Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:44 PM GMT

PDB ID	:	5E30
Title	:	Crystal structure of H5 hemagglutinin Q226L mutant from the influenza virus A/duck/Egypt/10185SS/2010 (H5N1) with LSTc
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2015-10-01
Resolution	:	2.70 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:

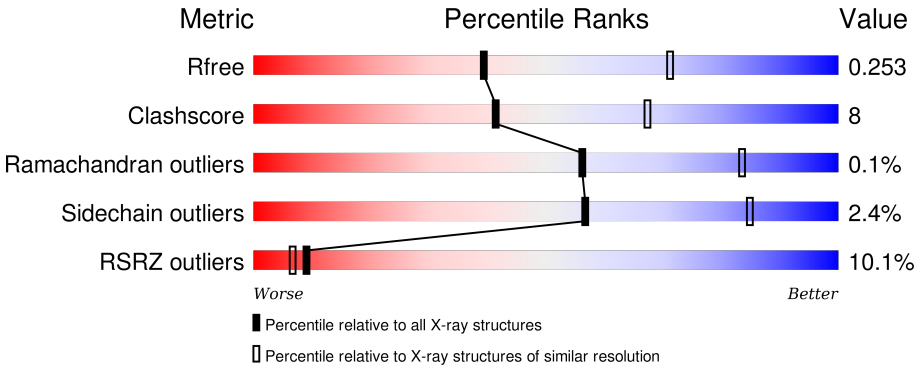
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	5% 79% 17%
1	C	333	4% 75% 21%
1	E	333	2% 81% 15%
2	B	180	14% 73% 24%
2	D	180	28% 71% 26%

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Mol	Chain	Length	Quality of chain
2	F	180	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1008	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12411 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	323	Total	C	N	O	S	0	0	0
			2558	1611	443	490	14			
1	A	323	Total	C	N	O	S	0	0	0
			2558	1611	443	490	14			
1	E	323	Total	C	N	O	S	0	0	0
			2558	1611	443	490	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	ALA	-	expression tag	UNP G8IPF0
C	8	ASP	-	expression tag	UNP G8IPF0
C	9	PRO	-	expression tag	UNP G8IPF0
C	10	GLY	-	expression tag	UNP G8IPF0
C	226	LEU	GLN	engineered mutation	UNP G8IPF0
A	7	ALA	-	expression tag	UNP G8IPF0
A	8	ASP	-	expression tag	UNP G8IPF0
A	9	PRO	-	expression tag	UNP G8IPF0
A	10	GLY	-	expression tag	UNP G8IPF0
A	226	LEU	GLN	engineered mutation	UNP G8IPF0
E	7	ALA	-	expression tag	UNP G8IPF0
E	8	ASP	-	expression tag	UNP G8IPF0
E	9	PRO	-	expression tag	UNP G8IPF0
E	10	GLY	-	expression tag	UNP G8IPF0
E	226	LEU	GLN	engineered mutation	UNP G8IPF0

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1418	880	248	282	8			

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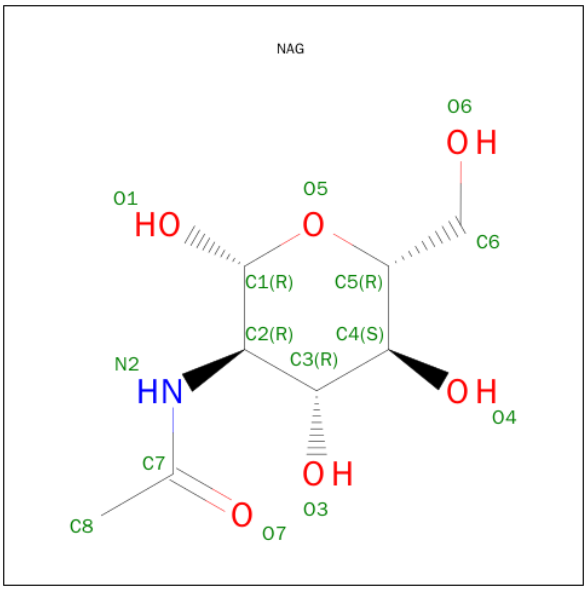
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1418	880	248	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1418	880	248	282	8			

There are 15 discrepancies between the modelled and reference sequences:

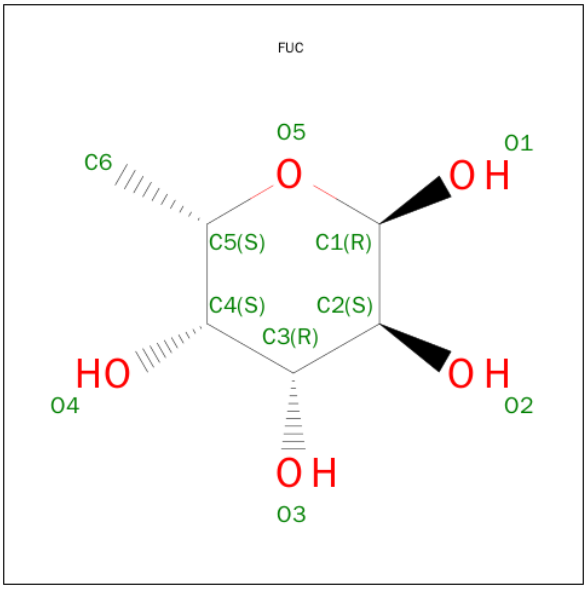
Chain	Residue	Modelled	Actual	Comment	Reference
D	176	ARG	-	expression tag	UNP G8IPF0
D	177	LEU	-	expression tag	UNP G8IPF0
D	178	VAL	-	expression tag	UNP G8IPF0
D	179	PRO	-	expression tag	UNP G8IPF0
D	180	ARG	-	expression tag	UNP G8IPF0
B	176	ARG	-	expression tag	UNP G8IPF0
B	177	LEU	-	expression tag	UNP G8IPF0
B	178	VAL	-	expression tag	UNP G8IPF0
B	179	PRO	-	expression tag	UNP G8IPF0
B	180	ARG	-	expression tag	UNP G8IPF0
F	176	ARG	-	expression tag	UNP G8IPF0
F	177	LEU	-	expression tag	UNP G8IPF0
F	178	VAL	-	expression tag	UNP G8IPF0
F	179	PRO	-	expression tag	UNP G8IPF0
F	180	ARG	-	expression tag	UNP G8IPF0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



