Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:44 PM GMT

PDB ID	:	4MHH
Title	:	Crystal structure of Fab H5M9 in complex with influenza virus hemagglutinin from A/Viet Nam/1203/2004 (H5N1)
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2013-08-29
Resolution	:	3.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

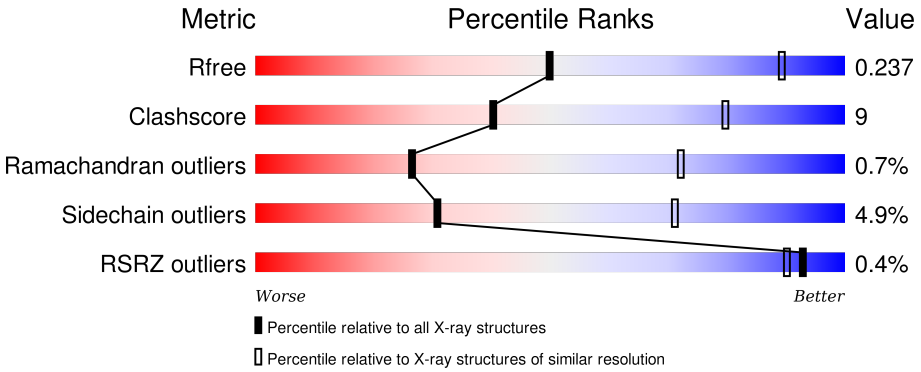
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.56 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	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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	334	76% 19%
1	C	334	79% 16%
1	E	334	75% 21%
2	I	218	80% 18%
2	K	218	78% 20%

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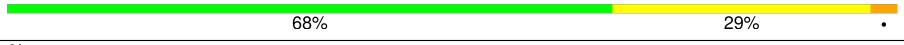
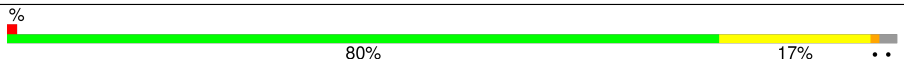
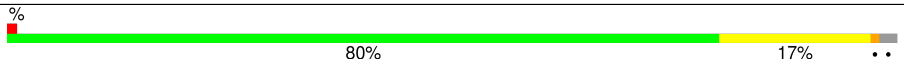
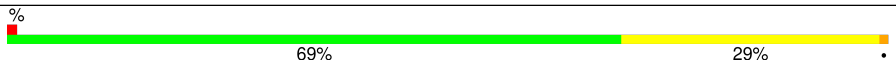
Mol	Chain	Length	Quality of chain
2	L	218	
3	B	181	
3	D	181	
3	F	181	
4	G	222	
4	H	222	
4	J	222	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2568	1622	443	488	15			
1	C	324	Total	C	N	O	S	0	0	0
			2568	1622	443	488	15			
1	E	324	Total	C	N	O	S	0	0	0
			2568	1622	443	488	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
A	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
A	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
A	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
C	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
C	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
C	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
C	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
E	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
E	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
E	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
E	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33

- Molecule 2 is a protein called H5M9 antibody, light chain (kappa).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1683	1044	291	342	6			
2	I	217	Total	C	N	O	S	0	0	0
			1683	1044	291	342	6			
2	K	217	Total	C	N	O	S	0	0	0
			1683	1044	291	342	6			

- Molecule 3 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
3	D	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
3	F	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
B	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
B	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
B	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
B	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
B	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
B	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
D	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
D	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
D	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
D	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
D	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
D	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
D	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
F	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
F	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
F	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
F	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
F	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
F	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
F	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33

- Molecule 4 is a protein called H5M9 antibody, heavy chain (IgG1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	222	Total	C	N	O	S	0	0	0
			1682	1062	277	334	9			
4	G	222	Total	C	N	O	S	0	0	0
			1682	1062	277	334	9			
4	J	222	Total	C	N	O	S	0	0	0
			1682	1062	277	334	9			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	5	Total	C	N	O	0	0
			61	34	2	25		
5	C	5	Total	C	N	O	0	0
			61	34	2	25		
5	E	5	Total	C	N	O	0	0
			61	34	2	25		

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

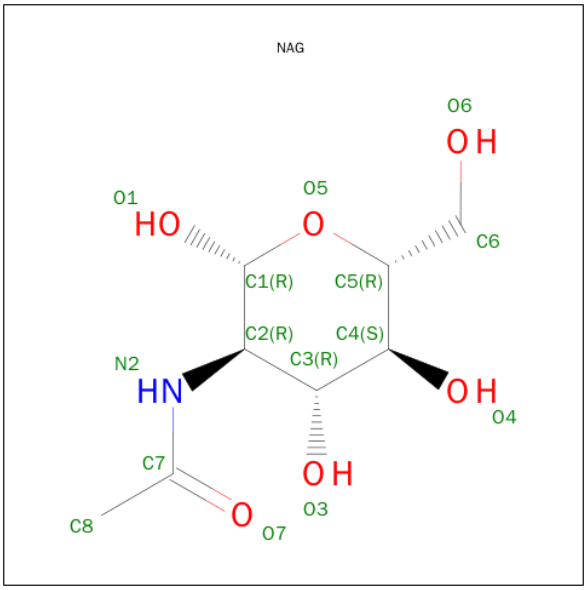
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	C	2	Total	C	N	O	0	0
			28	16	2	10		
6	C	2	Total	C	N	O	0	0
			28	16	2	10		
6	C	2	Total	C	N	O	0	0
			28	16	2	10		
6	C	2	Total	C	N	O	0	0
			28	16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

