Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:39 PM GMT

PDB ID	:	3UBN
Title	:	Influenza hemagglutinin from the 2009 pandemic in complex with ligand 6SLN
Authors	:	Xu, R.; Wilson, I.A.
Deposited on	:	2011-10-24
Resolution	:	2.51 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:

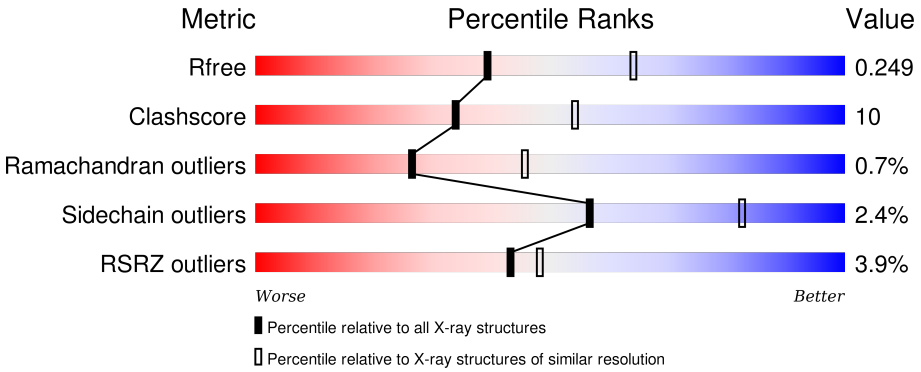
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.51 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	78% 19%
1	C	329	73% 23%
1	E	329	73% 23%
1	G	329	73% 24%
1	I	329	74% 22%

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Mol	Chain	Length	Quality of chain
1	K	329	2% 73% 22%
2	B	177	5% 78% 19%
2	D	177	15% 66% 29%
2	F	177	14% 72% 24%
2	H	177	12% 71% 24%
2	J	177	2% 73% 21%
2	L	177	% 73% 22%

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 7 unique types of molecules in this entry. The entry contains 24203 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	319	Total	C	N	O	S	0	0	0
			2495	1579	428	475	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	319	Total	C	N	O	S	0	0	0
			2492	1578	428	473	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	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	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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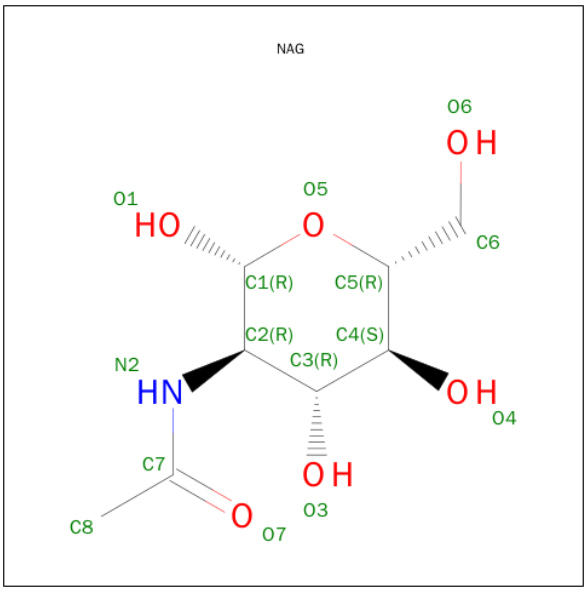
Chain	Residue	Modelled	Actual	Comment	Reference
L	175	SER	-	EXPRESSION TAG	UNP C3W5S1
L	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
L	177	ARG	-	EXPRESSION TAG	UNP C3W5S1

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			46	25	2	19		
3	C	3	Total	C	N	O	0	0
			46	25	2	19		
3	E	3	Total	C	N	O	0	0
			46	25	2	19		
3	I	3	Total	C	N	O	0	0
			46	25	2	19		
3	K	3	Total	C	N	O	0	0
			46	25	2	19		

- 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		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
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 (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	2	Total C N O 31 17 1 13	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	55	Total O 55 55	0	0
7	B	28	Total O 28 28	0	0
7	C	60	Total O 60 60	0	0
7	D	31	Total O 31 31	0	0
7	E	33	Total O 33 33	0	0
7	F	22	Total O 22 22	0	0

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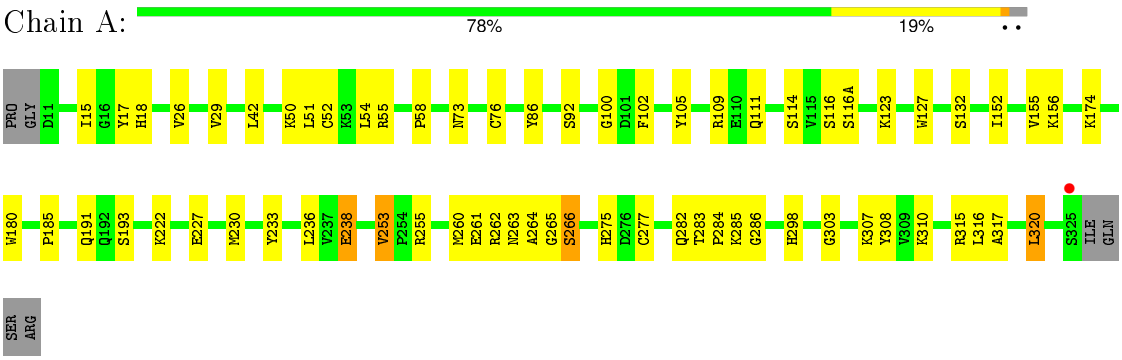
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	63	Total O 63 63	0	0
7	H	27	Total O 27 27	0	0
7	I	44	Total O 44 44	0	0
7	J	36	Total O 36 36	0	0
7	K	51	Total O 51 51	0	0
7	L	35	Total O 35 35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

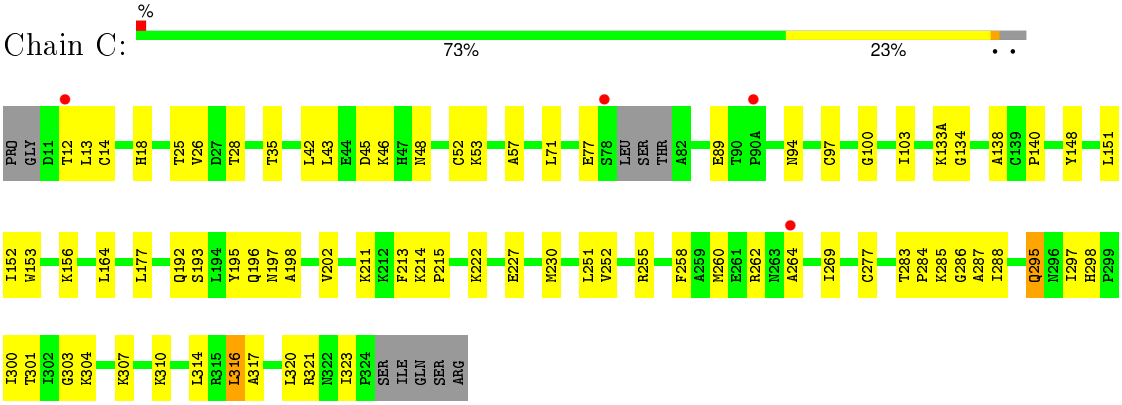
- Molecule 1: Hemagglutinin HA1

Chain A:



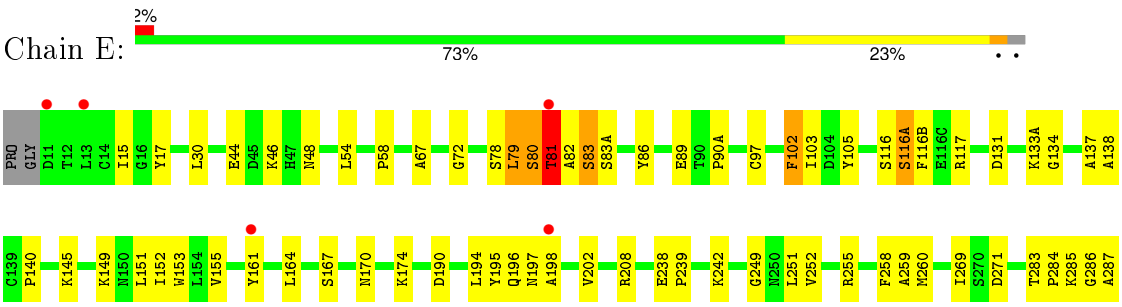
- Molecule 1: Hemagglutinin HA1

Chain C:



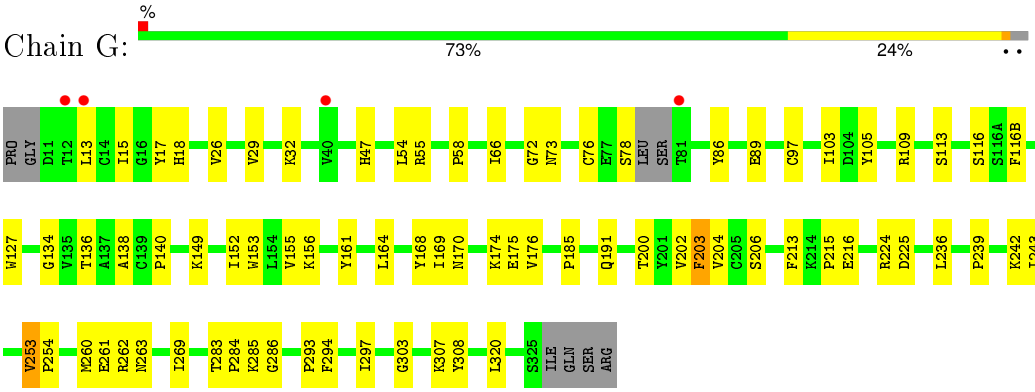
- Molecule 1: Hemagglutinin HA1

Chain E:



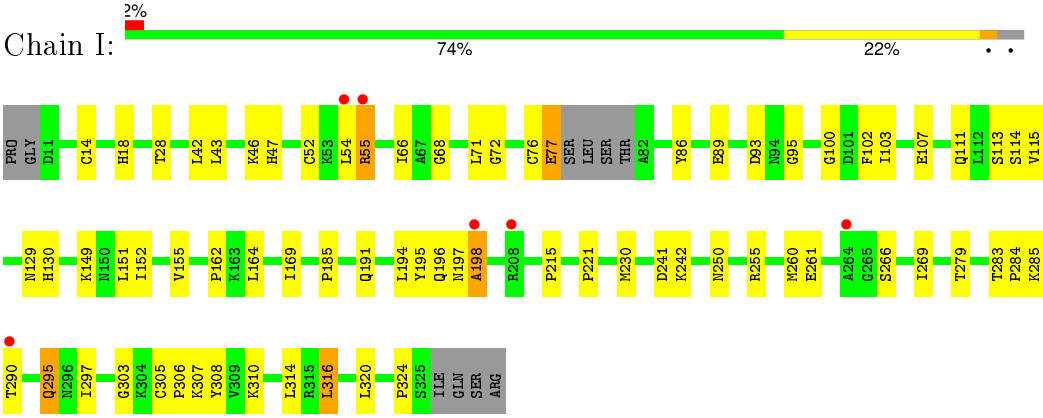
• Molecule 1: Hemagglutinin HA1

Chain G:



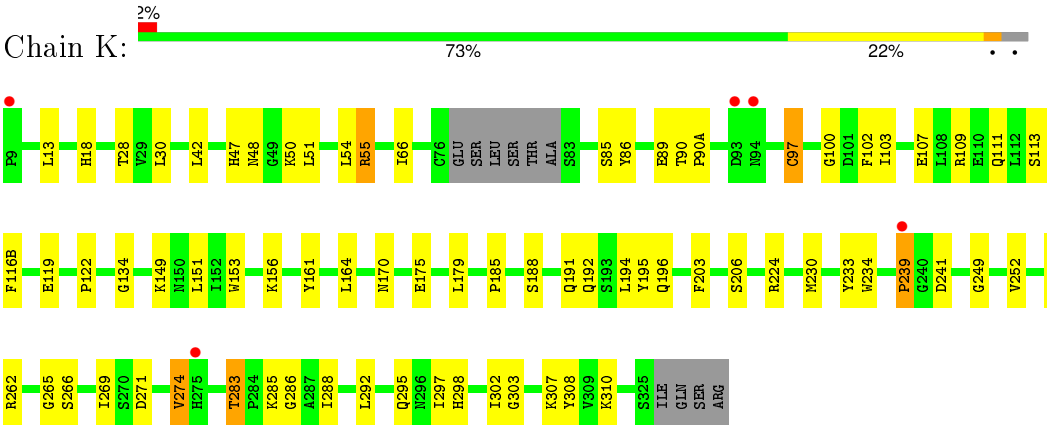
• Molecule 1: Hemagglutinin HA1

Chain I:



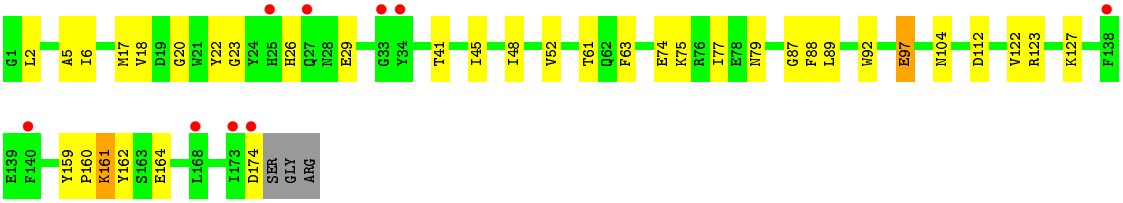
• Molecule 1: Hemagglutinin HA1

Chain K:

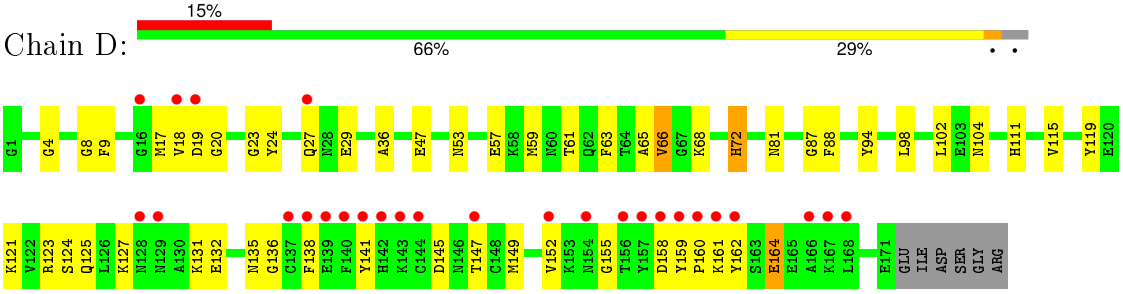


• Molecule 2: Hemagglutinin HA2

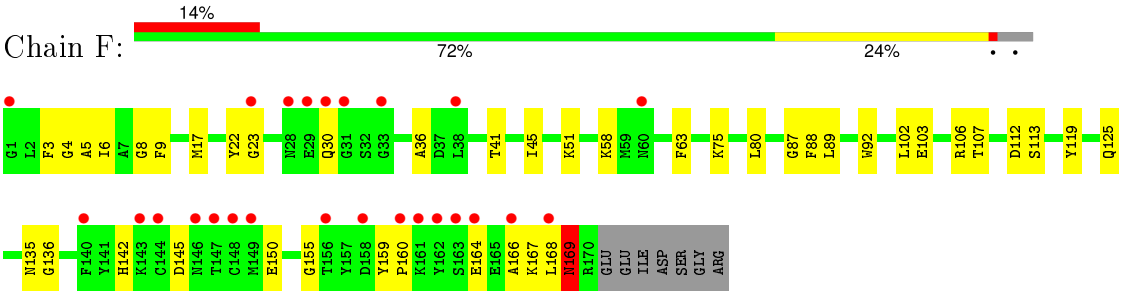
Chain B:



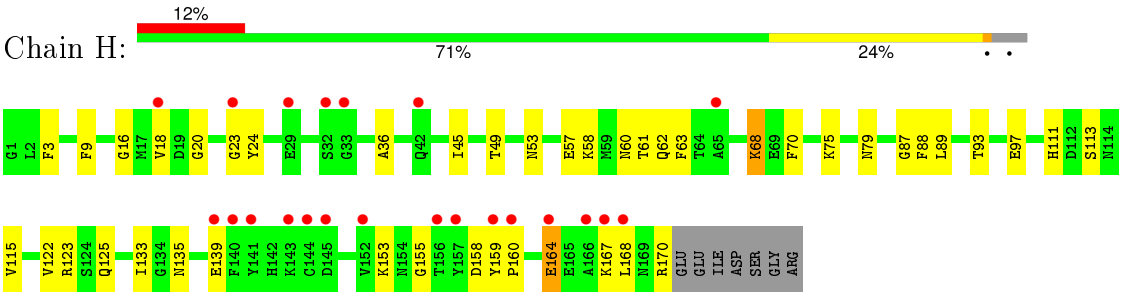
• Molecule 2: Hemagglutinin HA2



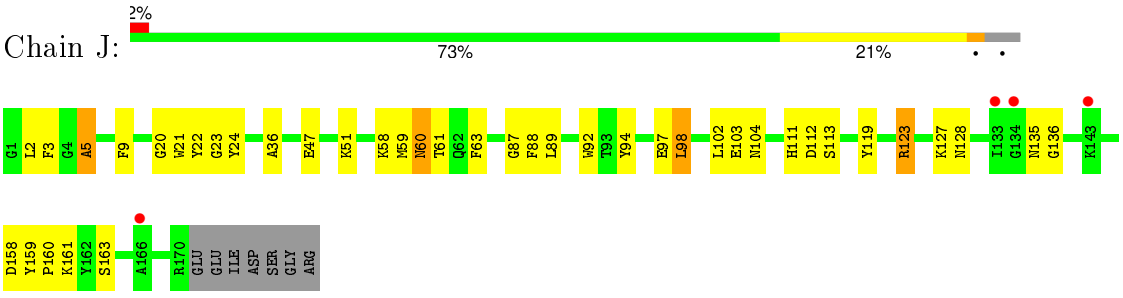
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

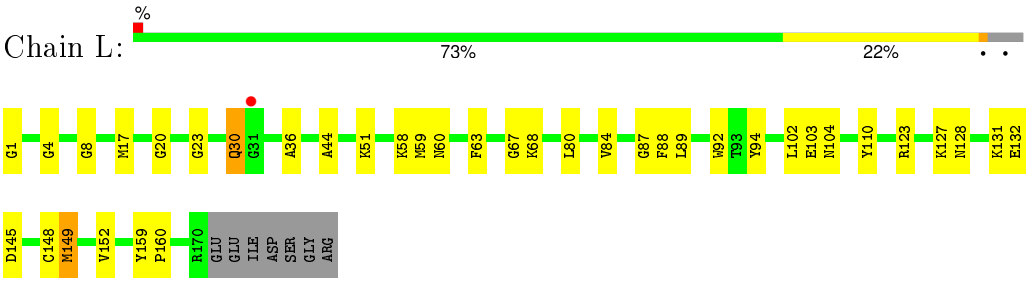


• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

Chain L:


%
73%
22%
G1 G4 G8 M17 G20 G23 Q30 G31 A36 A44 K51 K58 M59 N60 F63 G67 K68 L80 V84 G87 F88 L89 W92 T93 Y94 L102 E103 N104 Y110 R123 K127 N128 K131 E132 I133 F138 E139
D145 C148 M149 V152 Y159 P160 R170 GLU GLU ILE ASP SER GLY ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.00Å 116.71Å 119.66Å 60.61° 77.05° 80.38°	Depositor
Resolution (Å)	49.68 – 2.51 49.68 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.68-2.51) 80.1 (49.68-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.205 , 0.253 0.203 , 0.249	Depositor DCC
R_{free} test set	4909 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 99214 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24203	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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	0.22	0/2586	0.40	0/3516
1	C	0.22	0/2558	0.40	0/3476
1	E	0.22	0/2586	0.43	0/3516
1	G	0.22	0/2571	0.40	0/3494
1	I	0.22	0/2558	0.41	0/3476
1	K	0.22	0/2556	0.40	0/3473
2	B	0.22	0/1433	0.35	0/1931
2	D	0.22	0/1408	0.35	0/1897
2	F	0.22	0/1399	0.36	0/1885
2	H	0.22	0/1399	0.36	0/1885
2	J	0.23	0/1399	0.37	0/1885
2	L	0.23	0/1399	0.36	0/1885
All	All	0.22	0/23852	0.39	0/32319