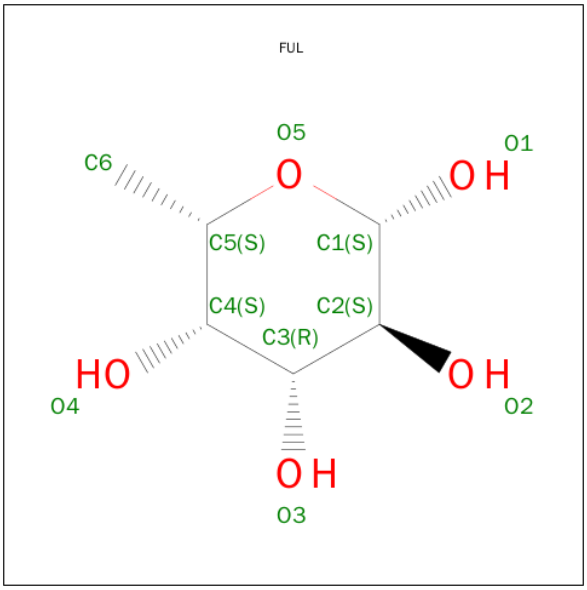
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1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

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



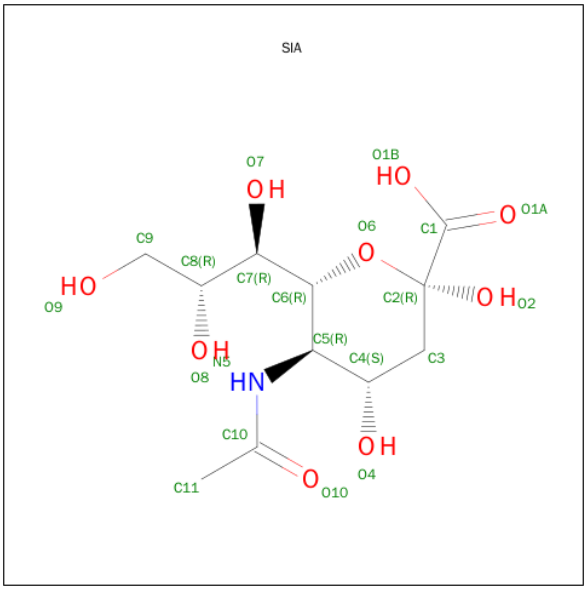
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is BETA-L-FUCOSE (three-letter code: FUL) (formula: $C_6H_{12}O_5$).



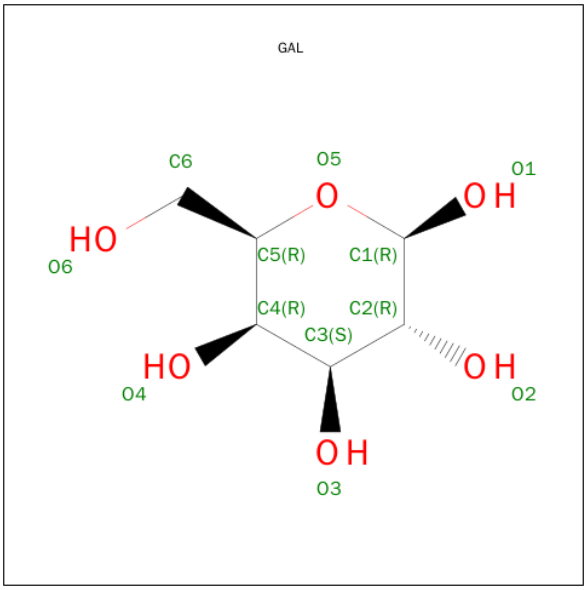
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 10 6 4	0	0
5	A	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0

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



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

- Molecule 7 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 11 6 5	0	0
7	C	1	Total C O 12 6 6	0	0
7	A	1	Total C O 11 6 5	0	0
7	A	1	Total C O 12 6 6	0	0
7	E	1	Total C O 11 6 5	0	0
7	E	1	Total C O 12 6 6	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	49	Total O 49 49	0	0

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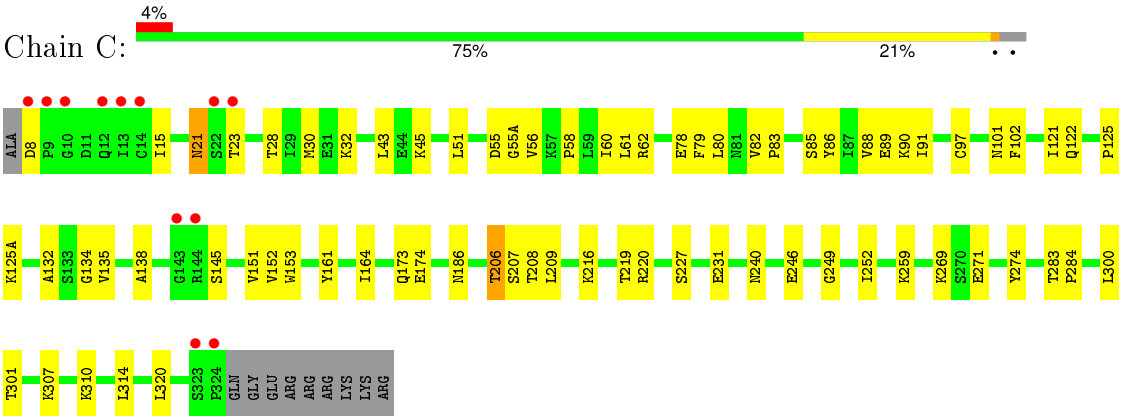
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	8	Total O 8 8	0	0
8	A	60	Total O 60 60	0	0
8	B	4	Total O 4 4	0	0
8	E	33	Total O 33 33	0	0
8	F	6	Total O 6 6	0	0

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.

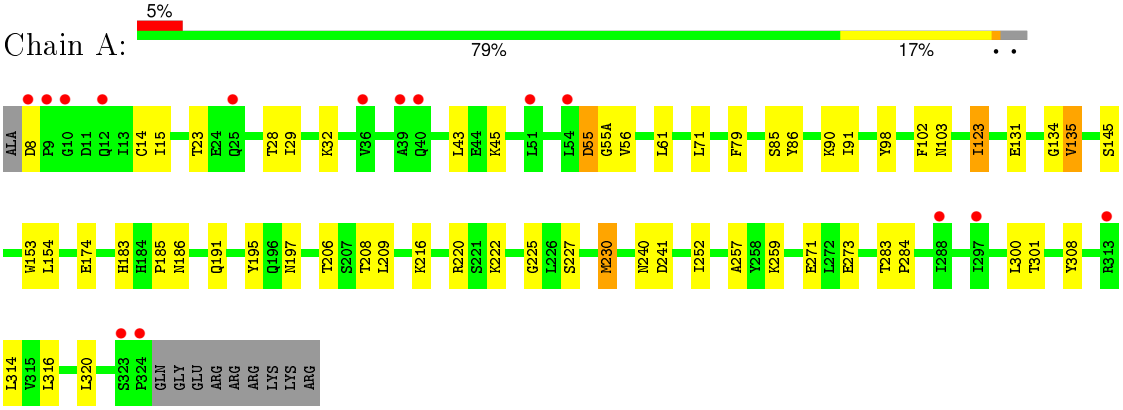
- Molecule 1: Hemagglutinin

Chain C:



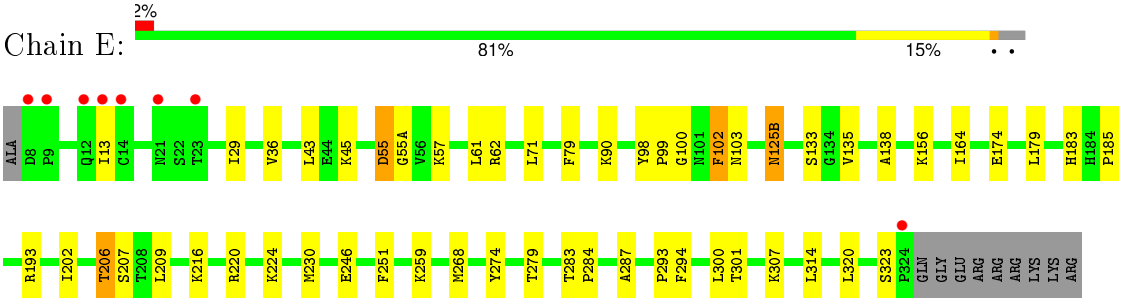
- Molecule 1: Hemagglutinin

Chain A:



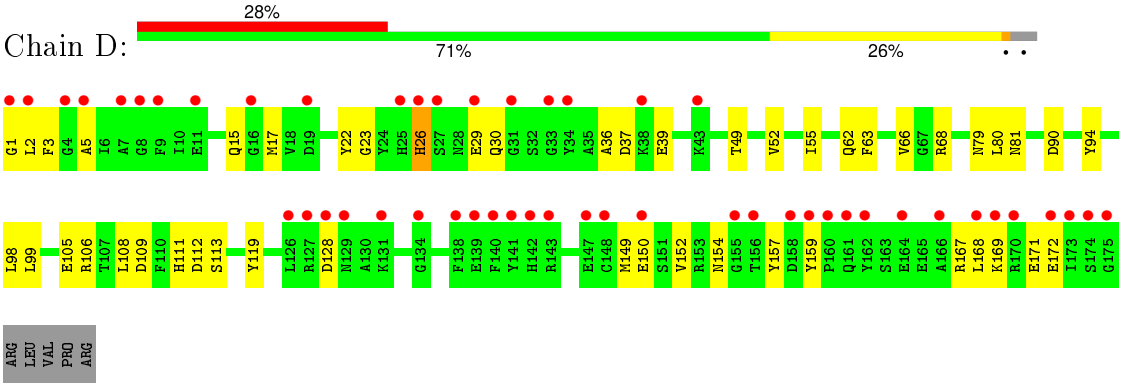
- Molecule 1: Hemagglutinin

Chain E:



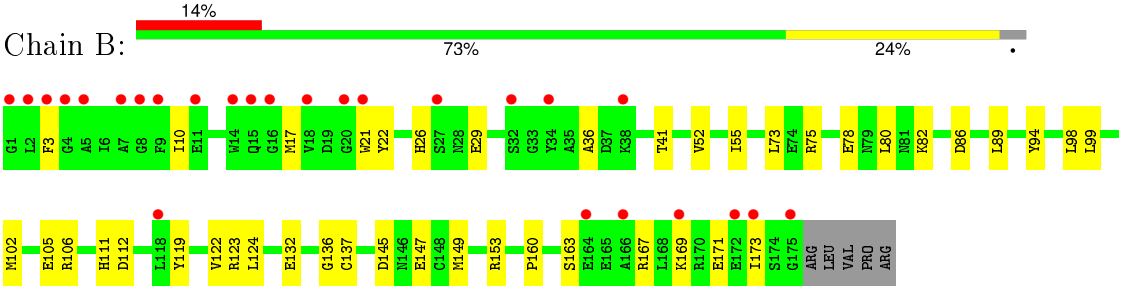
• Molecule 2: Hemagglutinin

Chain D:



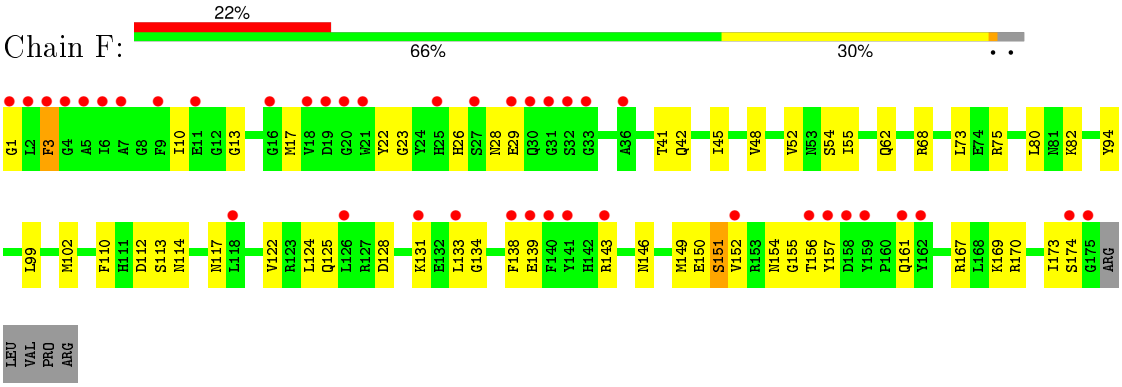
• Molecule 2: Hemagglutinin

Chain B:



• Molecule 2: Hemagglutinin

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.90Å 228.52Å 70.68Å 90.00° 114.29° 90.00°	Depositor
Resolution (Å)	49.19 – 2.70 49.19 – 2.69	Depositor EDS
% Data completeness (in resolution range)	94.8 (49.19-2.70) 94.8 (49.19-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.249 0.208 , 0.253	Depositor DCC
R_{free} test set	2669 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.5	EDS
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 52918 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12411	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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, FUL, FUC

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	0.53	0/2619	0.67	1/3559 (0.0%)
1	C	0.52	0/2619	0.65	0/3559
1	E	0.49	0/2619	0.64	0/3559
2	B	0.39	0/1445	0.53	0/1942
2	D	0.40	0/1445	0.59	0/1942
2	F	0.40	0/1445	0.53	0/1942
All	All	0.48	0/12192	0.62	1/16503 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	ILE	CG1-CB-CG2	-5.09	100.20	111.40