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		
7	E	3	Total	C	N	O	0	0
			39	22	2	15		
7	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	K	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

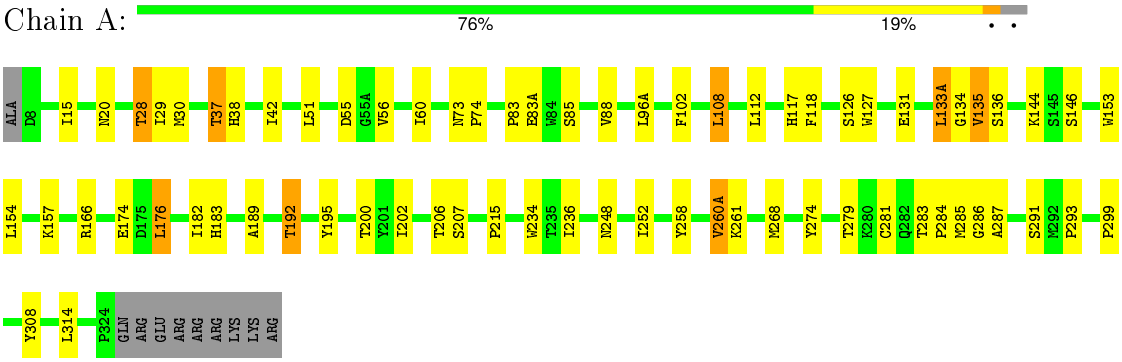
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	4	Total	C	N	O	0	0
			50	28	2	20		

3 Residue-property plots (i)

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

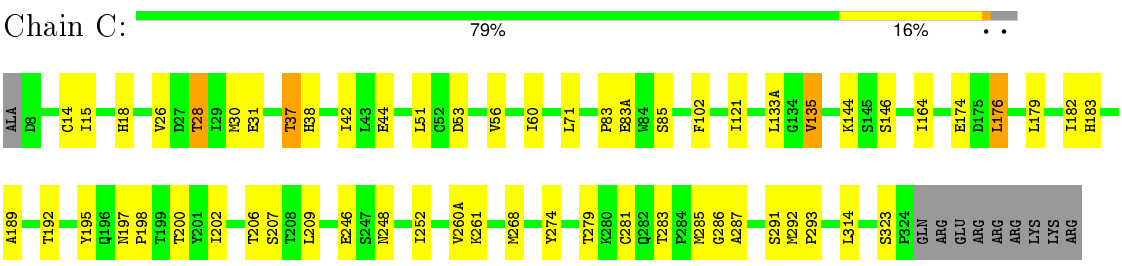
- Molecule 1: Hemagglutinin HA1 chain

Chain A:



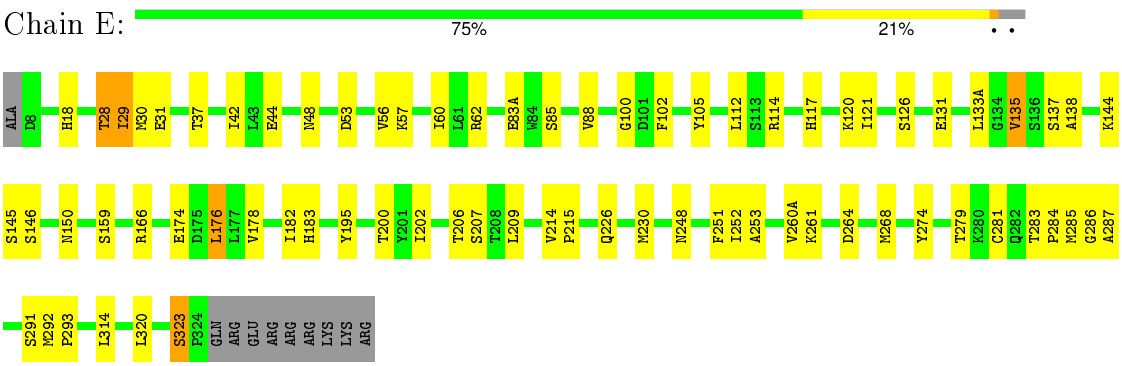
- Molecule 1: Hemagglutinin HA1 chain

Chain C:



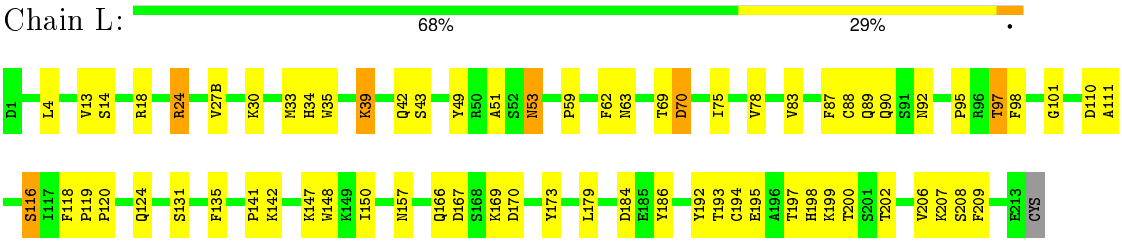
- Molecule 1: Hemagglutinin HA1 chain

Chain E:



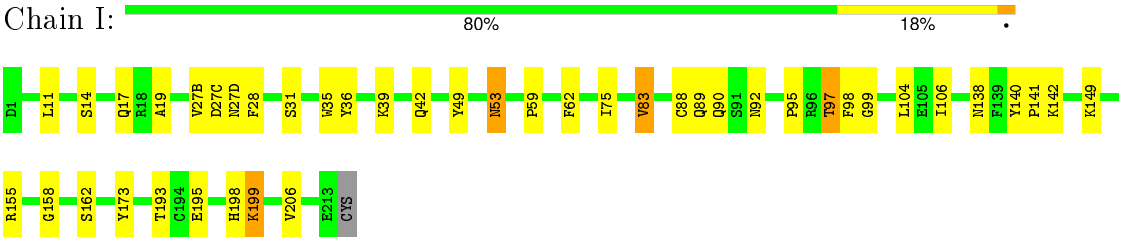
- Molecule 2: H5M9 antibody, light chain (kappa)

Chain L:



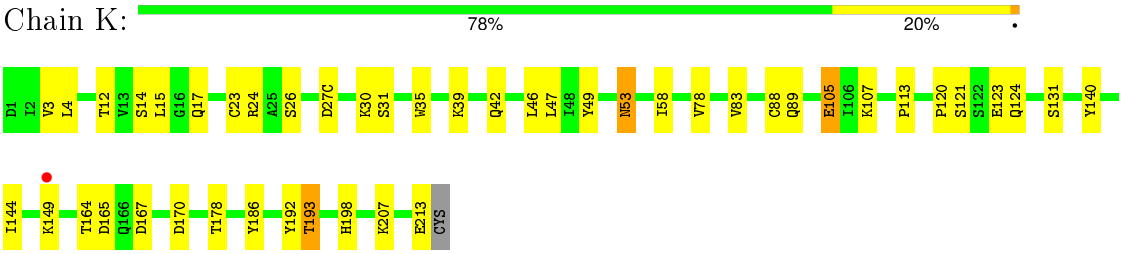
- Molecule 2: H5M9 antibody, light chain (kappa)

Chain I:



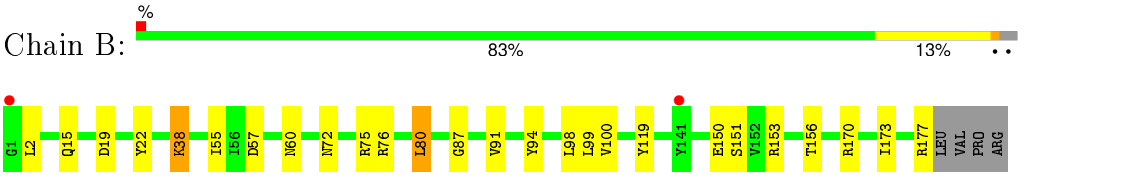
- Molecule 2: H5M9 antibody, light chain (kappa)

Chain K:



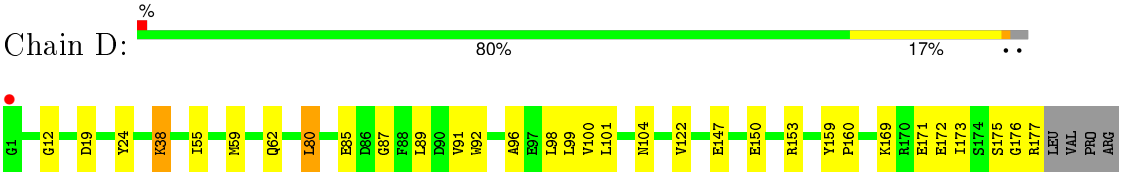
- Molecule 3: Hemagglutinin HA2 chain

Chain B:



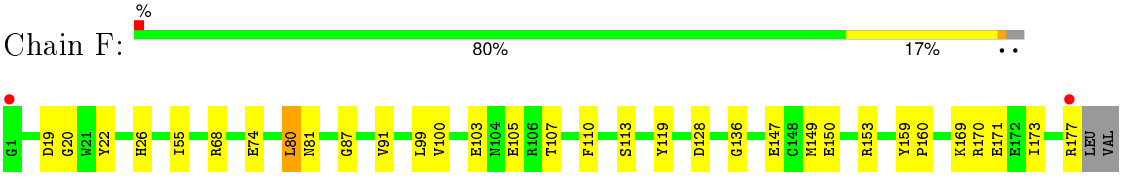
- Molecule 3: Hemagglutinin HA2 chain

Chain D:



- Molecule 3: Hemagglutinin HA2 chain

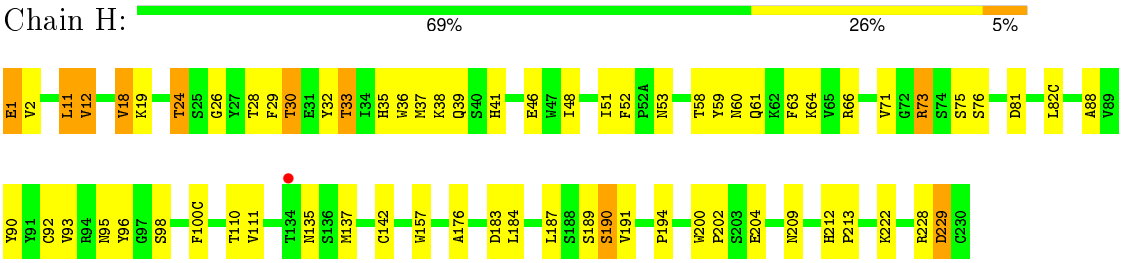
Chain F:



PRO
ARG

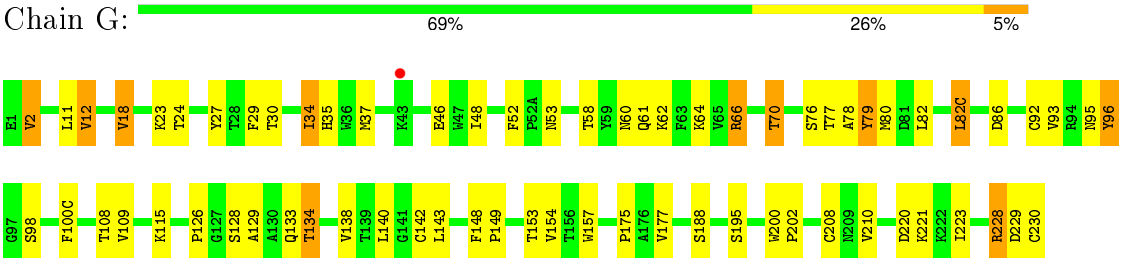
- Molecule 4: H5M9 antibody, heavy chain (IgG1)

Chain H:



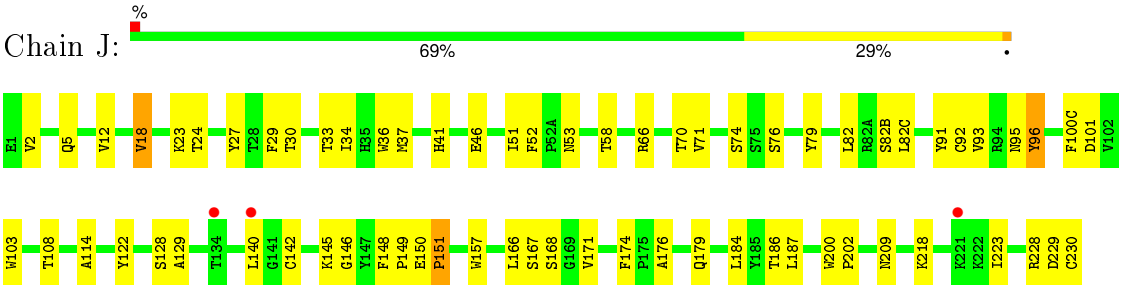
- Molecule 4: H5M9 antibody, heavy chain (IgG1)

Chain G:



- Molecule 4: H5M9 antibody, heavy chain (IgG1)

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.01Å 251.42Å 230.81Å 90.00° 107.01° 90.00°	Depositor
Resolution (Å)	47.30 – 3.56 47.30 – 3.56	Depositor EDS
% Data completeness (in resolution range)	91.5 (47.30-3.56) 91.7 (47.30-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.201 , 0.238 0.200 , 0.237	Depositor DCC
R_{free} test set	4212 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	126.7	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 98.5	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 84428 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22784	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: NAG, MAN

