Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:39 PM GMT

PDB ID	:	3UBE
Title	:	Influenza hemagglutinin from the 2009 pandemic in complex with ligand LSTc
Authors	:	Xu, R.; Wilson, I.A.
Deposited on	:	2011-10-24
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 (i) symbol.

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

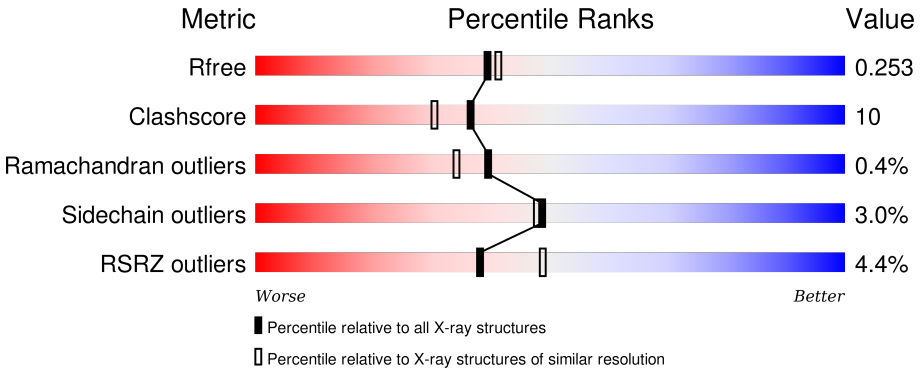
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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 <=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	329	81% 16%
1	C	329	83% 13%
1	E	329	76% 21%
1	G	329	3% 76% 21%
1	I	329	73% 21%

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Mol	Chain	Length	Quality of chain
1	K	329	2% 77% 18%
2	B	177	3% 78% 19%
2	D	177	16% 68% 26%
2	F	177	13% 73% 22%
2	H	177	15% 69% 27%
2	J	177	3% 67% 26% 5%
2	L	177	3% 80% 16%

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	336	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24588 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2522	1595	432	482	13			
1	C	320	Total	C	N	O	S	0	0	0
			2501	1582	429	477	13			
1	E	323	Total	C	N	O	S	0	0	0
			2522	1595	432	482	13			
1	G	321	Total	C	N	O	S	0	0	0
			2508	1586	430	479	13			
1	I	319	Total	C	N	O	S	0	0	0
			2495	1579	428	475	13			
1	K	320	Total	C	N	O	S	0	0	0
			2497	1581	429	474	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
A	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
A	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
A	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
C	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
C	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
C	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
C	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
E	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
E	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
E	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
E	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
G	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
G	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
G	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
G	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
I	9	PRO	-	EXPRESSION TAG	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
I	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
I	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
K	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
K	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
K	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
K	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1405	881	237	281	6			
2	D	171	Total	C	N	O	S	0	0	0
			1380	866	234	274	6			
2	F	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	H	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	J	169	Total	C	N	O	S	0	0	0
			1360	855	229	270	6			
2	L	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	EXPRESSION TAG	UNP C3W5S1
B	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
B	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
D	175	SER	-	EXPRESSION TAG	UNP C3W5S1
D	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
D	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
F	175	SER	-	EXPRESSION TAG	UNP C3W5S1
F	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
F	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
H	175	SER	-	EXPRESSION TAG	UNP C3W5S1
H	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
H	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
J	175	SER	-	EXPRESSION TAG	UNP C3W5S1
J	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
J	177	ARG	-	EXPRESSION TAG	UNP C3W5S1

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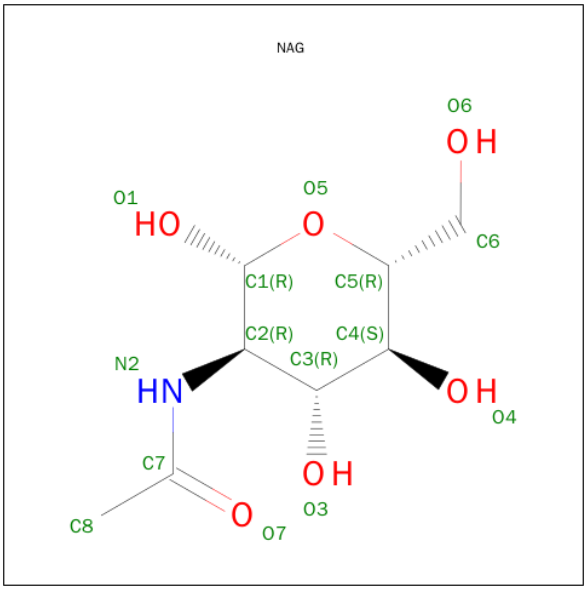
Chain	Residue	Modelled	Actual	Comment	Reference
L	175	SER	-	EXPRESSION TAG	UNP C3W5S1
L	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
L	177	ARG	-	EXPRESSION TAG	UNP C3W5S1

- 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
			57	31	2	24		
3	C	4	Total	C	N	O	0	0
			57	31	2	24		
3	K	4	Total	C	N	O	0	0
			57	31	2	24		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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	C	1	Total	C	N	O	0	0
			14	8	1	5		

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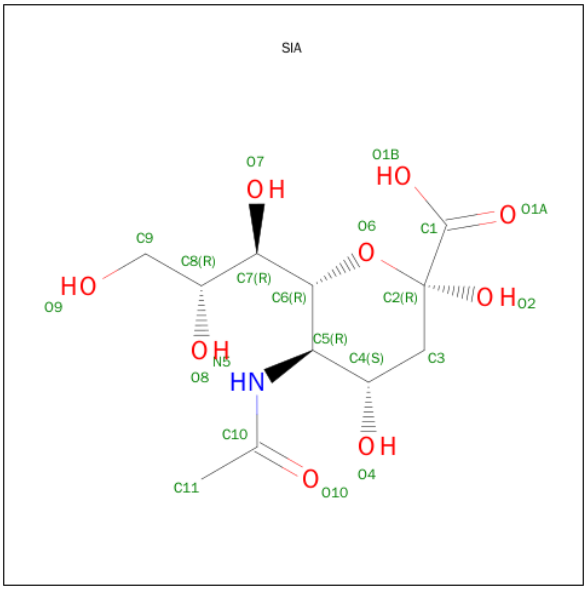
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0
4	K	1	Total C N O 14 8 1 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	3	Total C N O 45 25 2 18	0	0
5	I	3	Total C N O 45 25 2 18	0	0

- Molecule 6 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C N O 20 11 1 8	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	2	Total C N O 28 16 2 10	0	0

- Molecule 8 is water.

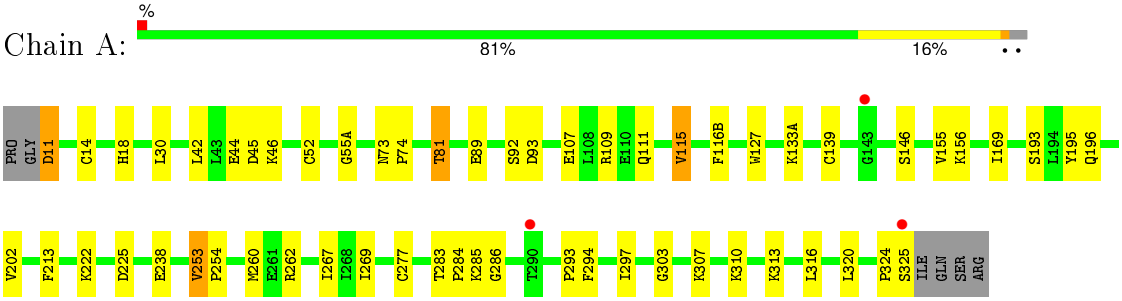
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	99	Total O 99 99	0	0
8	B	54	Total O 54 54	0	0
8	C	124	Total O 124 124	0	0
8	D	48	Total O 48 48	0	0
8	E	85	Total O 85 85	0	0
8	F	49	Total O 49 49	0	0
8	G	105	Total O 105 105	0	0
8	H	45	Total O 45 45	0	0
8	I	90	Total O 90 90	0	0
8	J	50	Total O 50 50	0	0
8	K	71	Total O 71 71	0	0
8	L	58	Total O 58 58	0	0

3 Residue-property plots

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.

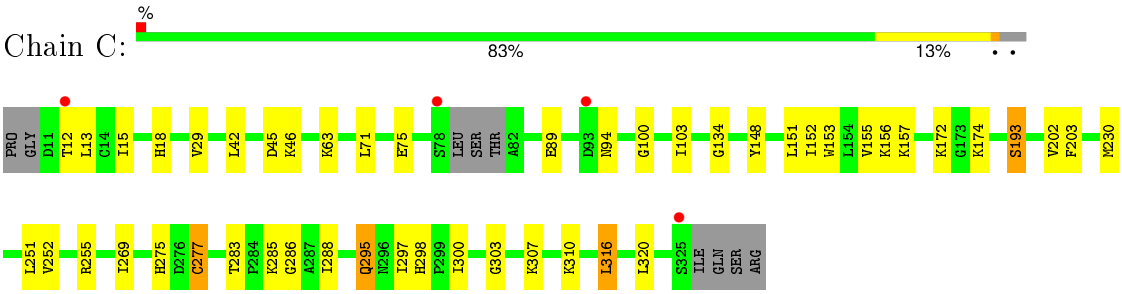
- Molecule 1: Hemagglutinin HA1

Chain A:



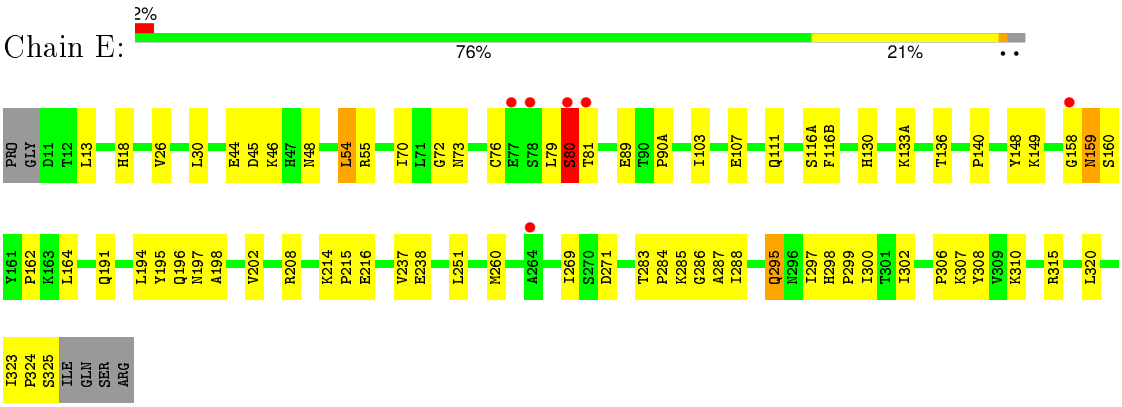
- Molecule 1: Hemagglutinin HA1

Chain C:



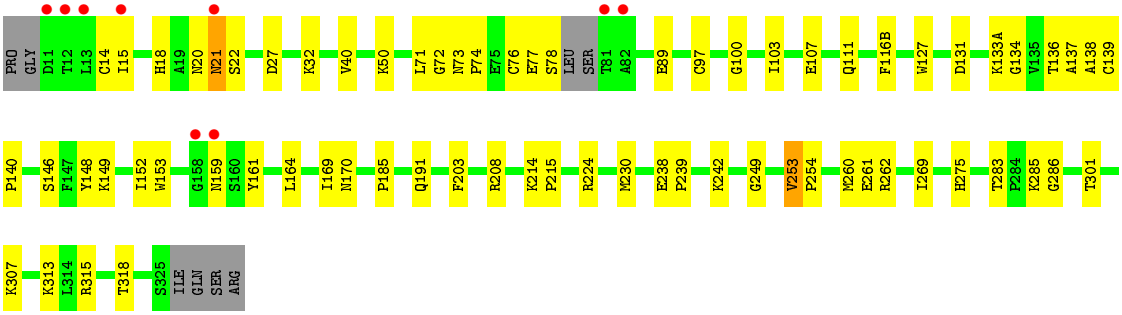
- Molecule 1: Hemagglutinin HA1

Chain E:



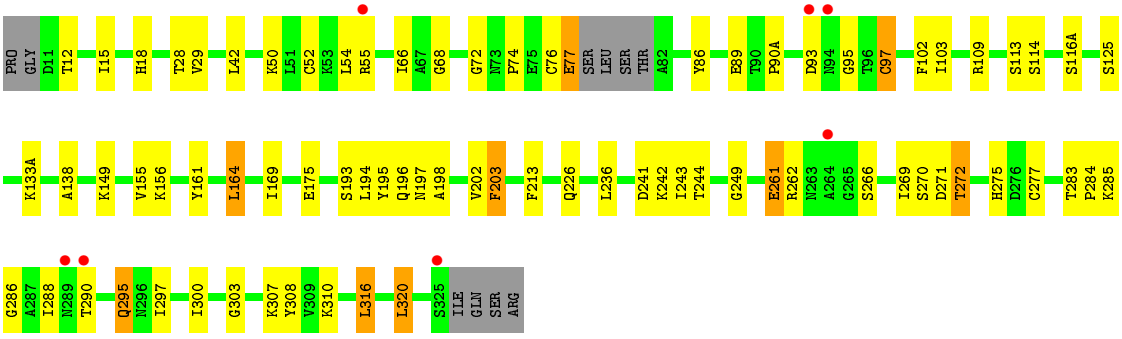
- Molecule 1: Hemagglutinin HA1

Chain G:



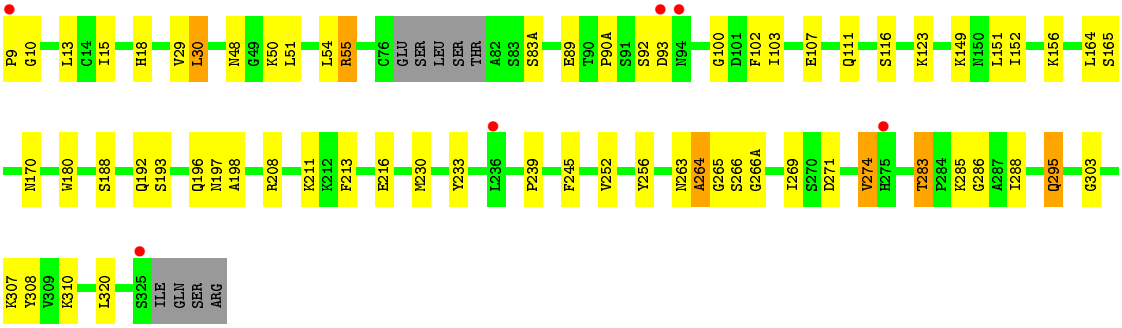
• Molecule 1: Hemagglutinin HA1

Chain I:



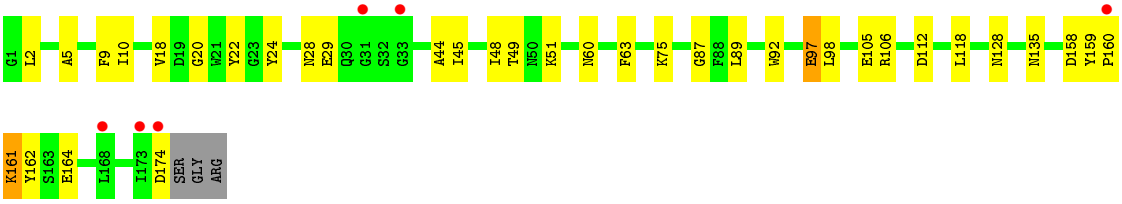
• Molecule 1: Hemagglutinin HA1

Chain K:



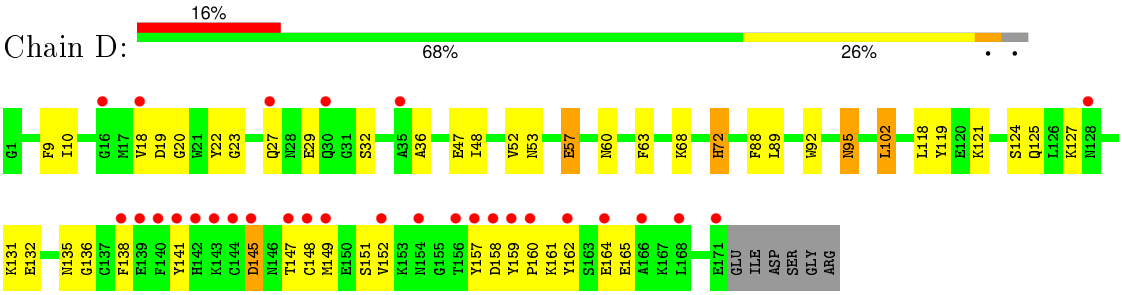
• Molecule 2: Hemagglutinin HA2

Chain B:



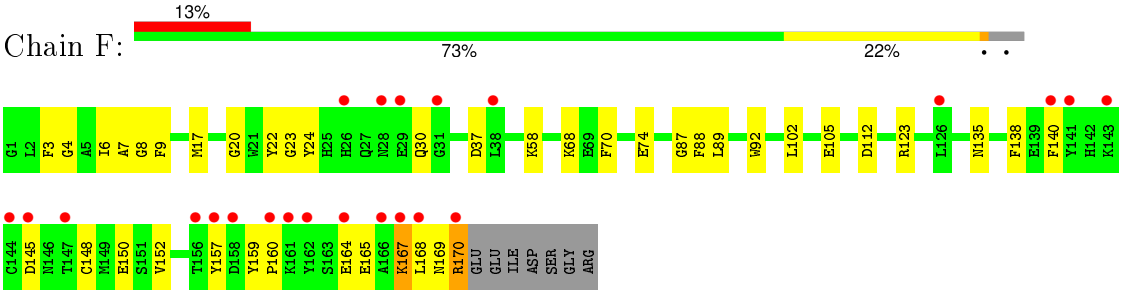
• Molecule 2: Hemagglutinin HA2

Chain D:



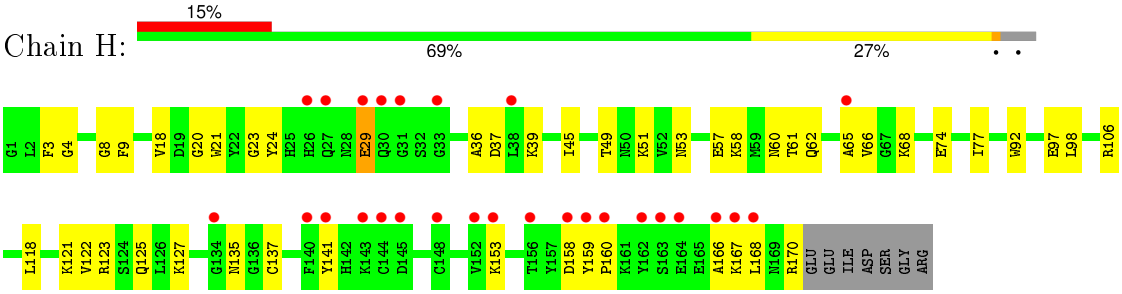
- Molecule 2: Hemagglutinin HA2

Chain F:



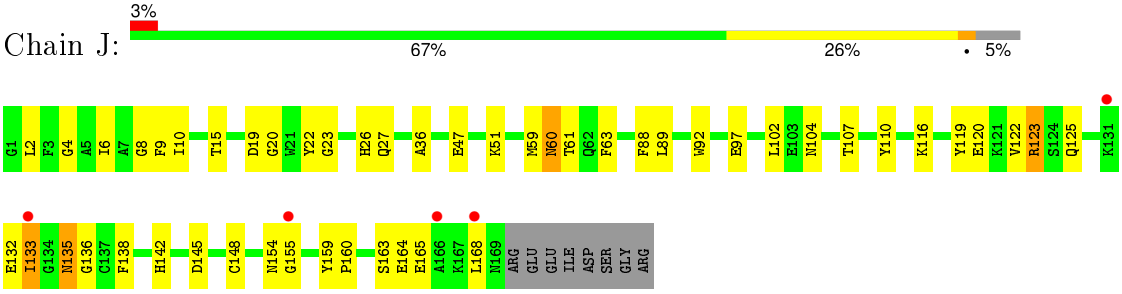
- Molecule 2: Hemagglutinin HA2

Chain H:



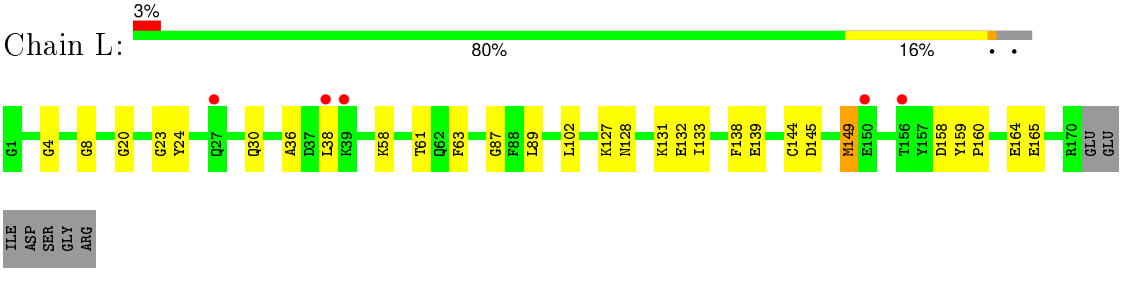
- Molecule 2: Hemagglutinin HA2

Chain J:



- Molecule 2: Hemagglutinin HA2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.78Å 116.59Å 118.72Å 60.86° 77.29° 80.71°	Depositor
Resolution (Å)	49.54 – 2.15 49.54 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.4 (49.54-2.15) 79.4 (49.54-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.193 , 0.252 0.192 , 0.253	Depositor DCC
R_{free} test set	7691 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 153138 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24588	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: SIA, GAL, 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	0.27	0/2586	0.46	0/3516
1	C	0.26	0/2564	0.46	0/3484
1	E	0.26	0/2586	0.47	0/3516
1	G	0.26	0/2571	0.45	0/3494
1	I	0.25	0/2558	0.46	0/3476
1	K	0.26	0/2561	0.47	0/3480
2	B	0.25	0/1433	0.40	0/1931
2	D	0.26	0/1408	0.41	0/1897
2	F	0.25	0/1399	0.40	0/1885
2	H	0.25	0/1399	0.41	0/1885
2	J	0.25	0/1388	0.42	0/1871
2	L	0.26	0/1399	0.40	0/1885
All	All	0.26	0/23852	0.44	0/32320

There are no bond length outliers.

There are no bond angle outliers.

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	2522	0	2465	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2501	0	2443	32	0
1	E	2522	0	2467	63	0
1	G	2508	0	2450	49	0
1	I	2495	0	2439	67	0
1	K	2497	0	2443	50	0
2	B	1405	0	1324	28	0
2	D	1380	0	1303	40	0
2	F	1371	0	1297	28	0
2	H	1371	0	1297	50	0
2	J	1360	0	1283	42	0
2	L	1371	0	1297	23	0
3	A	57	0	49	1	0
3	C	57	0	49	0	0
3	K	57	0	49	0	0
4	A	42	0	39	1	0
4	C	14	0	13	1	0
4	E	14	0	13	1	0
4	J	14	0	13	0	0
4	K	14	0	13	0	0
5	E	45	0	38	1	0
5	I	45	0	38	0	0
6	G	20	0	17	0	0
7	G	28	0	25	0	0
8	A	99	0	0	2	0
8	B	54	0	0	3	0
8	C	124	0	0	2	0
8	D	48	0	0	0	0
8	E	85	0	0	1	0
8	F	49	0	0	0	0
8	G	105	0	0	0	0
8	H	45	0	0	1	0
8	I	90	0	0	0	0
8	J	50	0	0	1	0
8	K	71	0	0	3	0
8	L	58	0	0	1	0
All	All	24588	0	22864	443	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 10.