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	2558	0	2493	38	0
1	C	2558	0	2492	47	0
1	E	2558	0	2492	33	0
2	B	1418	0	1322	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1418	0	1322	37	0
2	F	1418	0	1322	43	0
3	A	42	0	36	1	0
3	C	56	0	48	2	0
3	E	56	0	49	0	0
4	C	10	0	10	0	0
5	A	10	0	10	0	0
5	C	10	0	10	1	0
5	E	10	0	10	0	0
6	A	20	0	17	1	0
6	C	20	0	17	0	0
6	E	20	0	17	0	0
7	A	23	0	20	0	0
7	C	23	0	20	0	0
7	E	23	0	20	0	0
8	A	60	0	0	0	0
8	B	4	0	0	0	0
8	C	49	0	0	1	0
8	D	8	0	0	1	0
8	E	33	0	0	0	0
8	F	6	0	0	0	0
All	All	12411	0	11727	203	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 8.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:THR:HG22	1:C:208:THR:H	1.36	0.89
1:E:206:THR:HG22	1:E:209:LEU:H	1.36	0.88
1:E:174:GLU:HG3	1:E:259:LYS:HB3	1.61	0.82
1:E:29:ILE:HD11	2:F:102:MET:HA	1.66	0.78
2:B:123:ARG:NH1	2:B:132:GLU:OE1	2.20	0.75
1:C:216:LYS:O	1:C:220:ARG:NH2	2.20	0.73
1:A:206:THR:HG22	1:A:208:THR:H	1.54	0.72
1:C:121:ILE:HG21	1:C:259:LYS:HE3	1.72	0.71
1:A:29:ILE:HD11	2:B:102:MET:HA	1.76	0.67
1:C:28:THR:HB	2:D:105:GLU:HB2	1.76	0.67
1:E:125(B):ASN:OD1	1:E:125(B):ASN:N	2.28	0.67
1:E:216:LYS:O	1:E:220:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:HIS:HB2	2:F:149:MET:SD	2.36	0.66
1:A:28:THR:HB	2:B:105:GLU:HB2	1.79	0.65
1:C:206:THR:HB	1:C:209:LEU:HB3	1.78	0.65
2:F:128:ASP:O	2:F:170:ARG:NH2	2.31	0.64
2:B:22:TYR:OH	2:B:111:HIS:ND1	2.25	0.63
2:D:1:GLY:O	2:F:117:ASN:ND2	2.31	0.63
2:D:3:PHE:HD2	2:D:5:ALA:H	1.45	0.63
2:F:125:GLN:OE1	2:F:155:GLY:HA2	2.00	0.62
2:F:1:GLY:HA3	2:F:112:ASP:OD2	2.00	0.62
1:C:56:VAL:HB	1:C:85:SER:HB3	1.83	0.61
1:C:174:GLU:HG3	1:C:259:LYS:HB3	1.80	0.61
1:E:283:THR:HG22	1:E:301:THR:HG22	1.83	0.61
2:F:110:PHE:O	2:F:114:ASN:ND2	2.33	0.61
1:C:206:THR:HG22	1:C:208:THR:N	2.12	0.61
2:F:55:ILE:HG13	2:F:99:LEU:HD23	1.82	0.60
2:D:3:PHE:H	2:F:117:ASN:HD21	1.48	0.60
2:F:29:GLU:HG3	2:F:143:ARG:HH21	1.66	0.59
1:E:43:LEU:O	1:E:45:LYS:NZ	2.35	0.59
2:B:55:ILE:HG13	2:B:99:LEU:HD13	1.83	0.59
1:E:206:THR:HG22	1:E:209:LEU:N	2.12	0.58
1:C:186:ASN:ND2	1:C:227:SER:OG	2.30	0.58
2:F:150:GLU:OE2	2:F:154:ASN:ND2	2.35	0.58
2:D:26:HIS:HB2	2:D:149:MET:SD	2.45	0.56
1:C:206:THR:HG22	1:C:209:LEU:H	1.71	0.56
1:E:62:ARG:O	1:E:90:LYS:HD2	2.05	0.56
2:B:55:ILE:HD12	2:B:99:LEU:HD22	1.87	0.56
1:A:135:VAL:HG13	1:A:145:SER:HB3	1.87	0.56
2:D:55:ILE:HG13	2:D:99:LEU:HD23	1.88	0.56
1:E:268:MET:HG2	1:E:284:PRO:HG3	1.86	0.56
2:B:21:TRP:HB2	2:B:41:THR:HG23	1.87	0.55
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.87	0.55
1:E:307:LYS:HE2	2:F:62:GLN:HB3	1.89	0.55
2:D:29:GLU:HG3	2:D:30:GLN:HG3	1.87	0.55
2:B:167:ARG:NH1	2:F:173:ILE:O	2.39	0.54
1:A:206:THR:HB	1:A:209:LEU:HB3	1.89	0.54
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.07	0.54
1:C:62:ARG:O	1:C:90:LYS:HD2	2.08	0.54
1:E:284:PRO:HD3	1:E:300:LEU:O	2.07	0.54
1:A:43:LEU:HB2	1:A:314:LEU:HB2	1.90	0.54
2:B:82:LYS:NZ	2:B:86:ASP:OD2	2.34	0.54
2:D:3:PHE:N	2:F:117:ASN:HD21	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:HG	1:A:86:TYR:HD1	1.56	0.53
1:C:135:VAL:HG13	1:C:145:SER:HB3	1.91	0.53
1:E:323:SER:CB	2:F:13:GLY:H	2.21	0.52
2:B:26:HIS:HB2	2:B:149:MET:SD	2.50	0.52
2:B:167:ARG:HH12	2:F:173:ILE:HG22	1.74	0.52
2:F:151:SER:HB3	2:F:157:TYR:HA	1.92	0.52
2:D:1:GLY:HA3	2:D:3:PHE:CE1	2.45	0.51
2:D:94:TYR:CZ	2:D:98:LEU:HD22	2.46	0.51
2:B:80:LEU:HD22	2:F:80:LEU:HD21	1.92	0.51
2:F:3:PHE:CZ	2:F:113:SER:HA	2.45	0.51
1:E:133:SER:O	1:E:135:VAL:HG13	2.10	0.51
2:D:3:PHE:CG	2:D:112:ASP:OD2	2.64	0.51
1:C:186:ASN:OD1	1:C:219:THR:HG22	2.12	0.50
1:C:283:THR:HG22	1:C:301:THR:HG22	1.92	0.50
2:D:26:HIS:O	2:D:26:HIS:ND1	2.45	0.50
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.93	0.50
2:B:149:MET:O	2:B:153:ARG:HG3	2.12	0.50
2:B:124:LEU:HD22	2:F:134:GLY:HA2	1.93	0.50
2:D:106:ARG:NH2	2:B:106:ARG:HE	2.09	0.50
2:D:167:ARG:O	2:D:171:GLU:HG2	2.12	0.49
2:B:160:PRO:HA	2:B:163:SER:HB2	1.94	0.49
2:F:3:PHE:HZ	2:F:112:ASP:C	2.15	0.49
1:A:186:ASN:HD22	1:A:227:SER:CB	2.25	0.49
1:C:122:GLN:OE1	1:C:125:PRO:HA	2.13	0.49
2:B:3:PHE:HB2	2:B:112:ASP:OD1	2.13	0.49
1:E:138:ALA:O	1:E:224:LYS:NZ	2.29	0.49
2:D:99:LEU:HD13	2:B:98:LEU:HD21	1.95	0.48
1:E:202:ILE:HD11	1:E:251:PHE:HA	1.95	0.48
2:D:150:GLU:OE2	2:D:154:ASN:ND2	2.46	0.48
1:A:185:PRO:HG2	1:A:191:GLN:OE1	2.14	0.48
1:A:316:LEU:HD11	2:B:55:ILE:HG21	1.95	0.48
2:B:29:GLU:N	2:B:29:GLU:OE1	2.46	0.48
1:C:284:PRO:HD3	1:C:300:LEU:O	2.14	0.48
2:F:122:VAL:HG12	2:F:152:VAL:HG22	1.96	0.48
1:C:240:ASN:OD1	3:C:1002:NAG:H5	2.13	0.48
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.95	0.48
1:A:98:TYR:CD1	1:A:230:MET:HB2	2.48	0.47
2:F:29:GLU:OE2	2:F:143:ARG:HB3	2.14	0.47
1:A:284:PRO:HD3	1:A:300:LEU:O	2.14	0.47
2:D:37:ASP:OD1	2:D:39:GLU:HG3	2.13	0.47
2:D:2:LEU:HD12	2:D:109:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:LEU:HD11	2:F:139:GLU:HB2	1.95	0.47
1:E:55:ASP:HB3	1:E:55(A):GLY:H	1.54	0.47
1:A:216:LYS:O	1:A:220:ARG:NH2	2.47	0.47
2:F:22:TYR:H	2:F:41:THR:CG2	2.27	0.47