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	0.59	0/2631	0.83	2/3574 (0.1%)
1	C	0.56	0/2631	0.80	1/3574 (0.0%)
1	E	0.63	0/2631	0.86	1/3574 (0.0%)
2	I	0.52	0/1720	0.63	0/2332
2	K	0.48	0/1720	0.60	0/2332
2	L	0.65	0/1720	0.75	1/2332 (0.0%)
3	B	0.63	1/1460 (0.1%)	0.75	1/1961 (0.1%)
3	D	0.73	5/1460 (0.3%)	0.75	1/1961 (0.1%)
3	F	0.76	7/1460 (0.5%)	0.83	0/1961
4	G	0.56	0/1728	0.71	0/2361
4	H	0.62	0/1728	0.77	0/2361
4	J	0.47	0/1728	0.66	0/2361
All	All	0.60	13/22617 (0.1%)	0.76	7/30684 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	171	GLU	CD-OE1	5.94	1.32	1.25
3	D	171	GLU	CD-OE2	5.85	1.32	1.25
3	F	147	GLU	CD-OE2	5.77	1.32	1.25
3	F	177	ARG	CZ-NH1	5.68	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	171	GLU	CD-OE2	5.64	1.31	1.25
3	F	147	GLU	CG-CD	5.54	1.60	1.51
3	D	172	GLU	CD-OE2	5.44	1.31	1.25
3	F	147	GLU	CD-OE1	5.43	1.31	1.25
3	D	172	GLU	CD-OE1	5.38	1.31	1.25
3	D	147	GLU	CG-CD	5.26	1.59	1.51
3	F	171	GLU	CG-CD	5.18	1.59	1.51
3	F	177	ARG	CZ-NH2	5.16	1.39	1.33
3	B	177	ARG	CZ-NH1	5.07	1.39	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	195	TYR	N-CA-C	-7.95	89.55	111.00
1	A	195	TYR	N-CA-C	-7.07	91.91	111.00
1	C	195	TYR	N-CA-C	-6.46	93.54	111.00
2	L	63	ASN	N-CA-CB	5.57	120.62	110.60
1	A	108	LEU	CB-CG-CD1	-5.36	101.89	111.00
3	B	80	LEU	CA-CB-CG	5.13	127.10	115.30
3	D	80	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	323	SER	Peptide
1	E	323	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2568	0	2504	48	0
1	C	2568	0	2504	35	0
1	E	2568	0	2504	47	0
2	I	1683	0	1606	29	0
2	K	1683	0	1606	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1683	0	1606	45	0
3	B	1433	0	1339	18	0
3	D	1433	0	1339	18	0
3	F	1433	0	1339	21	0
4	G	1682	0	1632	41	0
4	H	1682	0	1632	49	0
4	J	1682	0	1632	41	0
5	A	61	0	52	0	0
5	C	61	0	52	0	0
5	E	61	0	52	1	0
6	A	84	0	75	3	0
6	C	112	0	100	1	0
6	E	84	0	75	0	0
7	A	39	0	34	0	0
7	B	39	0	34	2	0
7	E	39	0	34	0	0
8	F	14	0	13	0	0
8	I	14	0	13	0	0
8	K	14	0	13	0	0
8	L	14	0	13	0	0
9	D	50	0	43	1	0
All	All	22784	0	21846	388	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 9.