All (443) 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:J:59:MET:HA	2:J:60:ASN:CB	1.77	1.11
2:J:59:MET:CA	2:J:60:ASN:HB2	1.82	1.09
1:E:79:LEU:HA	1:E:80:SER:HB3	1.13	1.08
1:E:79:LEU:CA	1:E:80:SER:HB3	1.88	1.03
1:C:283:THR:HG22	1:C:285:LYS:H	1.27	0.99
1:I:283:THR:HG22	1:I:285:LYS:H	1.29	0.95
1:E:79:LEU:HA	1:E:80:SER:CB	1.99	0.93
2:H:58:LYS:HD2	2:J:97:GLU:HG2	1.52	0.92
1:E:298:HIS:HD2	1:E:300:ILE:H	1.13	0.89
2:H:53:ASN:O	2:H:57:GLU:HG2	1.71	0.89
1:G:283:THR:HG22	1:G:285:LYS:H	1.38	0.87
2:B:97:GLU:HG2	2:F:58:LYS:HD2	1.56	0.86
1:E:283:THR:HG22	1:E:285:LYS:H	1.40	0.85
1:I:270:SER:OG	1:I:272:THR:HG23	1.77	0.83
2:H:45:ILE:O	2:H:49:THR:HG23	1.80	0.82
1:G:283:THR:HB	1:G:286:GLY:O	1.81	0.81
1:C:283:THR:HB	1:C:286:GLY:O	1.79	0.81
1:E:283:THR:HB	1:E:286:GLY:O	1.80	0.81
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.62	0.80
1:E:72:GLY:HA3	1:E:149:LYS:H	1.44	0.80
1:A:283:THR:HB	1:A:286:GLY:O	1.81	0.80
2:H:97:GLU:HG2	2:L:58:LYS:HD2	1.65	0.79
2:J:59:MET:HA	2:J:60:ASN:HB2	0.87	0.77
2:H:62:GLN:HE21	1:I:310:LYS:NZ	1.81	0.77
1:A:283:THR:HG22	1:A:285:LYS:H	1.49	0.76
2:L:30:GLN:OE1	2:L:145:ASP:HB2	1.85	0.76
1:I:283:THR:HB	1:I:286:GLY:O	1.86	0.75
2:J:9:PHE:O	2:J:135:ASN:HA	1.87	0.74
1:K:211:LYS:HD3	1:K:213:PHE:CZ	2.23	0.73
2:D:149:MET:O	2:D:152:VAL:HG22	1.90	0.72
1:E:208:ARG:NH2	1:E:238:GLU:H	1.87	0.72
1:K:283:THR:CG2	1:K:285:LYS:H	2.03	0.71
1:E:160:SER:O	1:E:162:PRO:HD3	1.91	0.71
2:H:62:GLN:HE21	1:I:310:LYS:HZ3	1.40	0.68
1:C:12:THR:OG1	2:D:27:GLN:HG2	1.94	0.68
1:I:236:LEU:HD13	1:I:262:ARG:NH1	2.08	0.68
1:E:310:LYS:HG2	2:F:89:LEU:HD11	1.76	0.67
1:I:303:GLY:HA2	2:J:63:PHE:CE1	2.29	0.67
1:K:283:THR:HG22	1:K:285:LYS:H	1.58	0.67
2:L:127:LYS:HG3	2:L:128:ASN:H	1.60	0.67
2:H:123:ARG:HH12	2:J:123:ARG:HH21	1.43	0.67
1:E:158:GLY:O	1:E:159:ASN:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:VAL:HG11	1:E:251:LEU:HD13	1.79	0.65
2:L:144:CYS:SG	2:L:149:MET:HE3	2.37	0.65
2:J:47:GLU:HB3	1:K:30:LEU:HG	1.79	0.64
1:E:298:HIS:CD2	1:E:300:ILE:H	2.05	0.64
1:E:283:THR:HG22	1:E:285:LYS:N	2.13	0.63
1:K:211:LYS:HD3	1:K:213:PHE:CE1	2.34	0.63
1:E:26:VAL:HG12	1:E:315:ARG:HG3	1.80	0.62
2:B:60:ASN:HB3	8:B:749:HOH:O	1.98	0.62
1:I:116(A):SER:HB3	1:I:261:GLU:HG2	1.80	0.62
2:D:47:GLU:HB3	1:E:30:LEU:HG	1.80	0.62
2:D:27:GLN:HA	2:D:32:SER:HB3	1.81	0.62
1:G:77:GLU:O	1:G:78:SER:HB3	2.00	0.62
1:K:48:ASN:O	1:K:50:LYS:HG3	2.00	0.61
2:B:45:ILE:O	2:B:49:THR:HG23	2.00	0.61
1:K:288:ILE:HD12	1:K:295:GLN:HG3	1.82	0.61
1:I:18:HIS:HB2	2:J:20:GLY:O	2.00	0.61
1:E:72:GLY:HA3	1:E:149:LYS:N	2.16	0.61
2:H:167:LYS:HG3	2:H:170:ARG:NH1	2.15	0.61
1:I:283:THR:HG23	1:I:284:PRO:HD2	1.81	0.61
1:E:208:ARG:HH22	1:E:238:GLU:H	1.49	0.61
1:A:222:LYS:HD3	1:A:225:ASP:HA	1.83	0.60
2:H:167:LYS:HG3	2:H:170:ARG:HH12	1.66	0.60
1:A:310:LYS:HG3	2:B:89:LEU:HD11	1.82	0.60
2:D:158:ASP:OD2	2:D:160:PRO:HD2	2.01	0.60
1:C:18:HIS:HB2	2:D:20:GLY:O	2.01	0.60
1:I:74:PRO:HB3	1:I:149:LYS:HE3	1.83	0.60
2:B:161:LYS:HE3	2:B:162:TYR:CZ	2.37	0.60
1:C:13:LEU:HD22	2:D:152:VAL:HG21	1.84	0.59
1:C:42:LEU:HD11	1:C:316:LEU:HG	1.83	0.59
1:A:55(A):GLY:HA3	4:A:336:NAG:H83	1.85	0.59
1:E:140:PRO:HD2	4:E:333:NAG:H83	1.83	0.59
2:H:123:ARG:HH12	2:J:123:ARG:NH2	2.00	0.58
2:H:123:ARG:HH22	2:J:123:ARG:NH2	1.99	0.58
2:F:30:GLN:HE21	2:F:145:ASP:HB2	1.69	0.58
1:E:90(A):PRO:HD2	1:E:271:ASP:OD1	2.02	0.58
2:D:158:ASP:OD1	2:D:161:LYS:HB2	2.02	0.58
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.86	0.58
1:I:42:LEU:HD11	1:I:316:LEU:HG	1.86	0.58
1:I:28:THR:HG22	2:J:104:ASN:HB3	1.86	0.58
2:H:3:PHE:CZ	2:J:2:LEU:HG	2.39	0.58
2:H:125:GLN:O	2:H:127:LYS:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:PHE:O	2:D:135:ASN:HA	2.04	0.57
1:G:283:THR:CG2	1:G:285:LYS:HG2	2.33	0.57
1:G:262:ARG:HG2	1:G:262:ARG:HH11	1.69	0.57
1:C:275:HIS:HB3	8:C:819:HOH:O	2.04	0.57
1:A:42:LEU:HD11	1:A:316:LEU:HD22	1.87	0.57
1:K:283:THR:HG22	1:K:285:LYS:N	2.20	0.57
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.87	0.57
1:I:97:CYS:HB2	1:I:138:ALA:O	2.05	0.57
2:L:4:GLY:O	2:L:8:GLY:HA3	2.05	0.57
1:A:155:VAL:HG12	1:A:156:LYS:N	2.18	0.57
1:E:44:GLU:OE2	1:E:46:LYS:HG2	2.05	0.57
1:K:18:HIS:HB2	2:L:20:GLY:O	2.04	0.57
1:I:307:LYS:HE2	2:J:61:THR:HG22	1.87	0.56
1:E:208:ARG:HH22	1:E:237:VAL:HA	1.69	0.56
2:F:169:ASN:O	2:F:170:ARG:HB2	2.04	0.56
1:I:116(A):SER:HB3	1:I:261:GLU:CG	2.35	0.56
1:G:116(B):PHE:HE1	1:G:260:MET:HE1	1.71	0.56
1:I:288:ILE:HG21	1:I:297:ILE:HD13	1.86	0.56
1:I:89:GLU:O	1:I:269:ILE:HA	2.05	0.56
1:A:253:VAL:HG13	1:A:254:PRO:O	2.06	0.56
1:G:127:TRP:CH2	1:G:253:VAL:HG21	2.41	0.56
2:J:160:PRO:HA	2:J:163:SER:OG	2.06	0.56
2:F:165:GLU:O	2:F:168:LEU:HB2	2.06	0.56
1:A:18:HIS:HB2	2:B:20:GLY:O	2.06	0.56
1:I:283:THR:HG22	1:I:285:LYS:N	2.11	0.55
1:A:283:THR:HG23	1:A:284:PRO:HD2	1.88	0.55
2:L:149:MET:HA	2:L:149:MET:HE2	1.87	0.55
1:G:253:VAL:HG22	1:G:254:PRO:HD2	1.88	0.55
2:F:9:PHE:O	2:F:135:ASN:HA	2.07	0.55
1:C:63:LYS:NZ	1:C:75:GLU:HB3	2.21	0.55
1:E:288:ILE:CD1	1:E:295:GLN:HG3	2.37	0.55
2:H:62:GLN:NE2	1:I:310:LYS:NZ	2.53	0.55
2:L:132:GLU:HG2	2:L:138:PHE:CE2	2.40	0.55
1:K:170:ASN:O	1:K:239:PRO:O	2.25	0.54
1:C:288:ILE:HD13	1:C:295:GLN:HG3	1.88	0.54
2:H:153:LYS:HG2	2:H:153:LYS:O	2.07	0.54
1:A:238:GLU:HG2	8:A:362:HOH:O	2.06	0.54
1:G:169:ILE:HG13	1:G:242:LYS:HG3	1.90	0.54
2:H:4:GLY:O	2:H:8:GLY:HA3	2.08	0.54
2:H:24:TYR:CE1	2:H:153:LYS:HG3	2.43	0.54
1:K:54:LEU:O	1:K:55:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:GLN:NE2	2:F:145:ASP:HB2	2.21	0.54
1:G:18:HIS:HB2	2:H:20:GLY:O	2.08	0.54
2:J:19:ASP:OD2	2:J:36:ALA:HB3	2.08	0.53
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.90	0.53
1:G:214:LYS:HG3	1:G:215:PRO:HD2	1.88	0.53
2:H:24:TYR:CE1	2:H:37:ASP:HB2	2.44	0.53
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.43	0.53
2:D:132:GLU:HG2	2:D:138:PHE:CE2	2.43	0.53
2:H:158:ASP:OD1	2:H:160:PRO:HD2	2.08	0.53
2:B:87:GLY:HA3	2:F:88:PHE:CZ	2.44	0.53
1:G:131:ASP:OD1	1:G:133(A):LYS:HE2	2.08	0.53
2:D:53:ASN:O	2:D:57:GLU:CG	2.57	0.53
2:D:161:LYS:HD2	2:D:162:TYR:CZ	2.43	0.53
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.09	0.53
1:C:310:LYS:HE3	2:D:89:LEU:HD21	1.90	0.52
1:C:151:LEU:HB3	1:C:252:VAL:HG12	1.90	0.52
2:J:164:GLU:O	2:J:168:LEU:HG	2.09	0.52
1:K:310:LYS:HG2	1:K:310:LYS:O	2.09	0.52
2:B:75:LYS:HE3	8:E:562:HOH:O	2.09	0.52
2:F:164:GLU:O	2:F:168:LEU:HD13	2.09	0.52
1:K:307:LYS:HE2	2:L:61:THR:HG22	1.91	0.52
2:D:53:ASN:O	2:D:57:GLU:HG2	2.10	0.52
1:I:284:PRO:HD3	1:I:300:ILE:O	2.11	0.51
1:G:27:ASP:HA	1:G:32:LYS:O	2.10	0.51
2:H:51:LYS:HG3	1:I:29:VAL:HG22	1.92	0.51
1:K:89:GLU:O	1:K:269:ILE:HA	2.09	0.51
1:I:12:THR:OG1	2:J:27:GLN:HB3	2.10	0.51
1:I:72:GLY:O	1:I:149:LYS:HG2	2.10	0.51
1:K:156:LYS:HD2	1:K:196:GLN:HE21	1.76	0.51
1:I:290:THR:HG22	1:I:290:THR:O	2.09	0.51
1:A:81:THR:HG21	8:A:827:HOH:O	2.10	0.51
1:I:52:CYS:HB3	1:I:277:CYS:O	2.10	0.51
2:H:62:GLN:HE21	1:I:310:LYS:HZ2	1.57	0.51
2:L:149:MET:HA	2:L:149:MET:CE	2.41	0.51
1:A:127:TRP:CZ2	1:A:253:VAL:HG11	2.45	0.51
1:E:107:GLU:O	1:E:111:GLN:HG3	2.11	0.51
1:K:164:LEU:HD12	1:K:164:LEU:C	2.31	0.51
1:I:242:LYS:HG2	1:I:243:ILE:N	2.25	0.51
1:K:93:ASP:N	8:K:682:HOH:O	2.44	0.51
2:D:151:SER:OG	2:D:157:TYR:HA	2.12	0.50
1:E:214:LYS:HG3	1:E:215:PRO:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ASP:C	1:C:46:LYS:HD2	2.32	0.50
2:D:19:ASP:HB3	2:D:36:ALA:HB2	1.94	0.50
2:D:124:SER:O	2:D:127:LYS:HE3	2.12	0.50
1:A:155:VAL:CG1	1:A:156:LYS:N	2.75	0.50
2:L:23:GLY:HA3	2:L:36:ALA:HA	1.94	0.50
2:H:23:GLY:HA3	2:H:36:ALA:HA	1.94	0.50
2:L:127:LYS:HG3	2:L:128:ASN:N	2.27	0.50
1:I:133(A):LYS:HG3	1:I:133(A):LYS:O	2.12	0.50
2:B:9:PHE:O	2:B:135:ASN:HA	2.12	0.50
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.92	0.49
1:K:263:ASN:O	1:K:264:ALA:C	2.49	0.49
1:I:236:LEU:HD13	1:I:262:ARG:HH11	1.75	0.49
1:I:155:VAL:HG13	1:I:194:LEU:O	2.12	0.49
1:C:156:LYS:HE2	1:C:193:SER:O	2.11	0.49
1:G:97:CYS:O	1:G:224:ARG:HD3	2.11	0.49
2:F:17:MET:SD	2:F:23:GLY:HA3	2.52	0.49
1:K:54:LEU:C	1:K:55:ARG:HG3	2.33	0.49
2:B:106:ARG:HD3	8:B:190:HOH:O	2.11	0.49
1:G:137:ALA:O	1:G:140:PRO:HD3	2.11	0.49
2:B:2:LEU:HG	2:F:3:PHE:CZ	2.47	0.49
1:K:197:ASN:O	1:K:198:ALA:HB3	2.13	0.49
2:F:70:PHE:HB3	2:F:74:GLU:HB2	1.94	0.49
1:K:151:LEU:HB3	1:K:252:VAL:HG12	1.95	0.49
1:G:283:THR:HG22	1:G:285:LYS:N	2.18	0.49
2:H:168:LEU:HD23	2:H:168:LEU:O	2.11	0.49
2:H:65:ALA:O	2:H:66:VAL:HB	2.13	0.49
1:I:169:ILE:HD13	1:I:242:LYS:HB2	1.93	0.49
1:G:103:ILE:HD12	1:G:103:ILE:N	2.28	0.49
1:G:127:TRP:CZ2	1:G:253:VAL:HG21	2.47	0.49
1:K:303:GLY:HA2	2:L:63:PHE:CE1	2.48	0.49
1:A:109:ARG:HB3	1:A:267:ILE:CD1	2.43	0.49
1:K:308:TYR:CD2	2:L:89:LEU:HD13	2.48	0.49
1:I:164:LEU:C	1:I:164:LEU:HD12	2.33	0.49
2:F:148:CYS:O	2:F:152:VAL:HG23	2.13	0.49
2:H:9:PHE:O	2:H:135:ASN:HA	2.12	0.49
1:E:72:GLY:O	1:E:73:ASN:C	2.52	0.48
1:G:89:GLU:O	1:G:269:ILE:HA	2.13	0.48
1:K:149:LYS:HE2	1:K:256:TYR:CE1	2.48	0.48
1:C:295:GLN:OE1	1:C:297:ILE:N	2.46	0.48
1:E:89:GLU:O	1:E:269:ILE:HA	2.13	0.48
1:G:208:ARG:HG3	1:G:238:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:HIS:HB2	2:F:20:GLY:O	2.13	0.48
1:A:89:GLU:O	1:A:269:ILE:HA	2.13	0.48
2:H:123:ARG:HG2	2:H:123:ARG:HH11	1.77	0.48
1:E:54:LEU:C	1:E:55:ARG:HG2	2.34	0.48
2:J:119:TYR:CE1	2:J:136:GLY:HA2	2.48	0.48
1:E:79:LEU:CB	1:E:80:SER:HB3	2.44	0.48
2:F:4:GLY:O	2:F:8:GLY:HA3	2.14	0.48
1:G:73:ASN:HB3	1:G:76:CYS:SG	2.54	0.48
1:C:203:PHE:HE2	1:E:216:GLU:HB3	1.79	0.48
2:D:95:ASN:HD22	2:D:95:ASN:N	2.10	0.48
2:F:167:LYS:HG2	2:F:168:LEU:N	2.28	0.47
2:J:88:PHE:CZ	2:L:87:GLY:HA3	2.49	0.47
1:I:114:SER:HB2	1:I:266:SER:HB2	1.95	0.47
1:E:208:ARG:NH1	1:E:238:GLU:HG3	2.28	0.47
1:E:116(B):PHE:CE1	1:E:260:MET:HE2	2.50	0.47
1:K:50:LYS:O	1:K:286:GLY:HA2	2.14	0.47
2:L:159:TYR:N	2:L:160:PRO:HD2	2.30	0.47
2:J:4:GLY:O	2:J:8:GLY:HA3	2.13	0.47
2:D:131:LYS:HE3	2:D:141:TYR:OH	2.14	0.47
1:C:298:HIS:CE1	1:C:300:ILE:HB	2.50	0.47
1:A:115:VAL:HG11	1:A:116(B):PHE:HB2	1.96	0.47
1:E:164:LEU:C	1:E:164:LEU:HD12	2.35	0.47
2:J:132:GLU:HG2	2:J:138:PHE:CE2	2.50	0.47
1:G:107:GLU:O	1:G:111:GLN:HG3	2.15	0.47
1:G:15:ILE:HD11	2:H:122:VAL:HG21	1.96	0.47