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	2464	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2495	0	2437	50	0
1	E	2522	0	2467	74	0
1	G	2508	0	2450	56	0
1	I	2495	0	2439	54	0
1	K	2492	0	2438	55	0
2	B	1405	0	1324	28	0
2	D	1380	0	1303	44	0
2	F	1371	0	1297	33	0
2	H	1371	0	1297	38	0
2	J	1371	0	1296	35	0
2	L	1371	0	1297	31	0
3	A	46	0	40	0	0
3	C	46	0	40	1	0
3	E	46	0	40	2	0
3	I	46	0	40	0	0
3	K	46	0	40	1	0
4	A	56	0	52	0	0
4	C	28	0	26	1	0
4	E	14	0	13	1	0
4	J	14	0	13	0	0
4	K	14	0	13	0	0
5	G	31	0	26	0	0
6	G	28	0	25	2	0
7	A	55	0	0	1	0
7	B	28	0	0	0	0
7	C	60	0	0	1	0
7	D	31	0	0	0	0
7	E	33	0	0	0	0
7	F	22	0	0	1	0
7	G	63	0	0	0	0
7	H	27	0	0	0	0
7	I	44	0	0	0	0
7	J	36	0	0	1	0
7	K	51	0	0	0	0
7	L	35	0	0	1	0
All	All	24203	0	22877	470	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 (470) 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:79:LEU:HA	1:E:80:SER:CB	1.81	1.10
1:E:79:LEU:HA	1:E:80:SER:HB3	1.26	1.10
2:J:59:MET:HA	2:J:60:ASN:HB3	1.03	1.03
1:E:82:ALA:HB3	1:E:83:SER:HB2	1.41	1.00
2:J:59:MET:HA	2:J:60:ASN:CB	1.91	0.97
2:J:59:MET:CA	2:J:60:ASN:HB3	1.94	0.96
1:E:79:LEU:CA	1:E:80:SER:HB3	2.02	0.89
1:E:82:ALA:CB	1:E:83:SER:HB2	2.02	0.88
2:H:97:GLU:HG2	2:L:58:LYS:HD2	1.57	0.87
1:E:283:THR:HG22	1:E:285:LYS:H	1.37	0.87
1:I:283:THR:HG22	1:I:285:LYS:H	1.38	0.87
1:G:283:THR:HG22	1:G:285:LYS:H	1.41	0.85
1:C:283:THR:HG22	1:C:285:LYS:H	1.42	0.84
2:H:58:LYS:HD2	2:J:97:GLU:HG2	1.58	0.83
2:B:97:GLU:HG2	2:F:58:LYS:HD2	1.62	0.81
2:F:164:GLU:O	2:F:167:LYS:HG2	1.82	0.79
1:E:298:HIS:HD2	1:E:300:ILE:H	1.30	0.79
1:A:283:THR:HG22	1:A:285:LYS:H	1.45	0.79
1:E:72:GLY:HA3	1:E:149:LYS:H	1.48	0.77
1:A:283:THR:HB	1:A:286:GLY:O	1.87	0.75
1:I:283:THR:HB	1:I:286:GLY:O	1.87	0.74
2:H:24:TYR:CE1	2:H:153:LYS:HG3	2.22	0.74
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.73	0.71
1:E:190:ASP:O	1:E:194:LEU:HB2	1.92	0.69
2:L:23:GLY:HA3	2:L:36:ALA:HA	1.74	0.69
2:H:62:GLN:HE21	1:I:310:LYS:HZ3	1.40	0.69
1:K:114:SER:HB2	1:K:266:SER:HB2	1.75	0.69
2:H:167:LYS:HG3	2:H:170:ARG:HH12	1.59	0.68
1:K:283:THR:HG23	1:K:285:LYS:H	1.59	0.67
2:H:167:LYS:HG3	2:H:170:ARG:NH1	2.10	0.67
1:C:25:THR:HG22	1:C:35:THR:HG22	1.77	0.67
1:G:283:THR:HB	1:G:286:GLY:O	1.94	0.66
1:I:303:GLY:HA2	2:J:63:PHE:CE1	2.30	0.66
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.75	0.66
2:L:131:LYS:NZ	2:L:133:ILE:HG22	2.11	0.66
1:I:283:THR:HG23	1:I:284:PRO:HD2	1.78	0.66
1:E:298:HIS:CD2	1:E:300:ILE:H	2.12	0.65
1:E:72:GLY:HA3	1:E:149:LYS:N	2.12	0.65
2:J:9:PHE:O	2:J:135:ASN:HA	1.96	0.65
1:K:307:LYS:HG3	2:L:92:TRP:CE2	2.32	0.64
1:K:13:LEU:HB2	2:L:149:MET:HE1	1.79	0.64
1:E:174:LYS:HE3	1:E:259:ALA:HB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:119:TYR:CE1	2:J:136:GLY:HA2	2.33	0.64
1:I:89:GLU:O	1:I:269:ILE:HA	1.98	0.64
2:H:53:ASN:O	2:H:57:GLU:HG2	1.97	0.64
2:D:161:LYS:HD2	2:D:162:TYR:CZ	2.34	0.63
1:G:262:ARG:HG2	1:G:262:ARG:HH11	1.64	0.63
1:E:283:THR:HB	1:E:286:GLY:O	1.99	0.62
1:K:114:SER:HB2	1:K:266:SER:CB	2.29	0.62
2:B:75:LYS:NZ	2:B:79:ASN:HD21	1.98	0.61
1:I:28:THR:HG22	2:J:104:ASN:HB3	1.80	0.61
1:K:170:ASN:HB3	1:K:239:PRO:O	2.00	0.61
2:H:23:GLY:HA3	2:H:36:ALA:HA	1.83	0.61
1:E:82:ALA:CB	1:E:83:SER:CB	2.78	0.61
1:I:169:ILE:HD13	1:I:242:LYS:HB2	1.83	0.60
1:E:80:SER:O	1:E:81:THR:HG23	2.01	0.60
1:C:303:GLY:HA2	2:D:63:PHE:CE1	2.36	0.60
1:E:310:LYS:HG2	2:F:89:LEU:HD11	1.83	0.60
1:C:283:THR:HB	1:C:286:GLY:O	2.02	0.59
1:A:283:THR:HG23	1:A:284:PRO:HD2	1.83	0.59
2:H:9:PHE:O	2:H:135:ASN:HA	2.02	0.59
1:G:253:VAL:HG22	1:G:254:PRO:HD2	1.85	0.59
2:H:123:ARG:HH12	2:J:123:ARG:HH21	1.50	0.59
1:G:97:CYS:O	1:G:224:ARG:HD3	2.02	0.59
1:A:236:LEU:HD13	1:A:262:ARG:NH1	2.18	0.58
2:B:41:THR:O	2:B:45:ILE:HG13	2.02	0.58
2:J:59:MET:CA	2:J:60:ASN:CB	2.69	0.58
2:B:75:LYS:HZ3	2:B:79:ASN:HD21	1.50	0.58
2:D:149:MET:O	2:D:152:VAL:HG22	2.04	0.58
1:E:283:THR:HG23	1:E:284:PRO:HD2	1.86	0.58
1:A:303:GLY:HA2	2:B:63:PHE:CE1	2.39	0.58
1:E:167:SER:OG	1:E:242:LYS:HE2	2.04	0.58
2:B:123:ARG:NH1	2:D:123:ARG:HH22	2.02	0.58
2:D:65:ALA:O	2:D:66:VAL:HG12	2.04	0.57
1:G:15:ILE:HD11	2:H:122:VAL:HG21	1.86	0.57
1:G:283:THR:HG23	1:G:284:PRO:HD2	1.85	0.57
2:D:9:PHE:O	2:D:135:ASN:HA	2.04	0.57
1:A:174:LYS:HD2	1:A:261:GLU:HG3	1.87	0.57
1:E:202:VAL:HG11	1:E:251:LEU:HD13	1.86	0.57
1:I:115:VAL:HG12	1:I:116(A):SER:H	1.70	0.57
2:F:30:GLN:HE21	2:F:145:ASP:HB2	1.70	0.57
2:J:119:TYR:HE1	2:J:136:GLY:HA2	1.69	0.57
1:A:116:SER:HB3	1:A:263:ASN:HD21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:GLU:OE2	1:E:46:LYS:HG2	2.06	0.56
2:J:160:PRO:HA	2:J:163:SER:OG	2.06	0.56
2:B:87:GLY:HA3	2:F:88:PHE:CZ	2.41	0.56
2:H:123:ARG:HH12	2:J:123:ARG:NH2	2.03	0.56
1:K:303:GLY:HA2	2:L:63:PHE:CE1	2.41	0.56
1:G:307:LYS:HE2	2:H:61:THR:HG22	1.87	0.56
2:D:53:ASN:O	2:D:57:GLU:HG2	2.05	0.56
1:C:214:LYS:HG3	1:C:215:PRO:HD2	1.87	0.56
1:G:13:LEU:HD11	2:H:24:TYR:HB3	1.87	0.56
1:G:127:TRP:CH2	1:G:253:VAL:HG21	2.41	0.56
1:E:151:LEU:HB3	1:E:252:VAL:HG12	1.87	0.56
1:I:54:LEU:C	1:I:55:ARG:HG3	2.25	0.56
1:K:206:SER:HB2	1:K:241:ASP:OD2	2.06	0.56
1:E:79:LEU:HA	1:E:80:SER:OG	2.04	0.55
2:J:88:PHE:CZ	2:L:87:GLY:HA3	2.41	0.55
1:C:140:PRO:HD2	4:C:333:NAG:H83	1.89	0.55
1:I:52:CYS:HB2	1:I:279:THR:HG22	1.88	0.55
1:C:300:ILE:HA	2:D:66:VAL:HG11	1.88	0.55
1:K:115:VAL:HG11	1:K:116(B):PHE:HB2	1.88	0.55
1:G:303:GLY:HA2	2:H:63:PHE:CE1	2.41	0.55
1:K:283:THR:HG22	1:K:286:GLY:H	1.72	0.55
1:G:200:THR:OG1	1:G:215:PRO:HG3	2.07	0.55
1:I:307:LYS:HG3	2:J:92:TRP:CE2	2.41	0.55
1:G:170:ASN:HB3	1:G:239:PRO:O	2.07	0.54
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.42	0.54
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.89	0.54
2:L:4:GLY:O	2:L:8:GLY:HA3	2.06	0.54
1:C:288:ILE:HD13	1:C:295:GLN:HG3	1.90	0.54
1:A:111:GLN:O	1:A:262:ARG:HD2	2.07	0.54
1:I:290:THR:HG23	1:I:306:PRO:HD3	1.89	0.54
1:I:197:ASN:O	1:I:198:ALA:HB3	2.07	0.54
2:D:47:GLU:HB3	1:E:30:LEU:HG	1.87	0.54
1:G:116(B):PHE:HE1	1:G:260:MET:HE2	1.72	0.54
1:E:307:LYS:HG3	2:F:92:TRP:CE2	2.42	0.54
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.90	0.54
2:B:5:ALA:HB3	2:B:112:ASP:OD2	2.08	0.54
1:K:18:HIS:HB2	2:L:20:GLY:O	2.08	0.54
2:L:30:GLN:OE1	2:L:145:ASP:HB2	2.08	0.53
1:E:208:ARG:NH2	1:E:238:GLU:H	2.06	0.53
2:D:124:SER:O	2:D:127:LYS:HE3	2.08	0.53
1:K:107:GLU:O	1:K:111:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:PRO:HD2	4:E:333:NAG:H83	1.90	0.53
1:G:72:GLY:O	1:G:149:LYS:HG2	2.08	0.53
1:C:152:ILE:HD11	1:C:255:ARG:HD2	1.90	0.53
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.44	0.53
2:H:88:PHE:CZ	2:J:87:GLY:HA3	2.44	0.53
2:H:159:TYR:HB3	2:H:160:PRO:HD3	1.89	0.53
1:E:82:ALA:HB1	1:E:83:SER:CA	2.39	0.53
1:G:203:PHE:HD1	1:G:204:VAL:N	2.07	0.53
2:D:158:ASP:OD1	2:D:161:LYS:HB2	2.08	0.53
1:C:18:HIS:HB2	2:D:20:GLY:O	2.08	0.53
1:A:310:LYS:HE3	2:B:89:LEU:HD21	1.90	0.53
1:C:301:THR:H	2:D:66:VAL:HG11	1.74	0.52
2:L:1:GLY:HA3	7:L:280:HOH:O	2.09	0.52
1:E:283:THR:HG22	1:E:285:LYS:N	2.16	0.52
1:C:13:LEU:HD22	2:D:152:VAL:HG21	1.91	0.52
2:B:74:GLU:HB3	2:B:77:ILE:HD11	1.91	0.52
2:B:161:LYS:HE3	2:B:162:TYR:CE1	2.43	0.52
1:E:116(A):SER:O	1:E:260:MET:HA	2.09	0.52
1:E:90(A):PRO:HD2	1:E:271:ASP:OD1	2.09	0.52
1:A:152:ILE:HG13	1:A:255:ARG:HB2	1.90	0.52
1:G:283:THR:CG2	1:G:285:LYS:HG2	2.39	0.52
2:D:131:LYS:HE3	2:D:141:TYR:OH	2.10	0.52
1:G:47:HIS:HB3	1:G:297:ILE:HD13	1.92	0.51
1:E:72:GLY:CA	1:E:149:LYS:H	2.21	0.51
1:E:303:GLY:HA2	2:F:63:PHE:CE1	2.45	0.51
1:E:103:ILE:HD12	1:E:103:ILE:N	2.25	0.51
1:I:116(A):SER:HB3	1:I:261:GLU:HG2	1.92	0.51
2:H:123:ARG:HH22	2:J:123:ARG:HH22	1.58	0.51
1:A:155:VAL:HG12	1:A:156:LYS:N	2.24	0.51
2:L:131:LYS:HZ2	2:L:133:ILE:HG22	1.74	0.51
2:B:88:PHE:CZ	2:D:87:GLY:HA3	2.46	0.51
1:C:52:CYS:HB3	1:C:277:CYS:O	2.10	0.51
2:J:47:GLU:HB3	1:K:30:LEU:HG	1.93	0.51
1:E:195:TYR:O	1:E:196:GLN:HB3	2.11	0.51
1:A:116(A):SER:O	1:A:260:MET:HA	2.11	0.51
2:L:127:LYS:HG3	2:L:128:ASN:H	1.75	0.51
1:E:170:ASN:HB3	1:E:239:PRO:O	2.11	0.51
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.46	0.51
2:L:44:ALA:HA	2:L:110:TYR:OH	2.11	0.51
2:H:164:GLU:H	2:H:164:GLU:CD	2.14	0.51
2:J:58:LYS:O	2:L:94:TYR:HD1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:TYR:CD2	2:F:89:LEU:HD13	2.45	0.50
1:A:307:LYS:HE2	2:B:61:THR:HG22	1.93	0.50
2:D:59:MET:HG3	2:D:61:THR:HG23	1.93	0.50
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.46	0.50
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.92	0.50
1:A:50:LYS:HG2	1:A:275:HIS:ND1	2.27	0.50
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.94	0.50
1:E:295:GLN:O	1:E:308:TYR:HA	2.12	0.50
1:K:116(A):SER:O	1:K:260:MET:HA	2.12	0.50
2:D:132:GLU:HG2	2:D:138:PHE:CE2	2.46	0.50
1:C:28:THR:HG22	2:D:104:ASN:HB3	1.94	0.49
1:C:89:GLU:O	1:C:269:ILE:HA	2.12	0.49
1:E:48:ASN:HD21	1:E:287:ALA:HB3	1.76	0.49
1:G:89:GLU:O	1:G:269:ILE:HA	2.12	0.49
1:E:117:ARG:HD3	1:E:258:PHE:CE1	2.47	0.49
1:I:114:SER:HB2	1:I:266:SER:HB2	1.94	0.49
2:D:158:ASP:OD2	2:D:160:PRO:HD2	2.13	0.49
1:C:42:LEU:HD11	1:C:316:LEU:HG	1.93	0.49
1:E:131:ASP:HB3	1:E:155:VAL:HG23	1.95	0.49
1:E:82:ALA:HB1	1:E:83:SER:HA	1.94	0.49
1:C:304:LYS:HE2	2:D:61:THR:O	2.12	0.49
1:K:119:GLU:CD	1:K:122:PRO:HA	2.33	0.49
1:A:310:LYS:HG3	2:B:89:LEU:HD11	1.94	0.49
1:K:47:HIS:HB3	1:K:297:ILE:HD13	1.94	0.49
1:K:86:TYR:HA	1:K:113:SER:O	2.12	0.49
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.95	0.49
1:E:320:LEU:HD23	1:E:320:LEU:N	2.27	0.49
1:C:283:THR:HG23	1:C:284:PRO:HD2	1.93	0.49
1:I:42:LEU:HD11	1:I:316:LEU:HG	1.95	0.49
1:K:66:ILE:HD12	1:K:109:ARG:HG2	1.95	0.49
2:H:87:GLY:HA3	2:L:88:PHE:CZ	2.48	0.48
1:K:161:TYR:CZ	1:K:249:GLY:HA2	2.48	0.48
1:E:152:ILE:HG13	1:E:255:ARG:HB2	1.96	0.48
1:A:265:GLY:O	1:A:266:SER:HB3	2.12	0.48
1:C:103:ILE:N	1:C:103:ILE:HD12	2.28	0.48
2:F:17:MET:SD	2:F:23:GLY:HA3	2.53	0.48
1:E:152:ILE:HD11	1:E:255:ARG:HD2	1.94	0.48
1:K:28:THR:HG22	2:L:104:ASN:HB3	1.96	0.48
2:D:94:TYR:CZ	2:D:98:LEU:HD11	2.49	0.48
2:F:169:ASN:OD1	2:F:169:ASN:N	2.43	0.48
2:F:125:GLN:NE2	2:F:155:GLY:HA2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:ALA:CB	1:E:83:SER:CA	2.91	0.48
1:I:307:LYS:HE2	2:J:61:THR:HG22	1.96	0.48
1:E:103:ILE:H	1:E:103:ILE:HD12	1.77	0.48
1:K:156:LYS:HD2	1:K:196:GLN:HE21	1.79	0.48
6:G:431:NAG:H62	6:G:432:NAG:H82	1.96	0.48
1:I:130:HIS:CE1	1:I:164:LEU:HB3	2.49	0.48
2:F:6:ILE:HG13	2:F:112:ASP:HA	1.95	0.48
1:E:137:ALA:O	1:E:140:PRO:HD3	2.14	0.48
2:B:17:MET:SD	2:B:23:GLY:HA3	2.54	0.48
2:D:17:MET:C	2:D:19:ASP:H	2.16	0.48
1:C:45:ASP:O	1:C:46:LYS:HD2	2.14	0.48
1:E:283:THR:CG2	1:E:285:LYS:H	2.19	0.48
2:H:62:GLN:NE2	1:I:310:LYS:HZ3	2.10	0.48
1:I:68:GLY:HA3	1:I:95:GLY:HA2	1.95	0.47
1:G:105:TYR:CZ	1:G:109:ARG:HD2	2.49	0.47
2:H:75:LYS:HE3	2:H:79:ASN:HD21	1.79	0.47
1:K:48:ASN:O	1:K:50:LYS:HG3	2.14	0.47
1:I:71:LEU:HD22	1:I:151:LEU:HD11	1.96	0.47
1:I:18:HIS:HB2	2:J:20:GLY:O	2.14	0.47
2:H:45:ILE:O	2:H:49:THR:HG23	2.14	0.47
1:G:103:ILE:HD12	1:G:103:ILE:N	2.28	0.47
2:F:159:TYR:N	2:F:160:PRO:HD2	2.29	0.47
1:I:100:GLY:HA3	1:I:230:MET:O	2.14	0.47
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.48	0.47
1:G:293:PRO:HG2	1:G:294:PHE:CD2	2.49	0.47
1:A:105:TYR:CE2	1:A:109:ARG:HD2	2.50	0.47