All (388) 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:283:THR:HG22	1:C:285:MET:H	1.30	0.96
1:A:283:THR:HG22	1:A:285:MET:H	1.36	0.89
1:E:37:THR:HG22	1:E:320:LEU:H	1.37	0.88
1:E:283:THR:HG22	1:E:285:MET:H	1.43	0.82
1:A:131:GLU:HB3	1:A:133(A):LEU:HD23	1.66	0.78
4:H:48:ILE:HA	4:H:63:PHE:HD2	1.49	0.77
1:E:279:THR:HB	1:E:281:CYS:H	1.51	0.75
2:L:120:PRO:HB3	2:L:131:SER:H	1.50	0.75
4:G:66:ARG:NH2	4:G:86:ASP:OD1	2.20	0.75
1:E:279:THR:HG21	1:E:287:ALA:HB1	1.70	0.74
3:B:150:GLU:HB3	7:B:2001:NAG:H62	1.69	0.73
1:E:37:THR:CG2	1:E:320:LEU:H	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ILE:HD12	1:C:202:ILE:HD12	1.68	0.73
1:A:182:ILE:HD12	1:A:202:ILE:HD12	1.69	0.73
2:K:149:LYS:HB2	2:K:193:THR:HG22	1.71	0.72
2:K:120:PRO:HB3	2:K:131:SER:H	1.53	0.72
4:G:70:THR:HG23	4:G:79:TYR:HB2	1.72	0.71
4:G:154:VAL:HG22	4:G:210:VAL:HG22	1.74	0.70
1:A:314:LEU:HD22	3:B:100:VAL:HG21	1.74	0.69
2:L:119:PRO:HB2	4:H:228:ARG:HH21	1.57	0.68
1:E:283:THR:HB	1:E:286:GLY:O	1.93	0.68
4:J:24:THR:HG22	4:J:76:SER:O	1.93	0.68
2:L:90:GLN:HE21	2:L:97:THR:CG2	2.08	0.67
1:C:279:THR:HG21	1:C:287:ALA:HB1	1.76	0.67
1:A:283:THR:HB	1:A:286:GLY:O	1.94	0.67
1:E:314:LEU:HD22	3:F:100:VAL:HG21	1.79	0.64
1:A:28:THR:HG22	1:A:30:MET:H	1.61	0.64
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.78	0.64
4:H:12:VAL:HG21	4:H:82(C):LEU:HD13	1.80	0.64
3:D:176:GLY:O	3:D:177:ARG:HG3	1.98	0.64
1:E:37:THR:HG22	1:E:320:LEU:N	2.12	0.63
1:C:56:VAL:HB	1:C:85:SER:HB3	1.79	0.63
4:H:18:VAL:HG22	4:H:82(C):LEU:HD11	1.81	0.63
1:A:279:THR:HB	1:A:281:CYS:H	1.63	0.63
4:G:18:VAL:HG23	4:G:82:LEU:HB2	1.79	0.62
1:E:206:THR:HB	1:E:209:LEU:H	1.64	0.62
4:G:208:CYS:N	4:G:221:LYS:O	2.28	0.61
1:C:283:THR:HG22	1:C:285:MET:N	2.11	0.61
4:H:200:TRP:CD1	4:H:202:PRO:HA	2.36	0.61
1:E:135:VAL:HG22	1:E:146:SER:HA	1.81	0.61
2:K:120:PRO:O	4:J:228:ARG:NH2	2.34	0.60
1:C:283:THR:HB	1:C:286:GLY:O	2.01	0.60
1:E:126:SER:O	1:E:166:ARG:NH2	2.35	0.59
2:K:113:PRO:HD3	2:K:198:HIS:CD2	2.37	0.59
4:H:1:GLU:O	4:H:26:GLY:HA3	2.03	0.59
4:H:19:LYS:NZ	4:H:81:ASP:HB2	2.18	0.59
4:G:128:SER:OG	4:G:230:CYS:SG	2.61	0.59
1:C:121:ILE:HD11	1:C:176:LEU:HD11	1.84	0.58
4:G:142:CYS:HB2	4:G:157:TRP:CH2	2.39	0.58
4:H:200:TRP:CG	4:H:202:PRO:HA	2.38	0.58
2:L:90:GLN:HE21	2:L:97:THR:HG23	1.68	0.58
1:C:135:VAL:HG22	1:C:146:SER:HA	1.86	0.58
1:E:182:ILE:HD12	1:E:202:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:145:LYS:HD2	4:J:179:GLN:HE22	1.69	0.57
1:A:42:ILE:HB	1:A:293:PRO:HG2	1.86	0.57
3:D:59:MET:HE2	3:D:96:ALA:HB2	1.86	0.57
4:G:30:THR:HB	4:G:53:ASN:HB2	1.86	0.57
4:H:39:GLN:O	4:H:88:ALA:HB1	2.03	0.57
3:F:87:GLY:O	3:F:91:VAL:HG23	2.05	0.57
2:L:116:SER:HA	2:L:207:LYS:HD2	1.87	0.57
2:I:95:PRO:O	2:I:97:THR:HG22	2.04	0.56
1:A:206:THR:HG22	1:A:207:SER:H	1.69	0.56
1:A:56:VAL:HB	1:A:85:SER:HB3	1.87	0.56
3:D:55:ILE:HG12	3:D:99:LEU:HD21	1.86	0.56
4:H:59:TYR:HD2	4:H:64:LYS:HD3	1.70	0.56
2:I:155:ARG:HG2	2:I:155:ARG:HH11	1.70	0.56
1:E:53:ASP:OD2	4:H:98:SER:OG	2.23	0.56
1:E:62:ARG:NH2	4:H:28:THR:HG21	2.21	0.56
2:L:192:TYR:HB2	2:L:209:PHE:CE1	2.41	0.55
3:D:19:ASP:OD1	3:D:19:ASP:N	2.33	0.55
2:I:90:GLN:HE21	2:I:97:THR:HG23	1.71	0.55
6:A:2010:NAG:H83	3:B:15:GLN:HG3	1.89	0.55
1:E:120:LYS:HE2	1:E:150:ASN:OD1	2.05	0.55
4:G:133:GLN:NE2	4:G:134:THR:O	2.39	0.55