1:K:283:THR:HG22	1:K:286:GLY:H	1.80	0.47
2:J:15:THR:HG23	8:J:202:HOH:O	2.15	0.47
1:E:54:LEU:O	1:E:55:ARG:HG2	2.15	0.47
1:E:195:TYR:O	1:E:196:GLN:HB3	2.14	0.47
1:C:307:LYS:HG3	2:D:92:TRP:CE2	2.50	0.47
1:E:164:LEU:O	1:E:164:LEU:HD12	2.15	0.46
1:G:97:CYS:HB2	1:G:138:ALA:O	2.14	0.46
1:A:109:ARG:HB3	1:A:267:ILE:HD11	1.97	0.46
1:E:324:PRO:O	1:E:325:SER:C	2.54	0.46
1:G:71:LEU:O	1:G:148:TYR:HB3	2.15	0.46
1:E:283:THR:HG23	1:E:284:PRO:HD2	1.97	0.46
1:K:283:THR:HB	1:K:286:GLY:O	2.15	0.46
1:E:197:ASN:O	1:E:198:ALA:HB3	2.14	0.46
1:C:152:ILE:HD11	1:C:255:ARG:HD2	1.98	0.46
1:I:270:SER:HG	1:I:272:THR:HG23	1.79	0.46
1:E:72:GLY:H	1:E:148:TYR:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:LEU:HB2	2:F:105:GLU:OE1	2.16	0.46
2:F:152:VAL:HA	2:F:157:TYR:HB2	1.96	0.46
1:A:52:CYS:HB3	1:A:277:CYS:O	2.15	0.46
1:A:202:VAL:HB	1:A:213:PHE:HB2	1.98	0.46
1:C:277:CYS:HA	4:C:334:NAG:H82	1.98	0.46
1:K:92:SER:HA	8:K:682:HOH:O	2.15	0.46
2:D:121:LYS:O	2:D:125:GLN:HG3	2.15	0.46
1:I:68:GLY:HA3	1:I:95:GLY:HA2	1.97	0.46
1:K:165:SER:HA	1:K:245:PHE:O	2.16	0.46
1:G:283:THR:CG2	1:G:285:LYS:H	2.18	0.46
1:I:310:LYS:HG2	2:J:89:LEU:HD11	1.98	0.46
1:G:77:GLU:OE1	1:G:77:GLU:HA	2.14	0.46
1:K:90(A):PRO:HD2	1:K:271:ASP:OD1	2.15	0.46
2:J:51:LYS:HG3	1:K:29:VAL:CG2	2.46	0.46
2:L:164:GLU:CD	2:L:165:GLU:H	2.19	0.46
1:I:138:ALA:HB2	1:I:226:GLN:HE21	1.81	0.45
1:C:89:GLU:O	1:C:269:ILE:HA	2.16	0.45
2:B:158:ASP:OD2	2:B:160:PRO:HD2	2.17	0.45
1:I:288:ILE:CG2	1:I:297:ILE:HD13	2.46	0.45
1:K:107:GLU:O	1:K:111:GLN:HG3	2.16	0.45
1:A:30:LEU:HD12	2:B:105:GLU:OE2	2.17	0.45
1:K:266:SER:OG	1:K:266(A):GLY:N	2.48	0.45
2:H:74:GLU:HB3	2:H:77:ILE:HD11	1.99	0.45
1:I:15:ILE:N	1:I:15:ILE:HD12	2.32	0.45
1:A:195:TYR:O	1:A:196:GLN:HB3	2.16	0.45
2:D:29:GLU:OE1	2:D:29:GLU:HA	2.16	0.45
1:C:103:ILE:N	1:C:103:ILE:HD12	2.32	0.45
1:A:324:PRO:O	1:A:325:SER:HB3	2.17	0.45
1:I:295:GLN:O	1:I:308:TYR:HA	2.16	0.45
2:D:132:GLU:HG2	2:D:138:PHE:HE2	1.82	0.45
2:D:164:GLU:HG2	2:D:165:GLU:N	2.32	0.45
1:G:100:GLY:HA3	1:G:230:MET:O	2.17	0.45
1:K:13:LEU:HD11	2:L:24:TYR:HB3	1.99	0.45
1:I:241:ASP:OD1	1:I:242:LYS:N	2.49	0.45
1:A:260:MET:HE2	1:A:262:ARG:HG2	1.98	0.45
2:J:142:HIS:HB2	2:J:165:GLU:CD	2.37	0.45
2:H:51:LYS:HG3	1:I:29:VAL:CG2	2.47	0.44
2:H:62:GLN:NE2	1:I:310:LYS:HZ2	2.15	0.44
1:E:54:LEU:HD11	1:E:302:ILE:HG22	1.98	0.44
1:E:103:ILE:HD12	1:E:103:ILE:N	2.33	0.44
1:I:202:VAL:HB	1:I:213:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:ILE:HD11	2:J:122:VAL:HG21	2.00	0.44
1:I:161:TYR:CZ	1:I:249:GLY:HA2	2.53	0.44
1:A:11:ASP:OD1	2:B:28:ASN:HA	2.16	0.44
2:B:51:LYS:HG3	1:C:29:VAL:CG2	2.47	0.44
1:G:170:ASN:HB3	1:G:239:PRO:O	2.18	0.44
1:I:90(A):PRO:HD2	1:I:271:ASP:CG	2.37	0.44
2:J:125:GLN:OE1	2:J:155:GLY:HA2	2.18	0.44
1:K:103:ILE:HD12	1:K:103:ILE:N	2.32	0.44
1:K:9:PRO:HB2	1:K:10:GLY:H	1.64	0.44
1:K:123:LYS:HG3	1:K:152:ILE:HD13	2.00	0.44
2:L:131:LYS:NZ	2:L:133:ILE:HG22	2.33	0.44
2:D:72:HIS:CD2	2:D:72:HIS:H	2.36	0.44
2:H:141:TYR:CE1	2:H:170:ARG:HG3	2.53	0.43
1:E:295:GLN:O	1:E:308:TYR:HA	2.17	0.43
1:G:40:VAL:HG13	1:G:318:THR:HG21	2.00	0.43
1:A:293:PRO:HG2	1:A:294:PHE:CD2	2.53	0.43
1:A:107:GLU:O	1:A:111:GLN:HG3	2.18	0.43
1:E:133(A):LYS:O	5:E:330:SIA:H113	2.18	0.43
2:H:29:GLU:H	2:H:29:GLU:CD	2.22	0.43
2:H:39:LYS:HD2	2:H:39:LYS:HA	1.73	0.43
1:I:203:PHE:HE2	1:K:216:GLU:HB3	1.83	0.43
1:I:320:LEU:HD13	2:J:6:ILE:HD13	1.99	0.43
2:H:58:LYS:HD2	2:J:97:GLU:CG	2.37	0.43
1:I:68:GLY:CA	1:I:95:GLY:HA2	2.48	0.43
2:H:167:LYS:HE2	2:H:170:ARG:HH12	1.82	0.43
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.53	0.43
2:L:158:ASP:HB2	8:L:714:HOH:O	2.18	0.43
2:J:107:THR:O	2:J:110:TYR:HB3	2.18	0.43
1:G:14:CYS:HA	2:H:137:CYS:HA	1.99	0.43
2:F:123:ARG:HB2	2:F:138:PHE:HZ	1.84	0.43
2:H:21:TRP:CH2	2:H:45:ILE:HD13	2.54	0.43
1:A:156:LYS:HE2	1:A:193:SER:O	2.19	0.43
1:K:51:LEU:HB2	1:K:274:VAL:HA	2.01	0.43
2:B:105:GLU:HA	2:B:105:GLU:OE1	2.18	0.43
1:K:123:LYS:HG3	1:K:152:ILE:CD1	2.49	0.43
2:L:133:ILE:HD13	2:L:139:GLU:HB2	2.01	0.43
1:K:83(A):SER:HB3	1:K:116:SER:O	2.19	0.43
1:G:152:ILE:HB	1:G:253:VAL:HG12	2.01	0.43
1:I:155:VAL:CG1	1:I:156:LYS:N	2.82	0.43
2:D:164:GLU:CD	2:D:164:GLU:H	2.22	0.43
2:D:118:LEU:HA	2:D:118:LEU:HD12	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:ASN:OD1	1:G:21:ASN:N	2.50	0.43
2:H:106:ARG:HD3	8:H:388:HOH:O	2.18	0.43
1:I:50:LYS:NZ	1:I:275:HIS:CG	2.87	0.43
1:I:66:ILE:HD12	1:I:109:ARG:HG2	2.00	0.43
1:A:73:ASN:HA	1:A:74:PRO:HD3	1.94	0.43
1:C:310:LYS:HE2	1:C:310:LYS:HB3	1.62	0.43
2:D:148:CYS:O	2:D:151:SER:HB3	2.19	0.43
2:H:118:LEU:O	2:H:121:LYS:HB3	2.19	0.43
1:A:139:CYS:O	1:A:146:SER:HB3	2.19	0.43
2:H:123:ARG:HG2	2:H:123:ARG:NH1	2.34	0.42
1:I:203:PHE:CE2	1:K:216:GLU:HB3	2.54	0.42
1:G:20:ASN:OD1	1:G:22:SER:HB3	2.19	0.42
1:G:50:LYS:HD2	1:G:275:HIS:CE1	2.54	0.42
1:G:50:LYS:HD2	1:G:275:HIS:ND1	2.33	0.42
1:K:100:GLY:HA3	1:K:230:MET:O	2.19	0.42
2:B:5:ALA:HB3	2:B:112:ASP:OD2	2.19	0.42
1:I:103:ILE:HD12	1:I:103:ILE:N	2.34	0.42
1:G:161:TYR:CZ	1:G:249:GLY:HA2	2.54	0.42
1:I:76:CYS:O	1:I:77:GLU:C	2.58	0.42
1:E:191:GLN:HG2	1:E:198:ALA:HA	2.01	0.42
2:B:159:TYR:HB3	2:B:160:PRO:HD3	2.00	0.42
1:I:197:ASN:O	1:I:198:ALA:HB3	2.19	0.42
1:A:283:THR:HG22	1:A:285:LYS:HG2	2.01	0.42
1:K:283:THR:HG23	1:K:285:LYS:H	1.81	0.42
1:I:175:GLU:OE1	1:I:262:ARG:NH1	2.53	0.42
1:G:116(B):PHE:CE1	1:G:260:MET:HE1	2.51	0.42
2:H:18:VAL:HG12	2:H:18:VAL:O	2.20	0.42
2:F:68:LYS:HA	2:F:68:LYS:HD3	1.89	0.42
2:H:53:ASN:C	2:H:57:GLU:HG2	2.38	0.42
1:G:72:GLY:O	1:G:149:LYS:HG2	2.19	0.42
1:E:79:LEU:HD23	1:E:79:LEU:H	1.84	0.42
1:I:303:GLY:HA2	2:J:63:PHE:CD1	2.55	0.42
1:G:301:THR:O	2:H:65:ALA:O	2.37	0.42
1:C:15:ILE:HD12	1:C:15:ILE:N	2.34	0.42
1:G:283:THR:HG21	1:G:285:LYS:HG2	2.01	0.42
1:E:45:ASP:C	1:E:297:ILE:HD11	2.39	0.42
2:F:24:TYR:CE1	2:F:37:ASP:HB2	2.55	0.42
2:B:49:THR:HG22	8:B:684:HOH:O	2.20	0.42
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.55	0.42
2:D:145:ASP:OD2	2:D:147:THR:HG22	2.19	0.42
1:G:164:LEU:HD23	1:G:164:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:123:ARG:HH22	2:J:123:ARG:HH22	1.63	0.42
2:H:141:TYR:O	2:H:166:ALA:HA	2.20	0.42
1:G:313:LYS:HE2	1:G:313:LYS:HB3	1.82	0.42
1:K:188:SER:O	1:K:192:GLN:HG2	2.20	0.42
1:E:130:HIS:CE1	1:E:162:PRO:HD2	2.55	0.42
2:F:6:ILE:HG13	2:F:112:ASP:HA	2.02	0.42
1:G:307:LYS:HG3	2:H:92:TRP:CE2	2.55	0.42
1:A:313:LYS:HE3	1:A:313:LYS:HB2	1.88	0.42
2:F:159:TYR:N	2:F:160:PRO:HD2	2.34	0.42
2:J:119:TYR:HE1	2:J:136:GLY:HA2	1.84	0.41
1:E:13:LEU:HB2	2:F:140:PHE:HE1	1.85	0.41
1:K:15:ILE:HD12	1:K:15:ILE:N	2.35	0.41
1:C:63:LYS:HZ2	1:C:75:GLU:HB3	1.83	0.41
2:D:131:LYS:HE3	2:D:141:TYR:CZ	2.55	0.41
1:K:180:TRP:CE2	1:K:233:TYR:HB2	2.55	0.41
1:E:73:ASN:HB3	1:E:76:CYS:SG	2.61	0.41
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.55	0.41
1:I:307:LYS:HG3	2:J:92:TRP:CE2	2.55	0.41
2:J:159:TYR:N	2:J:160:PRO:HD2	2.35	0.41
1:E:48:ASN:HD21	1:E:287:ALA:HB3	1.85	0.41
1:C:303:GLY:HA2	2:D:63:PHE:CE1	2.55	0.41
2:J:116:LYS:O	2:J:120:GLU:HG3	2.20	0.41
1:K:208:ARG:HG3	8:K:357:HOH:O	2.20	0.41
2:B:44:ALA:O	2:B:48:ILE:HG12	2.20	0.41
2:B:118:LEU:HD12	2:B:118:LEU:HA	1.92	0.41
2:J:133:ILE:O	2:J:133:ILE:HD12	2.19	0.41
1:E:307:LYS:HG3	2:F:92:TRP:CE2	2.55	0.41
1:E:158:GLY:O	1:E:159:ASN:CB	2.65	0.41
1:E:295:GLN:HB2	1:E:306:PRO:HB2	2.02	0.41
1:K:149:LYS:HE2	1:K:256:TYR:HE1	1.86	0.41
1:E:54:LEU:O	1:E:55:ARG:CG	2.68	0.41
1:G:73:ASN:HA	1:G:74:PRO:HD3	1.92	0.41
2:D:88:PHE:CZ	2:F:87:GLY:HA3	2.55	0.41
1:A:14:CYS:O	2:B:24:TYR:HA	2.20	0.41
2:B:98:LEU:HA	2:B:98:LEU:HD23	1.84	0.41
1:C:202:VAL:HG11	1:C:251:LEU:HD13	2.03	0.41
1:K:156:LYS:HE2	1:K:193:SER:O	2.21	0.41
1:I:169:ILE:HD13	1:I:242:LYS:HG3	2.03	0.41
1:C:100:GLY:HA3	1:C:230:MET:O	2.21	0.41
2:D:48:ILE:O	2:D:52:VAL:HG23	2.20	0.41
1:E:298:HIS:CD2	1:E:299:PRO:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:VAL:O	2:B:18:VAL:HG22	2.21	0.41
2:J:9:PHE:CE1	2:J:10:ILE:HG13	2.56	0.41
1:A:307:LYS:HG3	2:B:92:TRP:CE2	2.55	0.41
1:C:157:LYS:HA	8:C:704:HOH:O	2.21	0.41
2:J:145:ASP:O	2:J:148:CYS:HB3	2.20	0.41
1:E:72:GLY:CA	1:E:149:LYS:H	2.24	0.41
1:I:156:LYS:HE2	1:I:193:SER:O	2.20	0.41
2:L:158:ASP:OD2	2:L:160:PRO:HD2	2.20	0.41
1:G:307:LYS:HE2	2:H:61:THR:HG22	2.03	0.41
1:A:169:ILE:HD12	1:A:169:ILE:N	2.35	0.41
1:G:139:CYS:O	1:G:146:SER:HB3	2.21	0.41
1:I:308:TYR:CD2	2:J:89:LEU:HD13	2.56	0.41
2:H:159:TYR:HB3	2:H:160:PRO:HD3	2.03	0.41
1:I:114:SER:HB2	1:I:266:SER:CB	2.50	0.41
1:A:44:GLU:OE1	1:A:46:LYS:HG2	2.21	0.41
1:A:303:GLY:HA2	2:B:63:PHE:CE1	2.56	0.41
1:I:195:TYR:O	1:I:196:GLN:HB3	2.21	0.41
1:I:86:TYR:HA	1:I:113:SER:O	2.21	0.40
1:E:323:ILE:HD11	2:F:7:ALA:HB2	2.02	0.40
2:D:18:VAL:O	2:D:18:VAL:HG22	2.21	0.40
1:E:72:GLY:O	1:E:149:LYS:HG3	2.21	0.40
2:L:127:LYS:CG	2:L:128:ASN:N	2.84	0.40
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.57	0.40
2:H:98:LEU:HD23	2:H:98:LEU:HA	1.90	0.40
1:A:133(A):LYS:O	3:A:330:SIA:H113	2.21	0.40
1:E:130:HIS:NE2	1:E:162:PRO:HD2	2.37	0.40
2:F:152:VAL:HG22	2:F:157:TYR:CD1	2.56	0.40
1:C:172:LYS:C	1:C:174:LYS:H	2.24	0.40
1:A:45:ASP:C	1:A:297:ILE:HD11	2.41	0.40
2:D:102:LEU:HD12	2:D:102:LEU:HA	1.95	0.40
1:C:71:LEU:O	1:C:148:TYR:HB3	2.21	0.40
1:E:70:ILE:HA	1:E:70:ILE:HD12	1.92	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	321/329 (98%)	303 (94%)	17 (5%)	1 (0%)	46 42
1	C	316/329 (96%)	304 (96%)	11 (4%)	1 (0%)	46 42
1	E	321/329 (98%)	303 (94%)	15 (5%)	3 (1%)	21 13
1	G	317/329 (96%)	299 (94%)	18 (6%)	0	100 100
1	I	315/329 (96%)	297 (94%)	17 (5%)	1 (0%)	46 42
1	K	316/329 (96%)	304 (96%)	10 (3%)	2 (1%)	30 21
2	B	172/177 (97%)	168 (98%)	4 (2%)	0	100 100
2	D	169/177 (96%)	159 (94%)	8 (5%)	2 (1%)	16 9
2	F	168/177 (95%)	155 (92%)	13 (8%)	0	100 100
2	H	168/177 (95%)	155 (92%)	13 (8%)	0	100 100
2	J	167/177 (94%)	157 (94%)	8 (5%)	2 (1%)	16 9
2	L	168/177 (95%)	163 (97%)	5 (3%)	0	100 100
All	All	2918/3036 (96%)	2767 (95%)	139 (5%)	12 (0%)	39 34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	116(A)	SER
1	E	159	ASN
1	A	92	SER
1	E	80	SER
1	I	93	ASP
2	J	60	ASN
1	K	265	GLY
2	D	60	ASN
2	J	135	ASN
1	K	264	ALA
1	C	94	ASN
2	D	145	ASP