1:C:58:PRO:HB3	1:C:86:TYR:CZ	2.49	0.47
1:C:307:LYS:HE2	2:D:62:GLN:HB3	1.96	0.47
1:C:62:ARG:NH1	1:C:78:GLU:OE2	2.48	0.47
5:C:1004:FUL:H61	3:C:1005:NAG:O7	2.15	0.46
1:E:293:PRO:HG2	1:E:294:PHE:HD2	1.80	0.46
2:D:68:ARG:NH1	2:D:81:ASN:OD1	2.49	0.46
1:A:29:ILE:H	1:A:29:ILE:HD12	1.80	0.46
1:A:283:THR:HG22	1:A:301:THR:HG22	1.98	0.46
1:E:164:ILE:O	1:E:246:GLU:HA	2.15	0.46
1:C:121:ILE:CG2	1:C:259:LYS:HE3	2.43	0.46
1:E:156:LYS:HE2	1:E:193:ARG:O	2.16	0.46
1:C:101:ASN:OD1	1:C:231:GLU:HG3	2.16	0.46
1:E:183:HIS:O	1:E:185:PRO:HD3	2.16	0.46
2:D:128:ASP:OD1	2:D:159:TYR:OH	2.22	0.46
1:C:132:ALA:HB1	1:C:152:VAL:HG11	1.98	0.46
2:D:3:PHE:CD1	2:D:112:ASP:OD2	2.70	0.45
1:E:43:LEU:HB2	1:E:314:LEU:HB2	1.99	0.45
2:B:17:MET:HE1	2:B:36:ALA:HA	1.98	0.45
1:E:13:ILE:HG22	2:F:138:PHE:HB2	1.98	0.45
2:B:75:ARG:NH1	2:B:78:GLU:OE1	2.48	0.45
2:B:99:LEU:HD12	2:F:94:TYR:OH	2.17	0.45
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.83	0.45
1:E:293:PRO:HG2	1:E:294:PHE:CD2	2.52	0.45
1:A:43:LEU:O	1:A:45:LYS:NZ	2.50	0.45
2:F:131:LYS:HG3	2:F:139:GLU:HB3	1.99	0.45
2:D:17:MET:HE3	2:D:36:ALA:HA	1.99	0.44
1:A:134:GLY:HA2	6:A:2004:SIA:H113	1.99	0.44
1:C:307:LYS:HB3	2:D:62:GLN:NE2	2.31	0.44
2:D:17:MET:HE3	2:D:23:GLY:HA3	1.98	0.44
2:D:2:LEU:HA	2:F:113:SER:CB	2.48	0.44
1:C:15:ILE:HG13	2:D:119:TYR:HA	1.99	0.44
2:B:73:LEU:HA	2:B:73:LEU:HD23	1.74	0.44
1:C:186:ASN:HD22	1:C:227:SER:CB	2.30	0.44
1:A:174:GLU:HG3	1:A:259:LYS:HB3	1.99	0.44
1:A:222:LYS:HD2	1:A:225:GLY:O	2.17	0.44
2:F:169:LYS:O	2:F:173:ILE:HG13	2.18	0.44
2:D:49:THR:O	2:D:52:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:TYR:CZ	2:B:98:LEU:HD22	2.52	0.43
2:F:48:VAL:O	2:F:52:VAL:HG23	2.18	0.43
1:C:206:THR:CG2	1:C:208:THR:H	2.17	0.43
1:C:310:LYS:NZ	2:D:90:ASP:OD1	2.25	0.43
2:F:73:LEU:HA	2:F:73:LEU:HD23	1.91	0.43
1:A:8:ASP:OD1	1:A:8:ASP:N	2.51	0.43
2:D:3:PHE:N	2:D:3:PHE:CD1	2.86	0.43
1:C:43:LEU:O	1:C:45:LYS:NZ	2.52	0.43
1:C:173:GLN:NE2	8:C:1104:HOH:O	2.49	0.43
1:E:57:LYS:HE3	1:E:274:TYR:CE2	2.54	0.43
1:A:123:ILE:HD12	1:A:257:ALA:HB2	2.00	0.43
1:E:279:THR:HG21	1:E:287:ALA:HB1	1.99	0.43
2:F:42:GLN:O	2:F:45:ILE:HG22	2.18	0.43
1:A:183:HIS:O	1:A:185:PRO:HD3	2.17	0.43
2:F:28:ASN:ND2	2:F:146:ASN:OD1	2.46	0.43
1:C:21:ASN:N	1:C:21:ASN:OD1	2.40	0.43
1:A:90:LYS:NZ	1:A:273:GLU:OE2	2.52	0.43
2:D:63:PHE:HB2	8:D:203:HOH:O	2.19	0.43
1:C:164:ILE:O	1:C:246:GLU:HA	2.18	0.43
1:E:206:THR:HG23	1:E:207:SER:N	2.34	0.43
1:A:61:LEU:HA	1:A:79:PHE:CZ	2.54	0.43
1:C:91:ILE:HG22	1:C:271:GLU:OE2	2.19	0.43
1:A:91:ILE:HD13	1:A:271:GLU:HG2	2.01	0.43
2:B:169:LYS:O	2:B:173:ILE:HG13	2.18	0.42
2:B:171:GLU:OE2	2:F:174:SER:OG	2.37	0.42
2:B:145:ASP:OD2	2:B:147:GLU:HG2	2.19	0.42
1:A:240:ASN:OD1	3:A:2001:NAG:H5	2.19	0.42
2:B:119:TYR:OH	2:B:132:GLU:OE2	2.29	0.42
1:C:51:LEU:HD13	1:C:88:VAL:HG21	2.02	0.42
1:C:60:ILE:HD12	1:C:274:TYR:HB2	2.02	0.42
1:A:56:VAL:HB	1:A:85:SER:HB3	2.01	0.42
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.55	0.42
1:E:98:TYR:HA	1:E:99:PRO:HD3	1.94	0.42
2:D:168:LEU:O	2:D:172:GLU:HG3	2.20	0.42
1:E:102:PHE:HZ	1:E:179:LEU:HD22	1.84	0.42
1:A:14:CYS:HA	2:B:137:CYS:HA	2.02	0.42
1:C:206:THR:CG2	1:C:207:SER:N	2.83	0.41
1:A:55:ASP:HB3	1:A:55(A):GLY:H	1.51	0.41
2:F:124:LEU:HA	2:F:124:LEU:HD23	1.91	0.41
2:F:82:LYS:HB2	2:F:82:LYS:HE2	1.94	0.41
1:E:61:LEU:HA	1:E:79:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ASP:N	2:D:169:LYS:HZ1	2.17	0.41
1:A:308:TYR:HD2	2:B:89:LEU:HD22	1.85	0.41
1:E:100:GLY:HA3	1:E:230:MET:O	2.20	0.41
1:C:314:LEU:HA	1:C:314:LEU:HD23	1.91	0.41
1:C:32:LYS:NZ	2:F:54:SER:OG	2.42	0.41
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.54	0.41
2:F:151:SER:O	2:F:156:THR:N	2.54	0.41
1:A:195:TYR:O	1:A:197:ASN:N	2.51	0.41
2:F:75:ARG:HH11	2:F:75:ARG:HG3	1.86	0.41
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.95	0.41
1:C:55:ASP:HB3	1:C:55(A):GLY:H	1.61	0.41
2:D:108:LEU:O	2:D:112:ASP:HB2	2.20	0.41
1:C:61:LEU:HA	1:C:79:PHE:CZ	2.56	0.41
1:C:151:VAL:HB	1:C:252:ILE:HG22	2.03	0.41
1:C:82:VAL:HA	1:C:83:PRO:HD3	1.92	0.41
2:D:22:TYR:OH	2:D:111:HIS:HA	2.20	0.41
1:A:28:THR:O	1:A:32:LYS:NZ	2.52	0.40
1:A:131:GLU:O	1:A:154:LEU:HA	2.20	0.40
2:F:17:MET:HE3	2:F:23:GLY:HA3	2.03	0.40
1:C:97:CYS:HB2	1:C:138:ALA:O	2.21	0.40
2:D:152:VAL:HG22	2:D:157:TYR:CD1	2.56	0.40
2:F:167:ARG:HA	2:F:170:ARG:CZ	2.52	0.40
2:B:52:VAL:HA	2:B:55:ILE:HG22	2.03	0.40
1:E:268:MET:HE3	1:E:284:PRO:HA	2.02	0.40
1:E:71:LEU:HD23	1:E:71:LEU:HA	1.94	0.40
1:C:89:GLU:OE1	1:C:269:LYS:NZ	2.45	0.40
2:D:79:ASN:OD1	2:F:68:ARG:NH2	2.46	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	321/333 (96%)	308 (96%)	13 (4%)	0	100 100
1	C	321/333 (96%)	309 (96%)	12 (4%)	0	100 100
1	E	321/333 (96%)	309 (96%)	12 (4%)	0	100 100
2	B	173/180 (96%)	162 (94%)	11 (6%)	0	100 100
2	D	173/180 (96%)	161 (93%)	12 (7%)	0	100 100
2	F	173/180 (96%)	164 (95%)	8 (5%)	1 (1%)	30 59
All	All	1482/1539 (96%)	1413 (95%)	68 (5%)	1 (0%)	56 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	3	PHE

