
2	B	136	GLY	18.8
1	E	3	ILE	18.7
2	B	33	GLY	18.4
2	F	22	TYR	18.3
2	B	32	SER	18.3
2	B	36	ALA	17.9
2	F	140	PHE	17.6
2	B	21	TRP	17.3
2	B	141	TYR	17.1
1	A	5	ILE	17.0
2	B	35	ALA	16.9

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Mol	Chain	Res	Type	RSRZ
2	F	27	SER	16.4
2	B	26	HIS	16.1
2	F	118	LEU	15.6
2	F	30	GLN	15.3
1	A	2	GLN	15.2
2	F	148	CYS	15.1
2	D	125	GLN	14.9
2	B	22	TYR	14.8
2	F	144	CYS	14.7
2	B	122	VAL	14.3
2	B	152	VAL	13.9
2	B	20	GLY	13.9
2	B	140	PHE	13.8
2	F	31	GLY	13.8
1	E	4	CYS	13.7
2	F	152	VAL	13.6
2	D	127	ARG	13.5
1	A	6	GLY	13.5
2	B	34	TYR	13.5
2	B	137	CYS	13.4
2	F	33	GLY	13.2
2	F	124	LEU	13.0
2	F	26	HIS	12.9
2	B	125	GLN	12.6
2	F	21	TRP	12.6
2	B	146	ASN	12.5
2	B	118	LEU	12.5
2	B	50	ASN	12.3
2	F	133	LEU	12.2
2	B	124	LEU	12.2
2	B	133	LEU	11.5
2	B	17	MET	11.4
2	F	24	TYR	11.3
2	B	126	LEU	11.2
2	B	19	ASP	11.2
2	B	154	ASN	11.2
2	B	24	TYR	10.8
2	B	148	CYS	10.6
2	F	32	SER	10.6
2	B	25	HIS	10.6
2	F	132	GLU	10.5
2	D	30	GLN	10.4

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Mol	Chain	Res	Type	RSRZ
2	F	150	GLU	10.4
2	B	30	GLN	10.4
2	B	16	GLY	10.3
2	F	35	ALA	10.3
2	F	126	LEU	10.3
2	B	14	TRP	10.2
2	D	126	LEU	10.2
2	F	123	ARG	10.2
2	F	146	ASN	10.1
2	D	131	LYS	10.1
2	B	28	ASN	9.9
2	F	125	GLN	9.8
2	D	33	GLY	9.6
2	F	47	GLY	9.5
2	B	27	SER	9.4
2	F	11	GLU	9.4
2	F	40	SER	9.4
2	B	15	GLN	9.4
2	B	147	GLU	9.4
2	B	128	ASP	9.3
1	C	6	GLY	9.2
1	E	2	GLN	9.2
1	A	1	ASP	9.2
2	B	153	ARG	9.2
2	F	44	ALA	9.1
2	F	128	ASP	9.1
2	F	20	GLY	9.0
2	F	137	CYS	9.0
2	F	147	GLU	9.0
2	F	25	HIS	9.0
2	F	154	ASN	9.0
2	F	130	ALA	9.0
2	D	19	ASP	8.9
2	F	149	MET	8.9
2	F	16	GLY	8.9
2	B	145	ASP	8.9
2	F	29	GLU	8.8
2	F	36	ALA	8.8
1	E	7	TYR	8.8
2	D	128	ASP	8.7
1	A	13	THR	8.7
2	F	141	TYR	8.6

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Mol	Chain	Res	Type	RSRZ
2	B	131	LYS	8.6
2	F	45	ILE	8.5
2	B	29	GLU	8.4
2	F	136	GLY	8.4
2	F	120	ASP	8.4
2	B	47	GLY	8.3
2	B	144	CYS	8.3
2	F	50	ASN	8.2
2	D	136	GLY	8.2
2	D	27	SER	8.1