1:I:130:HIS:CE1	1:I:162:PRO:HG2	2.49	0.47
1:G:18:HIS:HB2	2:H:20:GLY:O	2.14	0.47
1:G:202:VAL:HB	1:G:213:PHE:HB2	1.96	0.47
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.55	0.47
1:E:82:ALA:HB1	1:E:83:SER:CB	2.44	0.47
1:G:116(B):PHE:CE1	1:G:260:MET:HE2	2.48	0.47
1:E:48:ASN:ND2	1:E:287:ALA:HB3	2.29	0.47
1:G:78:SER:HB2	1:G:149:LYS:NZ	2.29	0.47
1:I:68:GLY:CA	1:I:95:GLY:HA2	2.44	0.47
1:A:185:PRO:HG2	1:A:191:GLN:OE1	2.14	0.47
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.14	0.47
1:C:156:LYS:HE2	1:C:193:SER:O	2.15	0.47
1:C:195:TYR:O	1:C:196:GLN:HB3	2.14	0.47
2:J:94:TYR:O	2:J:98:LEU:HB2	2.15	0.47
2:H:133:ILE:HD13	2:H:139:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:LEU:HD22	7:C:335:HOH:O	2.14	0.47
1:I:129:ASN:HB3	1:I:162:PRO:HG3	1.97	0.47
1:I:76:CYS:O	1:I:77:GLU:C	2.54	0.47
1:I:66:ILE:HG13	1:I:89:GLU:OE2	2.14	0.47
1:K:66:ILE:HG13	1:K:89:GLU:OE2	2.15	0.47
1:C:100:GLY:HA3	1:C:230:MET:O	2.15	0.47
1:C:151:LEU:HB3	1:C:252:VAL:HG12	1.98	0.46
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.95	0.46
1:E:164:LEU:C	1:E:164:LEU:HD12	2.36	0.46
1:I:107:GLU:O	1:I:111:GLN:HG3	2.16	0.46
1:C:202:VAL:HB	1:C:213:PHE:HB2	1.95	0.46
1:A:307:LYS:HG3	2:B:92:TRP:CE2	2.50	0.46
1:K:54:LEU:HB3	1:K:85:SER:HB2	1.95	0.46
1:A:54:LEU:O	1:A:55:ARG:HB2	2.14	0.46
2:B:161:LYS:HE3	2:B:162:TYR:CZ	2.50	0.46
1:G:164:LEU:O	1:G:246:GLU:HA	2.15	0.46
2:F:106:ARG:HD3	7:F:427:HOH:O	2.15	0.46
1:K:164:LEU:HD12	1:K:164:LEU:C	2.36	0.46
1:I:288:ILE:HG21	1:I:297:ILE:HD12	1.97	0.46
2:J:5:ALA:HB3	2:J:112:ASP:OD2	2.16	0.46
2:D:19:ASP:HB3	2:D:36:ALA:HB2	1.97	0.46
1:G:216:GLU:HB3	1:K:203:PHE:HE2	1.79	0.46
1:E:89:GLU:O	1:E:269:ILE:HA	2.15	0.46
1:G:308:TYR:CD2	2:H:89:LEU:HD13	2.51	0.46
1:E:116(B):PHE:CE1	1:E:260:MET:HE2	2.50	0.46
1:I:164:LEU:C	1:I:164:LEU:HD12	2.36	0.46
2:D:88:PHE:CZ	2:F:87:GLY:HA3	2.51	0.46
2:D:145:ASP:OD2	2:D:147:THR:HG22	2.16	0.46
2:H:125:GLN:OE1	2:H:155:GLY:HA2	2.16	0.46
1:G:175:GLU:OE1	1:G:236:LEU:HD13	2.16	0.46
1:C:45:ASP:C	1:C:297:ILE:HD11	2.36	0.46
1:A:17:TYR:CZ	2:B:6:ILE:HG23	2.51	0.46
2:F:4:GLY:O	2:F:8:GLY:HA3	2.16	0.46
2:F:9:PHE:O	2:F:135:ASN:HA	2.16	0.46
1:A:320:LEU:H	1:A:320:LEU:HD23	1.81	0.46
1:C:298:HIS:CE1	1:C:300:ILE:HB	2.51	0.45
1:K:185:PRO:HG2	1:K:191:GLN:OE1	2.16	0.45
1:I:47:HIS:HB3	1:I:288:ILE:HG22	1.98	0.45
1:C:12:THR:OG1	2:D:27:GLN:HG2	2.16	0.45
1:A:123:LYS:HE2	1:A:132:SER:O	2.16	0.45
1:G:73:ASN:HB3	1:G:76:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLU:HG2	2:F:58:LYS:CD	2.42	0.45
1:E:317:ALA:O	2:F:107:THR:HG21	2.15	0.45
2:H:168:LEU:HD23	2:H:168:LEU:O	2.16	0.45
2:F:30:GLN:NE2	2:F:145:ASP:HB2	2.30	0.45
1:E:197:ASN:O	1:E:198:ALA:HB3	2.17	0.45
1:E:46:LYS:N	1:E:297:ILE:HD11	2.31	0.45
2:L:148:CYS:O	2:L:152:VAL:HG23	2.17	0.45
1:E:164:LEU:O	1:E:164:LEU:HD12	2.17	0.45
1:C:71:LEU:O	1:C:148:TYR:HB3	2.16	0.45
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.97	0.45
1:G:320:LEU:HB3	2:H:111:HIS:CG	2.52	0.45
2:L:159:TYR:N	2:L:160:PRO:HD2	2.30	0.45
1:A:238:GLU:HG2	1:A:238:GLU:H	1.54	0.45
2:J:159:TYR:N	2:J:160:PRO:HD2	2.32	0.45
1:A:18:HIS:HB2	2:B:20:GLY:O	2.16	0.45
1:C:164:LEU:HD12	1:C:164:LEU:C	2.37	0.45
1:I:86:TYR:HA	1:I:113:SER:O	2.17	0.45
1:K:51:LEU:HB2	1:K:274:VAL:HA	1.99	0.45
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.98	0.45
1:C:177:LEU:HB3	1:C:258:PHE:HB2	1.99	0.45
2:J:127:LYS:HG2	2:J:128:ASN:N	2.32	0.45
1:C:53:LYS:HG2	1:C:57:ALA:HA	1.98	0.45
1:A:180:TRP:CE2	1:A:233:TYR:HB2	2.51	0.45
2:D:125:GLN:NE2	2:D:155:GLY:HA2	2.32	0.45
2:L:51:LYS:HE3	2:L:103:GLU:OE2	2.17	0.45
1:G:116:SER:HB3	1:G:263:ASN:OD1	2.16	0.45
2:J:158:ASP:CG	2:J:161:LYS:HB2	2.38	0.44
2:F:119:TYR:CE1	2:F:136:GLY:HA2	2.51	0.44
1:K:149:LYS:HE2	1:K:256:TYR:HE1	1.82	0.44
1:G:66:ILE:HG13	1:G:89:GLU:OE2	2.17	0.44
1:A:238:GLU:HG2	7:A:352:HOH:O	2.17	0.44
1:K:151:LEU:HB3	1:K:252:VAL:HG12	1.99	0.44
1:I:195:TYR:O	1:I:196:GLN:HB3	2.18	0.44
1:G:97:CYS:HB2	1:G:138:ALA:O	2.16	0.44
1:E:320:LEU:HD23	1:E:320:LEU:H	1.82	0.44
2:L:127:LYS:HG3	2:L:128:ASN:N	2.33	0.44
1:I:114:SER:HB2	1:I:266:SER:CB	2.47	0.44
1:K:103:ILE:HG12	1:K:233:TYR:CE2	2.52	0.44
1:K:308:TYR:CD2	2:L:89:LEU:HD13	2.53	0.44
2:L:67:GLY:O	2:L:68:LYS:HE3	2.18	0.44
1:C:43:LEU:HB2	1:C:314:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:ILE:HD12	1:G:169:ILE:N	2.33	0.44
1:G:161:TYR:CZ	1:G:249:GLY:HA2	2.53	0.44
1:A:156:LYS:HE2	1:A:193:SER:O	2.17	0.44
1:E:288:ILE:CD1	1:E:295:GLN:HG3	2.47	0.44
2:H:123:ARG:HH22	2:J:123:ARG:NH2	2.15	0.44
1:I:316:LEU:HD22	7:J:189:HOH:O	2.17	0.44
1:A:114:SER:HB2	1:A:266:SER:CB	2.48	0.44
1:A:51:LEU:HA	1:A:282:GLN:NE2	2.32	0.44
2:H:3:PHE:CZ	2:J:2:LEU:HG	2.53	0.44
2:L:133:ILE:HD13	2:L:139:GLU:HB2	2.00	0.44
1:E:288:ILE:HD11	1:E:306:PRO:HD2	1.99	0.44
1:I:116(A):SER:HB3	1:I:261:GLU:CG	2.48	0.44
2:D:18:VAL:O	2:D:18:VAL:HG22	2.18	0.43
1:K:54:LEU:O	1:K:55:ARG:HG3	2.18	0.43
1:K:97:CYS:O	1:K:224:ARG:HD3	2.19	0.43
2:B:2:LEU:HG	2:F:3:PHE:CZ	2.54	0.43
1:A:114:SER:OG	1:A:263:ASN:HB2	2.19	0.43
1:I:305:CYS:O	2:J:61:THR:HG21	2.18	0.43
1:E:145:LYS:NZ	3:E:330:SIA:H31	2.32	0.43
1:I:185:PRO:HG2	1:I:191:GLN:OE1	2.19	0.43
1:K:175:GLU:OE1	1:K:262:ARG:NH1	2.48	0.43
1:E:67:ALA:HB2	1:E:105:TYR:CE1	2.53	0.43
1:G:54:LEU:O	1:G:55:ARG:HB2	2.17	0.43
1:E:15:ILE:HD12	1:E:15:ILE:N	2.32	0.43
2:H:68:LYS:HB3	2:H:70:PHE:CE2	2.54	0.43
2:D:121:LYS:O	2:D:125:GLN:HG3	2.18	0.43
1:E:102:PHE:O	1:E:105:TYR:HB2	2.18	0.43
2:D:125:GLN:CD	2:D:155:GLY:HA2	2.39	0.43
1:A:308:TYR:CD2	2:B:89:LEU:HD13	2.54	0.43
1:E:133(A):LYS:O	3:E:330:SIA:H113	2.19	0.43
2:D:81:ASN:OD1	2:F:80:LEU:HD13	2.19	0.43
2:J:51:LYS:HE3	2:J:103:GLU:OE2	2.19	0.43
1:K:283:THR:OG1	1:K:298:HIS:HB3	2.18	0.43
2:B:127:LYS:HB2	2:B:159:TYR:CE1	2.53	0.43
2:F:3:PHE:CE1	2:F:113:SER:HB2	2.53	0.43
1:A:26:VAL:HB	2:B:104:ASN:ND2	2.34	0.43
1:K:179:LEU:HD23	1:K:234:TRP:HB3	2.01	0.43
2:D:4:GLY:O	2:D:8:GLY:HA3	2.19	0.43
1:K:283:THR:HG22	1:K:286:GLY:O	2.19	0.43
1:K:89:GLU:O	1:K:269:ILE:HA	2.18	0.43
1:G:120:ILE:HG13	1:G:168:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:SER:HA	1:I:221:PRO:HG2	2.01	0.43
2:H:93:THR:O	2:H:97:GLU:HB2	2.19	0.43
1:K:54:LEU:HD21	1:K:302:ILE:HG22	2.01	0.43
2:J:3:PHE:CE2	2:J:113:SER:HB2	2.53	0.43
1:I:241:ASP:OD1	1:I:242:LYS:N	2.50	0.42
2:D:131:LYS:HB3	2:D:141:TYR:CZ	2.54	0.42
2:F:75:LYS:HD3	2:F:75:LYS:HA	1.79	0.42
1:K:288:ILE:O	1:K:288:ILE:HG13	2.18	0.42
1:I:308:TYR:CD2	2:J:89:LEU:HD13	2.54	0.42
2:H:16:GLY:O	2:H:18:VAL:HG23	2.20	0.42
1:A:52:CYS:HB3	1:A:277:CYS:O	2.18	0.42
1:C:197:ASN:O	1:C:198:ALA:HB3	2.18	0.42
1:G:155:VAL:HG12	1:G:156:LYS:N	2.34	0.42
1:G:253:VAL:HA	1:G:254:PRO:HD3	1.93	0.42
1:I:116(A):SER:O	1:I:260:MET:HA	2.20	0.42
1:C:307:LYS:HE2	2:D:61:THR:HG22	2.00	0.42
1:K:288:ILE:HG21	1:K:297:ILE:HD12	2.00	0.42
1:A:127:TRP:CZ2	1:A:253:VAL:HG11	2.54	0.42
2:F:41:THR:O	2:F:45:ILE:HG13	2.19	0.42
1:I:72:GLY:HA3	1:I:149:LYS:H	1.85	0.42
1:C:14:CYS:O	2:D:24:TYR:HA	2.19	0.42
1:K:100:GLY:HA3	1:K:230:MET:O	2.19	0.42
1:I:14:CYS:O	2:J:24:TYR:HA	2.19	0.42
1:G:262:ARG:HG2	1:G:262:ARG:NH1	2.32	0.42
1:K:149:LYS:HE2	1:K:256:TYR:CE1	2.55	0.42
1:K:194:LEU:HD11	3:K:601:SIA:H91	2.00	0.42
1:G:86:TYR:HA	1:G:113:SER:O	2.18	0.42
2:B:18:VAL:O	2:B:18:VAL:HG22	2.19	0.42
2:H:158:ASP:OD1	2:H:160:PRO:HD2	2.19	0.42
1:C:321:ARG:HD2	1:C:323:ILE:HD11	2.01	0.42
1:K:188:SER:O	1:K:192:GLN:HG2	2.20	0.42
2:L:132:GLU:HG2	2:L:138:PHE:CE2	2.55	0.42
1:G:170:ASN:HD21	1:G:176:VAL:HG23	1.85	0.42
1:E:17:TYR:HB2	1:E:320:LEU:HD11	2.02	0.42
1:A:260:MET:HE2	1:A:262:ARG:HG2	2.02	0.42
1:I:46:LYS:N	1:I:297:ILE:HD11	2.35	0.42
2:L:17:MET:SD	2:L:23:GLY:HA3	2.60	0.42
2:B:48:ILE:O	2:B:52:VAL:HG23	2.20	0.42
1:I:155:VAL:HG13	1:I:194:LEU:O	2.20	0.42
1:G:242:LYS:HG2	1:G:243:ILE:N	2.35	0.42
1:G:164:LEU:HD23	1:G:164:LEU:C	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:GLN:O	2:D:27:GLN:HG3	2.20	0.41
1:K:42:LEU:O	1:K:292:LEU:HB3	2.20	0.41
1:A:42:LEU:HD11	1:A:316:LEU:HD22	2.01	0.41
2:L:131:LYS:HZ1	2:L:133:ILE:HG22	1.86	0.41
1:K:195:TYR:O	1:K:196:GLN:HB3	2.20	0.41
1:K:103:ILE:HD12	1:K:103:ILE:N	2.35	0.41
2:F:51:LYS:HE3	2:F:103:GLU:OE2	2.20	0.41
1:I:152:ILE:HG13	1:I:255:ARG:HB2	2.02	0.41
1:K:283:THR:CG2	1:K:285:LYS:H	2.31	0.41
1:I:43:LEU:HB2	1:I:314:LEU:HB2	2.02	0.41
1:G:29:VAL:CG2	2:L:51:LYS:HG3	2.51	0.41
2:D:111:HIS:O	2:D:115:VAL:HG23	2.20	0.41
1:E:83(A):SER:CB	1:E:116:SER:HA	2.50	0.41
1:E:310:LYS:HD3	2:F:89:LEU:HD21	2.03	0.41
1:G:140:PRO:HD2	6:G:431:NAG:H83	2.02	0.41
2:F:5:ALA:HB3	2:F:112:ASP:OD2	2.20	0.41
1:A:222:LYS:HE2	1:A:227:GLU:HG3	2.03	0.41
1:E:116(B):PHE:HE1	1:E:260:MET:HE2	1.86	0.41
1:C:164:LEU:O	1:C:164:LEU:HD12	2.20	0.41
1:G:155:VAL:CG1	1:G:156:LYS:N	2.83	0.41
1:I:215:PRO:HB3	1:I:250:ASN:ND2	2.35	0.41
1:G:17:TYR:HB3	2:H:115:VAL:HG21	2.02	0.41
1:C:211:LYS:HD3	1:C:213:PHE:CZ	2.55	0.41
2:F:142:HIS:HD2	2:F:166:ALA:HB2	1.85	0.41
2:F:167:LYS:HG3	2:F:168:LEU:HD12	2.02	0.41
1:K:47:HIS:HB3	1:K:288:ILE:HG22	2.03	0.41
1:C:202:VAL:HG11	1:C:251:LEU:HD13	2.03	0.41
1:G:58:PRO:HB3	1:G:86:TYR:CZ	2.56	0.41
1:C:222:LYS:NZ	1:C:227:GLU:HG3	2.36	0.41
1:E:97:CYS:HB2	1:E:138:ALA:O	2.21	0.41
2:D:164:GLU:CD	2:D:164:GLU:H	2.24	0.41
1:A:265:GLY:O	1:A:266:SER:CB	2.69	0.41
1:C:48:ASN:ND2	1:C:287:ALA:HB3	2.36	0.41
1:G:26:VAL:O	1:G:32:LYS:O	2.38	0.41
2:J:21:TRP:CE3	2:J:111:HIS:HE1	2.39	0.41
2:D:72:HIS:CD2	2:D:72:HIS:H	2.39	0.41
1:K:310:LYS:O	1:K:310:LYS:HG2	2.21	0.41
2:H:62:GLN:HE21	1:I:310:LYS:NZ	2.14	0.41
1:C:97:CYS:HB2	1:C:138:ALA:O	2.22	0.41
1:I:295:GLN:HE21	1:I:295:GLN:HB3	1.73	0.41
1:A:284:PRO:HG2	1:A:298:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:GLN:O	2:D:127:LYS:HD2	2.21	0.40
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.84	0.40
1:G:123:LYS:HB2	1:G:152:ILE:HD11	2.03	0.40
2:L:80:LEU:O	2:L:84:VAL:HG23	2.20	0.40
1:K:134:GLY:HA3	1:K:153:TRP:HB3	2.04	0.40
2:H:3:PHE:CE1	2:H:113:SER:HB2	2.57	0.40
2:L:123:ARG:HB2	2:L:138:PHE:HZ	1.86	0.40
1:A:29:VAL:CG2	2:F:51:LYS:HG3	2.52	0.40
1:C:310:LYS:HB3	1:C:310:LYS:HE2	1.74	0.40
1:A:100:GLY:HA3	1:A:230:MET:O	2.20	0.40
2:L:149:MET:HA	2:L:149:MET:CE	2.51	0.40
1:K:90(A):PRO:HD2	1:K:271:ASP:OD1	2.21	0.40
1:K:90:THR:HA	1:K:90(A):PRO:HD3	1.97	0.40
1:I:103:ILE:HD12	1:I:103:ILE:N	2.37	0.40
1:E:298:HIS:CG	1:E:299:PRO:HD2	2.57	0.40
1:A:26:VAL:HG21	1:A:317:ALA:HB2	2.03	0.40
1:C:133(A):LYS:O	3:C:330:SIA:H113	2.21	0.40
1:C:260:MET:CE	1:C:262:ARG:HG2	2.52	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%)	300 (94%)	18 (6%)	3 (1%)	21	37
1	C	315/329 (96%)	300 (95%)	13 (4%)	2 (1%)	30	50
1	E	321/329 (98%)	294 (92%)	22 (7%)	5 (2%)	12	21
1	G	317/329 (96%)	301 (95%)	16 (5%)	0	100	100
1	I	315/329 (96%)	291 (92%)	21 (7%)	3 (1%)	19	34
1	K	315/329 (96%)	297 (94%)	16 (5%)	2 (1%)	30	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	172/177 (97%)	167 (97%)	5 (3%)	0	100	100
2	D	169/177 (96%)	156 (92%)	13 (8%)	0	100	100
2	F	168/177 (95%)	157 (94%)	10 (6%)	1 (1%)	30	50
2	H	168/177 (95%)	159 (95%)	9 (5%)	0	100	100
2	J	168/177 (95%)	158 (94%)	8 (5%)	2 (1%)	16	29
2	L	168/177 (95%)	161 (96%)	5 (3%)	2 (1%)	16	29
All	All	2917/3036 (96%)	2741 (94%)	156 (5%)	20 (1%)	26	46