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	285/290 (98%)	279 (98%)	6 (2%)	61	65
1	C	282/290 (97%)	276 (98%)	6 (2%)	61	65
1	E	285/290 (98%)	278 (98%)	7 (2%)	55	58
1	G	283/290 (98%)	276 (98%)	7 (2%)	55	58
1	I	281/290 (97%)	267 (95%)	14 (5%)	30	25
1	K	281/290 (97%)	274 (98%)	7 (2%)	55	58
2	B	150/152 (99%)	143 (95%)	7 (5%)	32	28
2	D	147/152 (97%)	141 (96%)	6 (4%)	37	35
2	F	146/152 (96%)	141 (97%)	5 (3%)	44	42
2	H	146/152 (96%)	143 (98%)	3 (2%)	61	65
2	J	145/152 (95%)	139 (96%)	6 (4%)	37	35
2	L	146/152 (96%)	143 (98%)	3 (2%)	61	65
All	All	2577/2652 (97%)	2500 (97%)	77 (3%)	48	48

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	81	THR
1	A	93	ASP
1	A	115	VAL
1	A	253	VAL
1	A	320	LEU
2	B	22	TYR
2	B	29	GLU
2	B	97	GLU
2	B	128	ASN
2	B	161	LYS
2	B	164	GLU
2	B	174	ASP
1	C	155	VAL
1	C	193	SER
1	C	277	CYS
1	C	295	GLN
1	C	316	LEU