2	D	141	TYR	8.1
2	F	134	GLY	8.1
2	F	18	VAL	7.9
2	F	145	ASP	7.9
2	B	132	GLU	7.9
2	D	26	HIS	7.9
2	F	142	HIS	7.9
2	B	51	LYS	7.8
2	F	14	TRP	7.7
2	B	44	ALA	7.7
2	B	48	VAL	7.7
2	F	42	GLN	7.6
2	F	28	ASN	7.6
1	C	11	ASN	7.4
2	F	23	GLY	7.4
2	B	151	SER	7.4
1	E	12	SER	7.4
2	D	21	TRP	7.4
2	B	121	LYS	7.3
2	D	119	TYR	7.2
2	D	130	ALA	7.2
1	E	1	ASP	7.2
2	F	46	ASP	7.2
2	F	151	SER	7.2
2	B	149	MET	7.2
2	F	127	ARG	7.2
2	D	129	ASN	7.1
2	B	54	SER	7.1
2	B	31	GLY	7.1
2	B	143	ARG	6.9
2	D	47	GLY	6.9
1	E	319	ASN	6.9

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Mol	Chain	Res	Type	RSRZ
2	B	139	GLU	6.9
2	F	34	TYR	6.9
2	B	119	TYR	6.8
2	F	139	GLU	6.7
2	B	40	SER	6.7
2	B	142	HIS	6.7
2	D	143	ARG	6.7
2	D	16	GLY	6.5
1	A	8	HIS	6.5
1	E	27	THR	6.5
2	F	43	LYS	6.5
1	A	11	ASN	6.4
2	D	134	GLY	6.4
2	B	150	GLU	6.4
2	D	52	VAL	6.4
1	C	316	GLY	6.3
2	B	18	VAL	6.3
1	C	3	ILE	6.3
2	F	56	ILE	6.3
2	D	139	GLU	6.2
1	E	11	ASN	6.2
1	E	13	THR	6.2
2	F	17	MET	6.2
2	F	115	VAL	6.1
2	B	120	ASP	6.1
2	D	154	ASN	6.1
2	D	31	GLY	6.1
2	F	51	LYS	6.0
1	C	5	ILE	6.0
1	A	30	GLN	6.0
2	B	117	ASN	5.9
2	B	56	ILE	5.9
2	F	38	LYS	5.9
2	F	10	ILE	5.8
1	C	13	THR	5.8
2	B	38	LYS	5.8
2	D	122	VAL	5.7
2	B	45	ILE	5.7
2	F	19	ASP	5.7
2	D	142	HIS	5.7
2	D	42	GLN	5.7
2	D	118	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
2	B	42	GLN	5.6
2	D	46	ASP	5.6
1	E	6	GLY	5.6
2	D	28	ASN	5.6
2	B	49	THR	5.6
2	D	152	VAL	5.6
2	F	153	ARG	5.6
2	F	116	LYS	5.5
2	D	18	VAL	5.5
1	E	5	ILE	5.5
2	F	131	LYS	5.5
2	B	43	LYS	5.5
2	F	117	ASN	5.4
1	A	317	LEU	5.4
2	B	135	ASN	5.4
2	D	24	TYR	5.4
2	F	110	PHE	5.3
1	E	9	ALA	5.3
1	E	26	VAL	5.3
2	D	36	ALA	5.3
2	B	46	ASP	5.3
1	E	10	ASN	5.3
2	F	48	VAL	5.2
2	B	55	ILE	5.2
2	D	14	TRP	5.2
1	C	12	SER	5.2
1	A	29	ALA	5.2
2	D	56	ILE	5.1
2	D	132	GLU	5.1
1	A	12	SER	5.1
2	D	38	LYS	5.1
1	C	4	CYS	5.0
2	B	127	ARG	4.9
2	D	151	SER	4.9
2	F	119	TYR	4.9
1	A	10	ASN	4.9
2	D	137	CYS	4.9
1	C	28	HIS	4.9
2	D	121	LYS	4.8
1	A	316	GLY	4.8
1	C	9	ALA	4.7
1	A	7	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