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	60	ASN
1	C	264	ALA
1	E	80	SER
1	I	93	ASP
1	K	265	GLY
1	A	266	SER
1	C	94	ASN
1	E	78	SER
1	E	83	SER
1	E	116(A)	SER
1	I	198	ALA
2	J	5	ALA
1	A	92	SER
1	A	264	ALA
2	F	169	ASN
1	I	324	PRO
1	K	239	PRO
2	L	60	ASN
1	E	81	THR
2	L	59	MET

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%)	280 (98%)	5 (2%)	66	88
1	C	281/290 (97%)	276 (98%)	5 (2%)	66	88
1	E	285/290 (98%)	279 (98%)	6 (2%)	61	85
1	G	283/290 (98%)	277 (98%)	6 (2%)	61	85
1	I	281/290 (97%)	274 (98%)	7 (2%)	55	82
1	K	281/290 (97%)	275 (98%)	6 (2%)	61	85
2	B	150/152 (99%)	143 (95%)	7 (5%)	32	56
2	D	147/152 (97%)	141 (96%)	6 (4%)	37	63
2	F	146/152 (96%)	142 (97%)	4 (3%)	52	79
2	H	146/152 (96%)	143 (98%)	3 (2%)	61	85
2	J	146/152 (96%)	142 (97%)	4 (3%)	52	79
2	L	146/152 (96%)	143 (98%)	3 (2%)	61	85
All	All	2577/2652 (97%)	2515 (98%)	62 (2%)	57	82