2:L:110:ASP:OD2	2:L:199:LYS:HE2	2.07	0.55
4:H:48:ILE:HA	4:H:63:PHE:CD2	2.36	0.55
4:H:190:SER:O	4:H:190:SER:OG	2.22	0.55
4:J:51:ILE:HD13	4:J:71:VAL:HG23	1.89	0.55
3:B:72:ASN:OD1	3:B:75:ARG:NH2	2.40	0.55
4:G:18:VAL:HG22	4:G:82(C):LEU:HD11	1.88	0.55
1:E:56:VAL:HB	1:E:85:SER:HB3	1.89	0.55
1:C:279:THR:HB	1:C:281:CYS:H	1.72	0.54
1:A:283:THR:HG22	1:A:285:MET:N	2.15	0.54
1:C:15:ILE:HD11	3:D:122:VAL:HG21	1.87	0.54
1:C:206:THR:HG22	1:C:207:SER:H	1.72	0.54
4:J:30:THR:HB	4:J:53:ASN:HB2	1.90	0.54
4:J:24:THR:HG21	4:J:29:PHE:CD1	2.43	0.54
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.43	0.54
1:E:200:THR:HA	1:E:248:ASN:HD21	1.73	0.54
2:L:49:TYR:CE1	2:L:53:ASN:HB2	2.43	0.53
4:G:143:LEU:HD12	4:G:188:SER:HB3	1.88	0.53
2:K:213:GLU:HB3	4:J:230:CYS:SG	2.48	0.53
3:F:169:LYS:O	3:F:173:ILE:HG12	2.07	0.53
4:J:36:TRP:CZ3	4:J:92:CYS:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:157:TRP:HE1	4:H:189:SER:HG	1.55	0.53
1:A:83:PRO:HG3	4:J:96:TYR:CZ	2.44	0.53
2:I:19:ALA:HB3	2:I:75:ILE:HB	1.91	0.53
1:A:126:SER:O	1:A:166:ARG:NH2	2.40	0.53
1:A:206:THR:HG22	1:A:207:SER:N	2.24	0.53
2:L:193:THR:HG23	2:L:208:SER:HB3	1.90	0.53
3:D:87:GLY:O	3:D:91:VAL:HG23	2.09	0.53
3:B:55:ILE:HG12	3:B:99:LEU:HD21	1.91	0.52
3:B:150:GLU:HG2	3:B:153:ARG:HH12	1.74	0.52
1:C:28:THR:HG22	1:C:30:MET:H	1.74	0.52
2:K:12:THR:HG23	2:K:105:GLU:HB3	1.91	0.52
2:L:147:LYS:HE3	2:L:195:GLU:HB3	1.91	0.52
2:L:141:PRO:HD2	2:L:198:HIS:HE1	1.74	0.52
4:H:38:LYS:HB2	4:H:90:TYR:CE1	2.45	0.52
1:C:200:THR:HA	1:C:248:ASN:OD1	2.10	0.52
1:C:37:THR:HB	1:C:38:HIS:ND1	2.25	0.52
1:A:60:ILE:HD12	1:A:274:TYR:HB2	1.91	0.52
2:I:83:VAL:HG13	2:I:106:ILE:HG12	1.91	0.52
1:A:200:THR:HA	1:A:248:ASN:OD1	2.10	0.51
1:A:108:LEU:HB2	1:A:234:TRP:CZ2	2.46	0.51
4:H:33:THR:CG2	4:H:95:ASN:HD22	2.23	0.51
1:E:102:PHE:O	1:E:105:TYR:HB2	2.10	0.51
2:K:35:TRP:CZ3	2:K:88:CYS:HB3	2.46	0.51
4:G:24:THR:HG22	4:G:76:SER:O	2.11	0.51
2:L:124:GLN:NE2	2:L:131:SER:OG	2.38	0.51
1:E:121:ILE:HD11	1:E:176:LEU:HD11	1.93	0.51
4:J:142:CYS:HB2	4:J:157:TRP:CH2	2.46	0.51
2:L:193:THR:HG22	2:L:194:CYS:H	1.74	0.51
1:C:206:THR:HG22	1:C:207:SER:N	2.25	0.50
1:E:251:PHE:CE2	1:E:253:ALA:HB2	2.47	0.50
1:C:60:ILE:HD12	1:C:274:TYR:HB2	1.93	0.50
2:I:35:TRP:CZ3	2:I:88:CYS:HB3	2.47	0.50
4:H:12:VAL:HG23	4:H:111:VAL:HG22	1.93	0.50
4:J:36:TRP:CH2	4:J:92:CYS:HB2	2.46	0.50
3:F:19:ASP:OD1	3:F:19:ASP:N	2.44	0.50
1:C:206:THR:HB	1:C:209:LEU:H	1.77	0.50
2:I:89:GLN:HB2	2:I:98:PHE:CD2	2.47	0.50
1:E:60:ILE:HD12	1:E:274:TYR:HB2	1.94	0.50
1:E:18:HIS:HB2	3:F:20:GLY:O	2.12	0.50
4:J:176:ALA:HA	4:J:187:LEU:HB3	1.94	0.50
3:B:94:TYR:CZ	3:B:98:LEU:HD22	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:THR:HG22	1:E:207:SER:H	1.76	0.50
4:G:52:PHE:CE2	4:G:53:ASN:HB3	2.47	0.50
3:B:99:LEU:HD13	3:D:98:LEU:HD21	1.93	0.50
2:K:17:GLN:O	2:K:78:VAL:HG23	2.12	0.50
2:L:27(B):VAL:O	2:L:27(B):VAL:HG22	2.12	0.50
2:I:141:PRO:HD2	2:I:198:HIS:HE1	1.77	0.49
2:I:142:LYS:HB3	2:I:173:TYR:CZ	2.47	0.49
4:H:37:MET:HE3	4:H:46:GLU:O	2.12	0.49
3:F:150:GLU:HG2	3:F:153:ARG:HH12	1.77	0.49
2:L:166:GLN:HB2	2:L:173:TYR:CE1	2.47	0.49
2:I:198:HIS:ND1	2:I:199:LYS:N	2.59	0.49
4:G:138:VAL:HG12	4:G:195:SER:HA	1.93	0.49
2:L:13:VAL:HG11	2:L:78:VAL:HG21	1.93	0.49