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	290/298 (97%)	282 (97%)	8 (3%)	51 81
1	C	290/298 (97%)	282 (97%)	8 (3%)	51 81
1	E	290/298 (97%)	283 (98%)	7 (2%)	57 85
2	B	149/154 (97%)	148 (99%)	1 (1%)	88 96
2	D	149/154 (97%)	144 (97%)	5 (3%)	44 75
2	F	149/154 (97%)	146 (98%)	3 (2%)	63 87
All	All	1317/1356 (97%)	1285 (98%)	32 (2%)	57 85

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	ASN
1	C	23	THR
1	C	30	MET
1	C	80	LEU

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Mol	Chain	Res	Type
1	C	102	PHE
1	C	125(A)	LYS
1	C	206	THR
1	C	320	LEU
2	D	15	GLN
2	D	26	HIS
2	D	66	VAL
2	D	80	LEU
2	D	113	SER
1	A	23	THR
1	A	55	ASP
1	A	102	PHE
1	A	103	ASN
1	A	123	ILE
1	A	135	VAL
1	A	230	MET
1	A	320	LEU
2	B	10	ILE
1	E	36	VAL
1	E	55	ASP
1	E	102	PHE
1	E	103	ASN
1	E	125(B)	ASN
1	E	206	THR
1	E	320	LEU
2	F	10	ILE
2	F	151	SER
2	F	161	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	95	ASN
1	C	173	GLN
1	C	196	GLN
1	A	173	GLN
1	A	186	ASN
2	B	26	HIS
2	B	114	ASN
2	B	142	HIS
2	F	114	ASN
2	F	117	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	2001	1,3,5	14,14,15	0.76	1 (7%)	15,19,21	0.84	0
5	FUL	A	2002	3	10,10,11	1.35	2 (20%)	13,14,16	1.40	3 (23%)
3	NAG	A	2003	3	14,14,15	0.20	0	15,19,21	0.34	0
6	SIA	A	2004	7	17,20,21	0.40	0	18,28,31	1.30	1 (5%)
7	GAL	A	2005	3,6	11,11,12	0.95	1 (9%)	15,15,17	1.61	2 (13%)
3	NAG	A	2006	7	14,14,15	0.64	0	15,19,21	0.77	0
7	GAL	A	2007	3	12,12,12	1.48	1 (8%)	17,17,17	0.94	1 (5%)
3	NAG	C	1001	1	14,14,15	0.47	0	15,19,21	0.30	0
3	NAG	C	1002	1,3,5,4	14,14,15	1.06	1 (7%)	15,19,21	0.85	1 (6%)
4	FUC	C	1003	3	10,10,11	1.05	0	13,14,16	0.89	1 (7%)
5	FUL	C	1004	3	10,10,11	1.32	2 (20%)	13,14,16	1.12	0
3	NAG	C	1005	3	14,14,15	0.36	0	15,19,21	0.33	0
6	SIA	C	1006	7	17,20,21	0.60	0	18,28,31	1.49	3 (16%)
7	GAL	C	1007	3,6	11,11,12	1.11	1 (9%)	15,15,17	1.34	2 (13%)
3	NAG	C	1008	7	14,14,15	0.55	0	15,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GAL	C	1009	3	12,12,12	1.26	2 (16%)	17,17,17	0.95	0
3	NAG	E	1001	1	14,14,15	0.50	0	15,19,21	0.45	0
3	NAG	E	1002	1,3,5	14,14,15	1.08	1 (7%)	15,19,21	1.01	1 (6%)
5	FUL	E	1003	3	10,10,11	1.25	1 (10%)	13,14,16	0.92	0
3	NAG	E	1004	3	14,14,15	0.44	0	15,19,21	0.19	0
6	SIA	E	1005	7	17,20,21	0.44	0	18,28,31	1.60	3 (16%)
7	GAL	E	1006	3,6	11,11,12	1.00	1 (9%)	15,15,17	1.82	4 (26%)
3	NAG	E	1007	7	14,14,15	0.31	0	15,19,21	0.71	1 (6%)
7	GAL	E	1008	3	12,12,12	0.99	0	17,17,17	1.07	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2001	1,3,5	-	0/6/23/26	0/1/1/1
5	FUL	A	2002	3	-	0/0/17/20	0/1/1/1
3	NAG	A	2003	3	-	0/6/23/26	0/1/1/1
6	SIA	A	2004	7	-	0/14/34/38	0/1/1/1
7	GAL	A	2005	3,6	-	0/2/19/22	0/1/1/1
3	NAG	A	2006	7	-	0/6/23/26	0/1/1/1
7	GAL	A	2007	3	-	0/2/22/22	0/1/1/1
3	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1002	1,3,5,4	-	0/6/23/26	0/1/1/1
4	FUC	C	1003	3	-	0/0/17/20	0/1/1/1
5	FUL	C	1004	3	-	0/0/17/20	0/1/1/1
3	NAG	C	1005	3	-	0/6/23/26	0/1/1/1
6	SIA	C	1006	7	-	0/14/34/38	0/1/1/1
7	GAL	C	1007	3,6	-	0/2/19/22	0/1/1/1
3	NAG	C	1008	7	-	0/6/23/26	0/1/1/1
7	GAL	C	1009	3	-	0/2/22/22	0/1/1/1
3	NAG	E	1001	1	-	0/6/23/26	0/1/1/1
3	NAG	E	1002	1,3,5	-	0/6/23/26	0/1/1/1
5	FUL	E	1003	3	-	0/0/17/20	0/1/1/1
3	NAG	E	1004	3	-	0/6/23/26	0/1/1/1
6	SIA	E	1005	7	-	0/14/34/38	0/1/1/1
7	GAL	E	1006	3,6	-	0/2/19/22	0/1/1/1
3	NAG	E	1007	7	-	0/6/23/26	0/1/1/1
7	GAL	E	1008	3	-	0/2/22/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1002	NAG	O5-C1	-3.93	1.37	1.43
3	C	1002	NAG	O5-C1	-3.83	1.37	1.43
3	A	2001	NAG	O5-C1	-2.59	1.39	1.43
7	A	2005	GAL	O5-C1	-2.13	1.40	1.43
7	C	1009	GAL	C3-C2	2.01	1.57	1.52
5	C	1004	FUL	C4-C3	2.11	1.57	1.52
7	C	1009	GAL	C1-C2	2.13	1.57	1.52
7	E	1006	GAL	C1-C2	2.16	1.57	1.52
5	A	2002	FUL	C4-C5	2.43	1.57	1.53
5	A	2002	FUL	C4-C3	2.61	1.59	1.52
5	E	1003	FUL	C4-C5	2.65	1.58	1.53
5	C	1004	FUL	C4-C5	2.72	1.58	1.53
7	C	1007	GAL	C2-C3	2.93	1.56	1.52
7	A	2007	GAL	C4-C3	3.14	1.60	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1006	SIA	C7-C6-C5	-3.75	108.90	114.06
5	A	2002	FUL	C1-C2-C3	-3.12	105.78	109.55
6	E	1005	SIA	C6-C5-N5	-2.66	106.50	111.06