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	PHE
1	A	238	GLU
1	A	253	VAL
1	A	315	ARG
1	A	320	LEU
2	B	22	TYR
2	B	26	HIS
2	B	29	GLU
2	B	97	GLU
2	B	161	LYS
2	B	164	GLU
2	B	174	ASP
1	C	77	GLU
1	C	192	GLN
1	C	295	GLN
1	C	316	LEU
1	C	320	LEU
2	D	29	GLU
2	D	66	VAL
2	D	68	LYS
2	D	72	HIS
2	D	102	LEU

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Mol	Chain	Res	Type
2	D	164	GLU
1	E	54	LEU
1	E	79	LEU
1	E	81	THR
1	E	102	PHE
1	E	295	GLN
1	E	320	LEU
2	F	22	TYR
2	F	102	LEU
2	F	150	GLU
2	F	169	ASN
1	G	136	THR
1	G	174	LYS
1	G	203	PHE
1	G	225	ASP
1	G	253	VAL
1	G	261	GLU
2	H	60	ASN
2	H	68	LYS
2	H	164	GLU
1	I	55	ARG
1	I	77	GLU
1	I	102	PHE
1	I	125	SER
1	I	295	GLN
1	I	316	LEU
1	I	320	LEU
2	J	22	TYR
2	J	98	LEU
2	J	102	LEU
2	J	123	ARG
1	K	55	ARG
1	K	97	CYS
1	K	102	PHE
1	K	274	VAL
1	K	283	THR
1	K	295	GLN
2	L	30	GLN
2	L	102	LEU
2	L	149	MET

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

Mol	Chain	Res	Type
1	A	263	ASN
2	B	26	HIS
2	B	43	ASN
2	B	79	ASN
2	B	95	ASN
2	D	72	HIS
2	D	95	ASN
1	E	298	HIS
2	F	30	GLN
2	F	50	ASN
2	H	60	ASN
2	H	62	GLN
1	I	21	ASN
1	I	289	ASN
2	J	30	GLN
2	J	95	ASN
2	J	117	ASN
1	K	196	GLN
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

19 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	0.27	0	18,28,31	1.22	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GAL	A	331	3	11,11,12	0.69	0	14,15,17	0.77	0
3	NAG	A	332	3	15,15,15	0.45	0	17,21,21	0.56	0
3	SIA	C	330	3	16,20,21	0.25	0	18,28,31	1.06	2 (11%)
3	GAL	C	331	3	11,11,12	0.65	0	14,15,17	0.73	0
3	NAG	C	332	3	15,15,15	0.51	0	17,21,21	0.63	0
3	SIA	E	330	3	16,20,21	0.23	0	18,28,31	1.32	2 (11%)
3	GAL	E	331	3	11,11,12	0.60	0	14,15,17	0.60	0
3	NAG	E	332	3	15,15,15	0.48	0	17,21,21	0.76	0
5	SIA	G	401	5	16,20,21	0.21	0	18,28,31	1.10	1 (5%)
5	GAL	G	402	5	11,11,12	0.61	0	14,15,17	0.52	0
6	NAG	G	431	1,6	14,14,15	0.55	0	15,19,21	0.71	0
6	NAG	G	432	6	14,14,15	0.54	0	15,19,21	0.73	0
3	SIA	I	501	3	16,20,21	0.25	0	18,28,31	1.39	3 (16%)
3	GAL	I	502	3	11,11,12	0.62	0	14,15,17	0.64	0
3	NAG	I	503	3	15,15,15	0.53	0	17,21,21	0.67	0
3	SIA	K	601	3	16,20,21	0.25	0	18,28,31	1.27	2 (11%)
3	GAL	K	602	3	11,11,12	0.65	0	14,15,17	0.81	1 (7%)
3	NAG	K	603	3	15,15,15	0.47	0	17,21,21	0.65	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	-	0/2/19/22	0/1/1/1
3	NAG	A	332	3	-	0/6/26/26	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	-	0/6/26/26	0/1/1/1
3	SIA	E	330	3	-	0/14/34/38	0/1/1/1
3	GAL	E	331	3	-	0/2/19/22	0/1/1/1
3	NAG	E	332	3	-	0/6/26/26	0/1/1/1
5	SIA	G	401	5	-	0/14/34/38	0/1/1/1
5	GAL	G	402	5	-	0/2/19/22	0/1/1/1
6	NAG	G	431	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	432	6	-	0/6/23/26	0/1/1/1
3	SIA	I	501	3	-	0/14/34/38	0/1/1/1
3	GAL	I	502	3	-	0/2/19/22	0/1/1/1
3	NAG	I	503	3	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/6/26/26	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})
3	I	501	SIA	C7-C6-C5	-3.31	109.31	114.32
3	E	330	SIA	C7-C6-C5	-3.14	109.57	114.32
3	A	330	SIA	C7-C6-C5	-2.91	109.91	114.32
3	C	330	SIA	C7-C6-C5	-2.32	110.81	114.32
3	K	601	SIA	C7-C6-C5	-2.27	110.89	114.32
3	K	602	GAL	C1-O5-C5	-2.19	109.47	112.25
3	I	501	SIA	O6-C2-C3	2.24	114.17	109.86
3	C	330	SIA	O6-C6-C5	2.56	112.67	108.48
3	A	330	SIA	O6-C6-C5	2.94	113.31	108.48
3	K	601	SIA	O6-C6-C5	3.27	113.84	108.48
3	I	501	SIA	O6-C6-C5	3.33	113.93	108.48
5	G	401	SIA	O6-C6-C5	3.37	113.99	108.48
3	E	330	SIA	O6-C6-C5	3.59	114.36	108.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	330	SIA	1	0
3	E	330	SIA	2	0
6	G	431	NAG	2	0
6	G	432	NAG	1	0
3	K	601	SIA	1	0