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Mol	Chain	Res	Type
1	C	320	LEU
2	D	22	TYR
2	D	57	GLU
2	D	68	LYS
2	D	72	HIS
2	D	95	ASN
2	D	102	LEU
1	E	54	LEU
1	E	80	SER
1	E	81	THR
1	E	136	THR
1	E	194	LEU
1	E	295	GLN
1	E	320	LEU
2	F	22	TYR
2	F	102	LEU
2	F	150	GLU
2	F	167	LYS
2	F	170	ARG
1	G	21	ASN
1	G	136	THR
1	G	159	ASN
1	G	203	PHE
1	G	253	VAL
1	G	261	GLU
1	G	315	ARG
2	H	29	GLU
2	H	60	ASN
2	H	68	LYS
1	I	54	LEU
1	I	55	ARG
1	I	77	GLU
1	I	97	CYS
1	I	102	PHE
1	I	125	SER
1	I	164	LEU
1	I	203	PHE
1	I	244	THR
1	I	261	GLU
1	I	272	THR
1	I	295	GLN
1	I	316	LEU

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Mol	Chain	Res	Type
1	I	320	LEU
2	J	22	TYR
2	J	26	HIS
2	J	102	LEU
2	J	123	ARG
2	J	133	ILE
2	J	154	ASN
1	K	30	LEU
1	K	55	ARG
1	K	102	PHE
1	K	274	VAL
1	K	283	THR
1	K	295	GLN
1	K	320	LEU
2	L	38	LEU
2	L	102	LEU
2	L	149	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	79	ASN
2	B	95	ASN
1	C	263	ASN
2	D	43	ASN
2	D	72	HIS
2	D	95	ASN
1	E	298	HIS
2	F	30	GLN
1	G	159	ASN
2	H	43	ASN
2	H	60	ASN
2	H	62	GLN
2	H	142	HIS
1	I	289	ASN
2	J	95	ASN
1	K	196	GLN
1	K	263	ASN
2	L	62	GLN

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

20 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	330	3	16,20,21	0.28	0	18,28,31	0.97	1 (5%)
3	GAL	A	331	3	12,12,12	0.53	0	17,17,17	0.48	0
3	NAG	A	332	3	14,14,15	0.55	0	15,19,21	1.13	1 (6%)
3	GAL	A	333	3	11,11,12	0.60	0	14,15,17	0.79	1 (7%)
3	SIA	C	330	3	16,20,21	0.26	0	18,28,31	1.26	1 (5%)
3	GAL	C	331	3	11,11,12	0.65	0	14,15,17	0.76	0
3	NAG	C	332	3	14,14,15	0.59	0	15,19,21	0.98	1 (6%)
3	GAL	C	333	3	12,12,12	0.59	0	17,17,17	0.58	0
5	SIA	E	330	5	16,20,21	0.23	0	18,28,31	0.98	2 (11%)
5	NAG	E	331	5	14,14,15	0.54	0	15,19,21	0.76	0
5	GAL	E	332	5	11,11,12	0.57	0	14,15,17	0.81	0
7	NAG	G	431	1,7	14,14,15	0.52	0	15,19,21	0.85	0
7	NAG	G	432	7	14,14,15	0.62	0	15,19,21	1.40	3 (20%)
5	SIA	I	501	5	16,20,21	0.21	0	18,28,31	1.26	2 (11%)
5	GAL	I	502	5	11,11,12	0.64	0	14,15,17	0.71	0
5	NAG	I	503	5	14,14,15	0.54	0	15,19,21	0.67	0
3	SIA	K	601	3	16,20,21	0.31	0	18,28,31	1.33	1 (5%)
3	GAL	K	602	3	11,11,12	0.64	0	14,15,17	0.70	0
3	NAG	K	603	3	14,14,15	0.64	0	15,19,21	0.85	0
3	GAL	K	604	3	12,12,12	0.53	0	17,17,17	0.56	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	330	3	-	0/14/34/38	0/1/1/1
3	GAL	A	331	3	-	0/2/22/22	0/1/1/1
3	NAG	A	332	3	-	0/6/23/26	0/1/1/1
3	GAL	A	333	3	-	0/2/19/22	0/1/1/1
3	SIA	C	330	3	-	0/14/34/38	0/1/1/1
3	GAL	C	331	3	-	0/2/19/22	0/1/1/1
3	NAG	C	332	3	-	0/6/23/26	0/1/1/1
3	GAL	C	333	3	-	0/2/22/22	0/1/1/1
5	SIA	E	330	5	-	0/14/34/38	0/1/1/1
5	NAG	E	331	5	-	0/6/23/26	0/1/1/1
5	GAL	E	332	5	-	0/2/19/22	0/1/1/1
7	NAG	G	431	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	432	7	-	0/6/23/26	0/1/1/1
5	SIA	I	501	5	-	0/14/34/38	0/1/1/1
5	GAL	I	502	5	-	0/2/19/22	0/1/1/1
5	NAG	I	503	5	-	0/6/23/26	0/1/1/1
3	SIA	K	601	3	-	0/14/34/38	0/1/1/1
3	GAL	K	602	3	-	0/2/19/22	0/1/1/1
3	NAG	K	603	3	-	0/6/23/26	0/1/1/1
3	GAL	K	604	3	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	432	NAG	C2-N2-C7	-3.06	119.11	123.04
5	I	501	SIA	C7-C6-C5	-2.77	110.14	114.32
5	E	330	SIA	C7-C6-C5	-2.26	110.91	114.32
3	A	333	GAL	O5-C1-C2	-2.04	107.54	110.86
3	A	330	SIA	O6-C6-C5	2.44	112.49	108.48
7	G	432	NAG	C3-C4-C5	2.55	114.64	110.20
5	E	330	SIA	O6-C6-C5	2.58	112.71	108.48
7	G	432	NAG	C4-C3-C2	2.68	115.39	111.23
3	C	332	NAG	C1-O5-C5	2.73	115.72	112.25
3	C	330	SIA	O6-C6-C5	3.23	113.77	108.48
5	I	501	SIA	O6-C6-C5	3.39	114.04	108.48
3	A	332	NAG	C1-O5-C5	3.54	116.74	112.25
3	K	601	SIA	O6-C6-C5	3.80	114.71	108.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	330	SIA	1	0
5	E	330	SIA	1	0