6	C	1006	SIA	C3-C4-C5	-2.48	108.71	111.47
7	E	1006	GAL	O5-C5-C6	-2.45	102.08	107.34
7	A	2005	GAL	O5-C5-C6	-2.38	102.25	107.34
3	C	1002	NAG	O3-C3-C2	-2.07	104.94	109.37
4	C	1003	FUC	O2-C2-C1	2.05	113.34	109.23
6	E	1005	SIA	O6-C2-C3	2.07	113.82	109.77
7	E	1006	GAL	O2-C2-C1	2.23	113.71	109.23
5	A	2002	FUL	O5-C5-C4	2.23	113.45	109.58
5	A	2002	FUL	O2-C2-C1	2.34	113.93	109.23
7	C	1007	GAL	C6-C5-C4	2.35	118.86	112.99
7	A	2007	GAL	O5-C5-C4	2.36	114.17	109.67
3	E	1002	NAG	C3-C4-C5	2.39	114.49	110.23
7	C	1007	GAL	C1-C2-C3	2.40	112.46	109.55
3	E	1007	NAG	C1-O5-C5	2.48	115.79	112.14
7	E	1008	GAL	O5-C5-C4	2.58	114.59	109.67
7	E	1006	GAL	C1-C2-C3	2.87	113.03	109.55
6	C	1006	SIA	O6-C6-C5	3.42	114.08	108.48
6	A	2004	SIA	O6-C6-C5	3.97	114.98	108.48
7	A	2005	GAL	C1-O5-C5	4.28	118.43	112.14
7	E	1006	GAL	C1-O5-C5	4.44	118.66	112.14
6	E	1005	SIA	O6-C6-C5	4.57	115.96	108.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NAG	1	0
6	A	2004	SIA	1	0
3	C	1002	NAG	1	0
5	C	1004	FUL	1	0
3	C	1005	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	323/333 (96%)	0.22	15 (4%) 36 35	7, 23, 73, 115	0
1	C	323/333 (96%)	0.16	12 (3%) 45 45	8, 24, 62, 128	0
1	E	323/333 (96%)	0.19	8 (2%) 61 61	11, 30, 68, 129	0
2	B	175/180 (97%)	1.07	26 (14%) 3 2	8, 82, 105, 117	0
2	D	175/180 (97%)	1.56	50 (28%) 1 0	9, 86, 122, 130	0
2	F	175/180 (97%)	1.24	40 (22%) 1 1	7, 83, 112, 117	0
All	All	1494/1539 (97%)	0.58	151 (10%) 9 7	7, 34, 110, 130	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	324	PRO	10.5
2	B	175	GLY	10.2
1	E	324	PRO	9.9
2	D	9	PHE	9.7
2	D	160	PRO	9.6
2	F	33	GLY	9.4
2	D	5	ALA	8.6
2	B	9	PHE	8.2
2	F	31	GLY	7.5
2	D	8	GLY	7.0
1	C	9	PRO	6.5
2	B	3	PHE	6.4
1	E	9	PRO	6.3
1	C	10	GLY	6.1
2	D	27	SER	6.0
2	B	1	GLY	5.9
1	C	8	ASP	5.3
2	D	166	ALA	5.3
2	B	5	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	1	GLY	5.0
2	F	140	PHE	5.0
2	F	32	SER	4.9
2	D	4	GLY	4.9
2	B	8	GLY	4.9
2	B	7	ALA	4.8
2	D	159	TYR	4.8
2	D	129	ASN	4.8
2	D	29	GLU	4.8
2	D	141	TYR	4.8
2	D	175	GLY	4.7
2	F	7	ALA	4.6
2	D	25	HIS	4.5
2	D	33	GLY	4.4
2	D	138	PHE	4.2
2	D	156	THR	4.2
2	F	19	ASP	4.2
2	F	18	VAL	4.2
1	C	323	SER	4.1
2	D	11	GLU	4.1
2	F	156	THR	4.1
2	D	161	GLN	4.0
2	F	30	GLN	4.0
2	D	143	ARG	4.0
1	C	12	GLN	4.0
1	A	324	PRO	4.0
2	F	175	GLY	3.9
2	D	31	GLY	3.9
2	F	3	PHE	3.9
2	F	118	LEU	3.8
2	F	162	TYR	3.8
2	F	138	PHE	3.8
1	C	14	CYS	3.8
2	B	27	SER	3.8
2	D	174	SER	3.8
1	A	39	ALA	3.7
2	B	173	ILE	3.7
1	E	8	ASP	3.7
2	D	155	GLY	3.6
2	F	21	TRP	3.6
2	D	126	LEU	3.6
2	D	168	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	158	ASP	3.5
2	D	140	PHE	3.5
2	D	142	HIS	3.5
2	B	4	GLY	3.5
2	B	20	GLY	3.5
2	D	162	TYR	3.5
2	F	143	ARG	3.5
2	F	11	GLU	3.4
2	F	20	GLY	3.4
2	D	1	GLY	3.4
2	D	158	ASP	3.4
2	D	16	GLY	3.4
2	D	26	HIS	3.3
2	D	2	LEU	3.3
1	E	23	THR	3.3
2	B	15	GLN	3.3
1	E	13	ILE	3.3
1	A	8	ASP	3.3
2	B	38	LYS	3.2
1	C	23	THR	3.2
2	D	173	ILE	3.1
2	F	174	SER	3.1
2	F	25	HIS	3.1
2	D	128	ASP	3.1
2	F	131	LYS	3.0
1	A	323	SER	2.9
2	B	164	GLU	2.9
2	B	16	GLY	2.9
2	F	126	LEU	2.9
2	F	133	LEU	2.8
1	C	13	ILE	2.8
1	A	54	LEU	2.8
2	D	169	LYS	2.8
2	B	21	TRP	2.7
2	B	118	LEU	2.7
1	A	25	GLN	2.6
1	A	313	ARG	2.6
2	D	7	ALA	2.6
2	D	134	GLY	2.6
1	A	10	GLY	2.6
2	D	139	GLU	2.6
2	F	141	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	43	LYS	2.6
2	B	11	GLU	2.6
2	B	14	TRP	2.6
2	B	2	LEU	2.6
2	D	172	GLU	2.5
2	D	19	ASP	2.5
2	F	16	GLY	2.5
2	F	9	PHE	2.5
2	D	38	LYS	2.5
2	D	164	GLU	2.5
1	C	143	GLY	2.5
1	A	9	PRO	2.5
2	F	29	GLU	2.4
2	B	32	SER	2.4
2	F	152	VAL	2.4
2	F	139	GLU	2.4
2	F	157	TYR	2.4
2	D	131	LYS	2.4
2	F	159	TYR	2.3
2	F	4	GLY	2.3
1	E	21	ASN	2.3
1	A	288	ILE	2.3
2	F	6	ILE	2.3
2	B	166	ALA	2.3
1	A	51	LEU	2.3
1	A	40	GLN	2.3
1	C	144	ARG	2.2
1	A	36	VAL	2.2
2	B	18	VAL	2.2
2	F	36	ALA	2.2
1	A	12	GLN	2.2
2	F	27	SER	2.2
2	F	2	LEU	2.2
2	B	34	TYR	2.2
2	D	148	CYS	2.2
1	C	22	SER	2.1
2	D	127	ARG	2.1
2	F	161	GLN	2.1
2	D	34	TYR	2.1
2	D	147	GLU	2.1
2	D	170	ARG	2.1
1	A	297	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	150	GLU	2.1
1	E	14	CYS	2.0
2	F	5	ALA	2.0
1	E	12	GLN	2.0
2	B	172	GLU	2.0
2	B	169	LYS	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)