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	333	1	14,14,15	0.51	0	15,19,21	0.77	0
4	NAG	A	334	1	14,14,15	0.48	0	15,19,21	0.71	0
4	NAG	A	335	1	14,14,15	0.48	0	15,19,21	0.86	0
4	NAG	A	336	1	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
4	NAG	C	333	1	14,14,15	0.48	0	15,19,21	0.79	0
4	NAG	C	334	1	14,14,15	0.50	0	15,19,21	0.68	0
4	NAG	E	333	1	14,14,15	0.51	0	15,19,21	0.68	0
4	NAG	J	561	2	14,14,15	0.48	0	15,19,21	0.65	0
4	NAG	K	641	1	14,14,15	0.47	0	15,19,21	0.99	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
4	NAG	A	333	1	-	0/6/23/26	0/1/1/1
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	333	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
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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	641	NAG	C1-O5-C5	2.09	114.90	112.25
4	A	336	NAG	C1-O5-C5	2.16	114.99	112.25

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
4	C	333	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%)	0.07	1 (0%) 94 95	30, 44, 60, 79	0
1	C	319/329 (96%)	-0.11	4 (1%) 79 82	30, 41, 60, 85	0
1	E	323/329 (98%)	0.05	5 (1%) 76 79	35, 49, 67, 88	0
1	G	321/329 (97%)	0.00	4 (1%) 81 83	28, 41, 61, 83	0
1	I	319/329 (96%)	-0.00	7 (2%) 65 69	32, 46, 62, 81	0
1	K	319/329 (96%)	0.03	5 (1%) 74 78	28, 42, 60, 85	0
2	B	174/177 (98%)	0.26	9 (5%) 31 35	34, 58, 80, 95	0
2	D	171/177 (96%)	0.67	27 (15%) 3 2	30, 57, 90, 103	0
2	F	170/177 (96%)	0.58	25 (14%) 3 3	32, 55, 94, 105	0
2	H	170/177 (96%)	0.65	22 (12%) 5 4	31, 51, 88, 99	0
2	J	170/177 (96%)	0.10	4 (2%) 62 66	31, 49, 69, 81	0
2	L	170/177 (96%)	-0.00	1 (0%) 90 91	30, 46, 62, 69	0
All	All	2949/3036 (97%)	0.14	114 (3%) 43 48	28, 46, 79, 105	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	168	LEU	5.9
2	D	16	GLY	5.1
1	C	12	THR	4.8
2	D	168	LEU	4.7
2	F	160	PRO	4.7
2	D	147	THR	4.7
2	F	29	GLU	4.6
2	D	144	CYS	4.3
2	B	33	GLY	4.2
2	D	157	TYR	4.1
2	J	133	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	162	TYR	4.1
2	F	164	GLU	4.0
2	F	161	LYS	4.0
1	K	94	ASN	4.0
2	D	160	PRO	4.0
2	D	142	HIS	3.9
2	D	138	PHE	3.9
2	H	143	LYS	3.9
2	H	144	CYS	3.8
2	F	158	ASP	3.7
2	D	143	LYS	3.7
2	D	140	PHE	3.6
2	D	156	THR	3.6
2	D	141	TYR	3.4
2	D	128	ASN	3.4
1	I	264	ALA	3.4
2	F	147	THR	3.4
2	H	141	TYR	3.3
2	D	129	ASN	3.3
2	B	173	ILE	3.3
2	H	164	GLU	3.3
2	J	143	LYS	3.2
2	H	167	LYS	3.2
1	G	13	LEU	3.2
2	F	38	LEU	3.2
2	H	159	TYR	3.2
2	H	140	PHE	3.2
2	H	29	GLU	3.1
2	F	156	THR	3.1
1	C	264	ALA	3.0
2	D	19	ASP	2.9
2	F	166	ALA	2.9
2	D	27	GLN	2.9
2	F	30	GLN	2.9
1	I	54	LEU	2.9
1	C	90(A)	PRO	2.9
1	I	55	ARG	2.9
1	G	12	THR	2.9
2	D	159	TYR	2.8
2	H	23	GLY	2.8
2	F	162	TYR	2.8
2	H	18	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	33	GLY	2.7
2	J	166	ALA	2.7
1	K	93	ASP	2.7
2	B	174	ASP	2.7
1	E	161	TYR	2.7
2	D	166	ALA	2.7
1	C	78	SER	2.7
1	A	325	SER	2.6
2	D	137	CYS	2.6
2	H	168	LEU	2.6
2	F	31	GLY	2.6
1	E	198	ALA	2.6
2	H	42	GLN	2.6
1	I	208	ARG	2.6
2	D	154	ASN	2.5
1	E	13	LEU	2.5
1	G	81	THR	2.5
2	H	65	ALA	2.5
2	H	166	ALA	2.5
2	B	138	PHE	2.5
2	D	152	VAL	2.5
2	F	60	ASN	2.5
2	J	134	GLY	2.5
2	F	23	GLY	2.5
1	E	81	THR	2.4
2	B	168	LEU	2.4
2	F	144	CYS	2.4
1	I	290	THR	2.4
2	F	148	CYS	2.4
2	H	157	TYR	2.4
2	H	145	ASP	2.4
2	F	163	SER	2.4
2	F	149	MET	2.4
2	H	160	PRO	2.3
2	F	140	PHE	2.3
2	B	34	TYR	2.3
1	I	198	ALA	2.3
2	B	27	GLN	2.3
2	F	28	ASN	2.2
2	F	143	LYS	2.2
1	K	275	HIS	2.2
2	B	25	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	152	VAL	2.2
1	K	239	PRO	2.2
2	H	139	GLU	2.2
2	D	161	LYS	2.2
1	K	9	PRO	2.2
1	G	40	VAL	2.2
1	E	11	ASP	2.2
2	B	140	PHE	2.2
2	D	18	VAL	2.2
1	I	288	ILE	2.2
2	F	146	ASN	2.1
2	H	156	THR	2.1
2	F	33	GLY	2.1
2	D	139	GLU	2.1
2	F	1	GLY	2.1
2	H	32	SER	2.1
2	D	167	LYS	2.0
2	D	158	ASP	2.0
2	L	31	GLY	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
6	NAG	G	432	14/15	0.84	0.21	1.90	48,57,64,68	0
3	SIA	K	601	20/21	0.93	0.23	1.44	47,59,66,68	0
3	GAL	K	602	11/12	0.84	0.27	0.89	64,73,82,85	0
5	GAL	G	402	11/12	0.93	0.22	0.86	55,67,74,76	0
3	SIA	E	330	20/21	0.94	0.17	0.70	49,55,62,66	0
6	NAG	G	431	14/15	0.92	0.15	0.25	38,50,56,56	0
3	SIA	A	330	20/21	0.96	0.15	-0.03	36,43,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SIA	I	501	20/21	0.96	0.12	-0.70	31,46,52,52	0
3	SIA	C	330	20/21	0.96	0.13	-0.71	33,39,43,47	0
5	SIA	G	401	20/21	0.95	0.12	-0.93	35,45,51,52	0
3	NAG	K	603	15/15	0.87	0.29	-	58,77,81,85	0
3	NAG	C	332	15/15	0.93	0.16	-	47,53,64,65	0
3	NAG	A	332	15/15	0.77	0.30	-	57,69,76,78	0
3	GAL	C	331	11/12	0.94	0.11	-	44,51,54,58	0
3	GAL	I	502	11/12	0.93	0.13	-	48,51,56,58	0
3	NAG	E	332	15/15	0.90	0.18	-	55,63,66,68	0
3	NAG	I	503	15/15	0.90	0.14	-	45,54,65,66	0
3	GAL	A	331	11/12	0.92	0.12	-	49,59,66,73	0
3	GAL	E	331	11/12	0.94	0.08	-	51,58,61,61	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
4	NAG	A	336	14/15	0.82	0.26	2.14	71,76,80,83	0
4	NAG	A	334	14/15	0.71	0.20	0.77	65,74,89,90	0
4	NAG	J	561	14/15	0.81	0.18	0.19	76,78,83,84	0
4	NAG	E	333	14/15	0.93	0.14	0.10	48,56,60,60	0
4	NAG	C	334	14/15	0.87	0.15	-0.04	62,76,83,84	0
4	NAG	C	333	14/15	0.94	0.12	-0.58	47,56,67,69	0
4	NAG	A	335	14/15	0.87	0.13	-1.18	48,52,58,61	0
4	NAG	A	333	14/15	0.76	0.44	-	70,84,86,87	0
4	NAG	K	641	14/15	0.78	0.28	-	71,81,89,91	0

6.5 Other polymers

There are no such residues in this entry.