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
4	NAG	A	334	1	14,14,15	0.56	0	15,19,21	0.88	0
4	NAG	A	335	1	14,14,15	0.41	0	15,19,21	1.13	2 (13%)
4	NAG	A	336	1	14,14,15	0.58	0	15,19,21	0.84	0
4	NAG	C	334	1	14,14,15	0.48	0	15,19,21	0.80	0
4	NAG	E	333	1	14,14,15	0.47	0	15,19,21	0.92	0
6	SIA	G	401	-	16,20,21	0.26	0	18,28,31	0.95	2 (11%)
4	NAG	J	561	2	14,14,15	0.47	0	15,19,21	0.79	0
4	NAG	K	641	1	14,14,15	0.40	0	15,19,21	1.56	3 (20%)

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	NAG	A	334	1	-	0/6/23/26	0/1/1/1
4	NAG	A	335	1	-	0/6/23/26	0/1/1/1
4	NAG	A	336	1	-	0/6/23/26	0/1/1/1
4	NAG	C	334	1	-	0/6/23/26	0/1/1/1
4	NAG	E	333	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SIA	G	401	-	-	0/14/34/38	0/1/1/1
4	NAG	J	561	2	-	0/6/23/26	0/1/1/1
4	NAG	K	641	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	641	NAG	C4-C3-C2	-2.85	106.80	111.23
4	K	641	NAG	C2-N2-C7	-2.77	119.49	123.04
4	A	335	NAG	C2-N2-C7	-2.21	120.20	123.04
6	G	401	SIA	C7-C6-C5	-2.03	111.25	114.32
6	G	401	SIA	O6-C6-C5	2.45	112.50	108.48
4	A	335	NAG	C1-O5-C5	2.70	115.68	112.25
4	K	641	NAG	C1-O5-C5	3.98	117.30	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	336	NAG	1	0
4	C	334	NAG	1	0
4	E	333	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	323/329 (98%)	0.08	3 (0%) 85 89	21, 34, 52, 71	0
1	C	320/329 (97%)	-0.16	4 (1%) 79 84	20, 33, 51, 76	0
1	E	323/329 (98%)	0.07	6 (1%) 70 78	24, 38, 58, 80	0
1	G	321/329 (97%)	0.04	9 (2%) 56 66	22, 35, 56, 71	0
1	I	319/329 (96%)	-0.00	7 (2%) 65 73	28, 41, 57, 77	0
1	K	320/329 (97%)	0.07	6 (1%) 70 78	22, 35, 53, 71	0
2	B	174/177 (98%)	0.17	6 (3%) 49 59	24, 43, 66, 82	0
2	D	171/177 (96%)	0.69	29 (16%) 2 4	23, 43, 76, 96	0
2	F	170/177 (96%)	0.70	23 (13%) 4 7	22, 44, 80, 95	0
2	H	170/177 (96%)	0.86	27 (15%) 3 4	23, 47, 84, 95	0
2	J	169/177 (95%)	0.31	5 (2%) 54 64	22, 46, 68, 77	0
2	L	170/177 (96%)	0.24	5 (2%) 55 65	22, 41, 61, 69	0
All	All	2950/3036 (97%)	0.18	130 (4%) 38 49	20, 38, 68, 96	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	168	LEU	7.6
2	H	144	CYS	6.0
2	D	160	PRO	5.9
2	D	152	VAL	5.5
2	H	164	GLU	5.3
2	H	29	GLU	5.2
2	H	143	LYS	4.9
2	H	160	PRO	4.8
2	H	168	LEU	4.7
2	D	147	THR	4.6
2	F	29	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	166	ALA	4.5
1	K	94	ASN	4.5
1	I	290	THR	4.4
2	D	156	THR	4.4
2	H	159	TYR	4.4
1	I	264	ALA	4.4
2	F	144	CYS	4.3
1	G	81	THR	4.2
2	D	144	CYS	4.2
1	G	12	THR	4.2
2	J	166	ALA	4.2
2	F	156	THR	4.1
2	H	140	PHE	4.1
2	D	143	LYS	4.0
2	B	173	ILE	4.0
2	D	158	ASP	4.0
2	F	162	TYR	3.9
2	F	161	LYS	3.9
2	F	166	ALA	3.8
2	H	33	GLY	3.8
2	F	160	PRO	3.7
2	H	166	ALA	3.7
2	D	168	LEU	3.6
2	J	168	LEU	3.6
2	F	31	GLY	3.5
1	K	93	ASP	3.4
2	H	141	TYR	3.4
2	H	167	LYS	3.4
1	I	325	SER	3.3
1	E	81	THR	3.3
1	I	55	ARG	3.3
2	H	158	ASP	3.2
2	D	159	TYR	3.2
1	G	13	LEU	3.2
1	A	325	SER	3.2
2	D	148	CYS	3.2
2	F	147	THR	3.2
2	D	145	ASP	3.1
1	E	78	SER	3.1
2	D	16	GLY	3.1
2	D	157	TYR	3.1
2	D	162	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	140	PHE	3.1
2	F	158	ASP	3.0
2	D	140	PHE	3.0
1	E	80	SER	3.0
2	F	143	LYS	3.0
2	J	133	ILE	3.0
2	D	138	PHE	3.0
2	H	38	LEU	2.9
2	H	152	VAL	2.9
1	K	9	PRO	2.9
2	H	31	GLY	2.9
1	I	289	ASN	2.9
2	D	27	GLN	2.9
1	G	21	ASN	2.9
2	H	156	THR	2.9
2	D	128	ASN	2.8
2	F	26	HIS	2.8
1	A	143	GLY	2.8
2	B	174	ASP	2.8
2	F	28	ASN	2.8
2	D	164	GLU	2.8
2	F	167	LYS	2.8
1	C	12	THR	2.8
1	A	290	THR	2.7
1	G	82	ALA	2.7
1	I	94	ASN	2.6
2	D	35	ALA	2.6
2	H	148	CYS	2.6
1	C	78	SER	2.6
2	D	154	ASN	2.6
2	H	162	TYR	2.6
2	D	142	HIS	2.6
2	F	170	ARG	2.6
2	J	155	GLY	2.5
2	L	156	THR	2.5
1	G	159	ASN	2.5
2	B	168	LEU	2.5
1	E	158	GLY	2.5
2	D	30	GLN	2.4
2	B	33	GLY	2.4
2	H	30	GLN	2.4
2	B	31	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	65	ALA	2.3
1	E	77	GLU	2.3
2	L	150	GLU	2.3
1	K	236	LEU	2.3
2	B	160	PRO	2.3
2	F	38	LEU	2.3
2	H	153	LYS	2.3
2	J	131	LYS	2.3
2	F	126	LEU	2.3
2	L	38	LEU	2.3
2	L	27	GLN	2.3
1	K	275	HIS	2.3
2	D	18	VAL	2.3
1	G	15	ILE	2.3
1	K	325	SER	2.2
2	F	164	GLU	2.2
2	H	26	HIS	2.2
1	G	11	ASP	2.2
1	G	158	GLY	2.2
2	H	163	SER	2.2
2	F	157	TYR	2.2
1	C	93	ASP	2.1
1	C	325	SER	2.1
1	E	264	ALA	2.1
2	H	27	GLN	2.1
2	F	141	TYR	2.1
2	H	145	ASP	2.1
2	D	141	TYR	2.1
2	L	39	LYS	2.1
2	D	139	GLU	2.1
2	D	171	GLU	2.1
2	D	149	MET	2.1
2	H	134	GLY	2.0
2	F	145	ASP	2.0
1	I	93	ASP	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
3	SIA	A	330	20/21	0.95	0.11	-0.08	31,37,42,46	0
3	GAL	K	602	11/12	0.90	0.16	-0.10	40,56,61,69	0
3	SIA	K	601	20/21	0.96	0.11	-0.35	33,40,45,46	0
3	GAL	A	333	11/12	0.93	0.13	-0.37	39,52,58,62	0
5	SIA	I	501	20/21	0.96	0.10	-0.49	29,38,42,42	0
5	SIA	E	330	20/21	0.94	0.10	-0.55	32,45,50,53	0
7	NAG	G	431	14/15	0.95	0.10	-0.98	32,39,46,46	0
3	SIA	C	330	20/21	0.96	0.08	-1.44	27,33,39,42	0
3	GAL	C	333	12/12	0.80	0.21	-	55,70,76,89	0
5	NAG	I	503	14/15	0.89	0.11	-	35,44,51,51	0
3	NAG	K	603	14/15	0.79	0.19	-	46,62,67,67	0
5	GAL	I	502	11/12	0.95	0.08	-	38,43,48,54	0
7	NAG	G	432	14/15	0.80	0.23	-	48,55,66,75	0
3	GAL	A	331	12/12	0.84	0.32	-	63,71,82,83	0
5	NAG	E	331	14/15	0.89	0.15	-	47,51,56,60	0
3	NAG	C	332	14/15	0.93	0.13	-	39,49,55,57	0
5	GAL	E	332	11/12	0.92	0.10	-	41,50,54,62	0
3	GAL	K	604	12/12	0.84	0.23	-	67,76,84,88	0
3	NAG	A	332	14/15	0.85	0.21	-	49,60,65,65	0
3	GAL	C	331	11/12	0.95	0.13	-	39,44,53,59	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, 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	A	336	14/15	0.79	0.30	2.72	62,69,71,76	0
4	NAG	A	335	14/15	0.88	0.13	0.56	34,46,56,58	0
4	NAG	E	333	14/15	0.89	0.12	-0.06	44,51,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	SIA	G	401	20/21	0.93	0.11	-0.10	29,38,45,46	0
4	NAG	J	561	14/15	0.87	0.15	-0.41	62,69,76,78	0
4	NAG	C	334	14/15	0.84	0.17	-	50,63,74,75	0
4	NAG	A	334	14/15	0.70	0.38	-	78,80,93,93	0
4	NAG	K	641	14/15	0.90	0.27	-	65,75,84,88	0

6.5 Other polymers

There are no such residues in this entry.