There are no carbohydrates in this entry.

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
3	NAG	E	1002	14/15	0.90	0.20	0.38	46,58,69,73	0
3	NAG	C	1002	14/15	0.93	0.19	0.34	29,43,61,71	0
6	SIA	C	1006	20/21	0.94	0.21	0.25	33,44,48,49	0
6	SIA	E	1005	20/21	0.94	0.17	-0.03	22,30,36,43	0
3	NAG	C	1008	14/15	0.80	0.42	-0.18	67,78,89,91	0
3	NAG	A	2001	14/15	0.93	0.15	-0.46	26,36,40,47	0
6	SIA	A	2004	20/21	0.96	0.14	-0.57	7,14,18,20	0
3	NAG	C	1005	14/15	0.89	0.39	-	47,65,73,78	0
3	NAG	C	1001	14/15	0.69	0.24	-	79,93,95,98	0
7	GAL	C	1009	12/12	0.77	0.39	-	73,90,103,110	0
7	GAL	E	1008	12/12	0.84	0.33	-	60,70,74,76	0
3	NAG	E	1001	14/15	0.83	0.27	-	83,94,99,100	0
5	FUL	C	1004	10/11	0.90	0.26	-	49,53,57,59	0
4	FUC	C	1003	10/11	0.77	0.47	-	76,94,98,101	0
3	NAG	A	2003	14/15	0.91	0.27	-	36,49,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	GAL	A	2005	11/12	0.94	0.13	-	21,30,33,37	0
7	GAL	C	1007	11/12	0.87	0.24	-	51,68,77,77	0
3	NAG	E	1007	14/15	0.83	0.41	-	46,60,62,63	0
5	FUL	A	2002	10/11	0.88	0.48	-	46,53,65,66	0
3	NAG	A	2006	14/15	0.95	0.12	-	34,43,52,57	0
5	FUL	E	1003	10/11	0.85	0.37	-	73,77,83,84	0
7	GAL	A	2007	12/12	0.76	0.32	-	56,70,78,81	0
7	GAL	E	1006	11/12	0.90	0.28	-	40,53,58,58	0
3	NAG	E	1004	14/15	0.78	0.30	-	66,80,87,88	0

6.5 Other polymers (i)

There are no such residues in this entry.