2	F	121	LYS	4.7
1	C	7	TYR	4.7
1	E	8	HIS	4.6
1	E	19	ILE	4.6
2	D	23	GLY	4.6
1	E	28	HIS	4.5
1	C	294	ILE	4.5
2	D	15	GLN	4.4
2	F	41	THR	4.4
2	F	135	ASN	4.4
1	E	20	MET	4.4
2	D	150	GLU	4.4
2	B	52	VAL	4.3
2	D	50	ASN	4.3
2	D	20	GLY	4.3
2	F	52	VAL	4.3
1	A	27	THR	4.3
2	F	61	THR	4.2
2	B	11	GLU	4.2
2	B	123	ARG	4.2
2	F	39	GLU	4.2
1	C	33	LEU	4.2
2	F	55	ILE	4.1
1	E	15	GLN	4.1
1	C	15	GLN	4.1
2	F	15	GLN	4.1
1	C	2	GLN	4.1
2	D	51	LYS	4.0
2	B	134	GLY	4.0
2	F	114	ASN	3.9
2	D	17	MET	3.9
1	C	8	HIS	3.8
2	D	145	ASP	3.8
2	D	29	GLU	3.8
2	F	37	ASP	3.8
1	C	10	ASN	3.8
2	F	129	ASN	3.8
2	D	123	ARG	3.7
2	B	37	ASP	3.7
2	D	35	ALA	3.7
1	C	312	VAL	3.7
2	D	117	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	315	THR	3.6
1	C	27	THR	3.6
2	D	32	SER	3.6
2	F	53	ASN	3.6
2	D	48	VAL	3.5
2	D	115	VAL	3.5
2	D	61	THR	3.5
1	C	229	PHE	3.5
2	D	133	LEU	3.5
1	E	140	ARG	3.5
2	D	43	LYS	3.4
2	F	12	GLY	3.4
2	F	107	THR	3.3
1	C	29	ALA	3.3
2	D	124	LEU	3.3
2	F	13	GLY	3.3
2	D	135	ASN	3.3
2	D	73	LEU	3.2
2	B	59	MET	3.2
1	A	15	GLN	3.2
2	D	59	MET	3.2
1	C	37	HIS	3.2
2	D	41	THR	3.1
1	A	319	ASN	3.1
1	C	14	GLU	3.1
2	D	54	SER	3.1
1	A	312	VAL	3.1
2	F	143	ARG	3.1
1	C	38	ASN	3.1
1	C	40	LYS	3.1
2	D	25	HIS	3.0
2	D	148	CYS	3.0
2	B	53	ASN	3.0
1	C	20	MET	3.0
2	D	77	ILE	3.0
2	D	13	GLY	2.9
1	C	30	GLN	2.9
1	E	104	LEU	2.9
1	C	282	ILE	2.9
2	F	111	HIS	2.9
1	C	46	GLY	2.9
2	D	149	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	114	ASN	2.8
2	B	39	GLU	2.8
2	D	11	GLU	2.8
1	C	144	PHE	2.8
1	C	284	ALA	2.8
1	A	14	GLU	2.8
1	C	1	ASP	2.8
1	E	30	GLN	2.8
2	B	61	THR	2.7
1	A	310	ARG	2.7
2	F	60	ASN	2.7
1	A	315	THR	2.7
2	D	12	GLY	2.7
2	D	147	GLU	2.7
1	E	310	ARG	2.6
1	C	147	VAL	2.6
2	D	70	PHE	2.6
1	E	14	GLU	2.6
1	A	28	HIS	2.6
2	F	101	LEU	2.6
1	E	108	ILE	2.6
1	A	26	VAL	2.6
2	F	100	VAL	2.6
1	C	319	ASN	2.6
1	A	209	LEU	2.6
1	C	272	GLY	2.6
2	B	13	GLY	2.6
1	E	154	ASP	2.6
1	C	273	ASN	2.5
1	C	169	GLN	2.5
2	D	44	ALA	2.5
1	E	24	VAL	2.5
1	C	274	CYS	2.5
2	D	144	CYS	2.5
1	C	271	TYR	2.5
1	A	24	VAL	2.5
2	D	45	ILE	2.5
2	F	98	LEU	2.5
2	D	53	ASN	2.5
2	D	22	TYR	2.4
2	D	34	TYR	2.4
2	D	40	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	62	LEU	2.4
1	C	286	ASN	2.4
1	C	25	THR	2.4
2	B	99	LEU	2.4
1	C	45	ASP	2.4
2	B	41	THR	2.4
2	B	70	PHE	2.4
1	E	23	ASN	2.4
1	E	32	ILE	2.3
2	F	49	THR	2.3
2	F	58	LYS	2.3
2	F	108	LEU	2.3
2	F	77	ILE	2.3
1	C	31	ASP	2.3
2	B	110	PHE	2.3
1	C	289	MET	2.3
2	D	10	ILE	2.3
1	C	317	LEU	2.3
1	C	26	VAL	2.3
2	B	115	VAL	2.3
1	C	176	TRP	2.3
2	F	92	TRP	2.3
1	E	288	SER	2.2
2	F	70	PHE	2.2
2	B	130	ALA	2.2
1	C	137	TYR	2.2
1	E	95	PHE	2.2
1	C	248	ILE	2.2
1	A	20	MET	2.2
1	A	37	HIS	2.2
1	C	41	LEU	2.2
1	A	270	GLU	2.2
2	B	116	LYS	2.2
1	E	83	ILE	2.2
1	E	105	LEU	2.1
2	D	120	ASP	2.1
1	C	104	LEU	2.1
1	A	95	PHE	2.1
1	C	230	TRP	2.1
2	B	57	ASP	2.1
2	B	58	LYS	2.1
1	C	89	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	209	LEU	2.1
1	C	287	SER	2.1
1	C	24	VAL	2.1
1	C	36	THR	2.0
1	E	158	PRO	2.0
1	A	23	ASN	2.0
1	C	23	ASN	2.0
1	C	65	PRO	2.0
1	E	229	PHE	2.0
1	A	254	TYR	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
4	GAL	A	1322	11/12	0.83	0.16	2.71	30,36,37,40	0
4	SIA	E	1321	20/21	0.91	0.13	-0.26	34,40,46,46	0
4	SIA	C	1321	20/21	0.90	0.13	-1.60	23,25,29,30	0
4	SIA	A	1321	20/21	0.91	0.12	-1.74	26,31,33,34	0
4	GAL	E	1322	11/12	0.90	0.11	-2.16	47,50,54,56	0
4	NAG	A	1323	15/15	0.87	0.20	-	46,56,64,66	0
4	NAG	C	1323	15/15	0.84	0.26	-	43,56,66,68	0
4	GAL	C	1322	11/12	0.88	0.13	-	28,32,34,36	0
4	NAG	E	1323	15/15	0.88	0.26	-	62,73,76,78	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
5	PO4	E	1324	5/5	0.85	0.38	10.54	64,71,74,75	0
5	PO4	A	1325	5/5	0.77	0.39	9.88	66,71,78,80	0
5	PO4	C	1324	5/5	0.83	0.34	6.55	53,65,67,67	0
5	PO4	A	1324	5/5	0.93	0.22	1.02	63,63,67,68	0
3	NAG	C	1320	14/15	0.83	0.16	0.12	37,40,47,49	0
3	NAG	E	1320	14/15	0.88	0.15	-0.11	35,37,46,50	0
3	NAG	A	1320	14/15	0.89	0.15	-	36,39,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.