4:J:145:LYS:HG3	4:J:186:THR:OG1	2.12	0.49
1:A:200:THR:OG1	1:A:215:PRO:HG3	2.12	0.49
1:E:57:LYS:HE3	4:H:32:TYR:CE2	2.47	0.49
1:C:164:ILE:O	1:C:246:GLU:HA	2.12	0.49
4:H:93:VAL:HG11	4:H:100(C):PHE:HB3	1.94	0.49
2:L:148:TRP:CE3	2:L:179:LEU:HD13	2.47	0.49
1:A:15:ILE:HG12	3:B:119:TYR:HA	1.95	0.49
4:G:200:TRP:CG	4:G:202:PRO:HA	2.48	0.49
4:G:140:LEU:HD22	4:G:223:ILE:HG21	1.94	0.49
1:E:206:THR:HG22	1:E:207:SER:N	2.27	0.48
4:J:18:VAL:HG23	4:J:82:LEU:HB2	1.95	0.48
4:J:52:PHE:CE2	4:J:53:ASN:HB3	2.48	0.48
3:B:151:SER:HB2	3:B:156:THR:HG22	1.94	0.48
2:I:59:PRO:HG2	2:I:62:PHE:CE2	2.48	0.48
1:A:189:ALA:O	1:A:192:THR:HG22	2.12	0.48
3:D:150:GLU:HG2	3:D:153:ARG:HH12	1.77	0.48
4:H:51:ILE:HD13	4:H:71:VAL:HG23	1.96	0.48
4:J:34:ILE:HG22	4:J:51:ILE:HG22	1.96	0.48
4:G:35:HIS:CD2	4:G:95:ASN:HB3	2.49	0.48
4:J:150:GLU:OE1	4:J:151:PRO:HA	2.14	0.48
4:G:34:ILE:HD13	4:G:93:VAL:O	2.13	0.47
4:G:37:MET:HE3	4:G:46:GLU:O	2.14	0.47
1:A:268:MET:HG2	1:A:284:PRO:HG3	1.95	0.47
9:D:2002:NAG:H4	9:D:2003:MAN:O2	2.13	0.47
1:C:83:PRO:HG3	4:G:96:TYR:CZ	2.50	0.47
1:A:28:THR:HG22	1:A:30:MET:N	2.29	0.47
2:L:135:PHE:CD2	4:H:190:SER:HB2	2.49	0.47
2:I:88:CYS:O	2:I:99:GLY:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:LEU:HD23	1:C:179:LEU:HD23	1.96	0.47
2:K:49:TYR:CE1	2:K:53:ASN:HB2	2.49	0.47
4:G:12:VAL:HG21	4:G:82(C):LEU:HD13	1.97	0.47
2:L:195:GLU:HG3	2:L:206:VAL:HG22	1.96	0.47
4:H:183:ASP:O	4:H:184:LEU:HD23	2.15	0.47
3:D:169:LYS:O	3:D:173:ILE:HG13	2.14	0.47
3:F:26:HIS:HB2	3:F:149:MET:HE3	1.96	0.47
1:A:127:TRP:CZ2	1:A:154:LEU:HD11	2.49	0.47
4:G:208:CYS:O	4:G:220:ASP:HA	2.14	0.47
2:K:121:SER:OG	2:K:123:GLU:OE1	2.32	0.47
4:J:200:TRP:CG	4:J:202:PRO:HA	2.50	0.47
4:J:140:LEU:HD22	4:J:223:ILE:HG21	1.96	0.47
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.97	0.47
4:H:48:ILE:HG12	4:H:63:PHE:CD2	2.50	0.47
4:J:36:TRP:HA	4:J:91:TYR:O	2.15	0.47
2:I:90:GLN:HE21	2:I:97:THR:CG2	2.27	0.46
2:I:27(B):VAL:HG23	2:I:92:ASN:HB2	1.98	0.46
4:H:29:PHE:CD2	4:H:76:SER:HA	2.50	0.46
4:G:66:ARG:HB2	4:G:66:ARG:HE	1.47	0.46
2:L:53:ASN:N	2:L:53:ASN:OD1	2.47	0.46
4:J:114:ALA:HB3	4:J:148:PHE:CE2	2.50	0.46
4:G:23:LYS:HG3	4:G:77:THR:OG1	2.15	0.46
2:L:169:LYS:HD2	2:L:169:LYS:HA	1.79	0.46
1:C:18:HIS:HD2	1:C:37:THR:HG21	1.81	0.46
2:L:33:MET:HB3	2:L:51:ALA:HB2	1.96	0.46
2:I:11:LEU:O	2:I:104:LEU:HD12	2.16	0.46
2:K:14:SER:OG	2:K:17:GLN:HG3	2.15	0.46
2:L:24:ARG:NH1	2:L:70:ASP:HB3	2.31	0.46
2:L:89:GLN:NE2	4:H:100(C):PHE:HE1	2.13	0.46
1:A:56:VAL:HG23	2:K:30:LYS:HZ1	1.81	0.46
4:J:18:VAL:HG22	4:J:82(C):LEU:HD11	1.97	0.46
2:I:149:LYS:HB2	2:I:193:THR:HB	1.96	0.46
4:J:37:MET:HE3	4:J:46:GLU:O	2.16	0.46
5:E:3003:NAG:H61	5:E:3004:NAG:HN2	1.80	0.46
2:I:27(C):ASP:OD2	2:I:31:SER:OG	2.24	0.46
3:D:175:SER:OG	3:D:177:ARG:O	2.34	0.46
1:E:137:SER:HA	1:E:145:SER:HB2	1.97	0.46
4:H:60:ASN:OD1	4:H:61:GLN:N	2.49	0.46
1:A:51:LEU:HD13	1:A:88:VAL:HG21	1.98	0.46
2:L:167:ASP:HB3	2:L:170:ASP:OD1	2.16	0.46
1:A:55:ASP:HB2	2:K:30:LYS:HZ3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:GLY:HA3	1:E:230:MET:O	2.16	0.46
4:J:33:THR:CG2	4:J:95:ASN:HD22	2.28	0.46
3:B:87:GLY:O	3:B:91:VAL:HG23	2.17	0.45
2:K:144:ILE:HD13	2:K:198:HIS:CD2	2.52	0.45
1:A:135:VAL:HG22	1:A:146:SER:HA	1.98	0.45
4:H:19:LYS:HZ3	4:H:81:ASP:HB2	1.81	0.45
2:I:36:TYR:OH	4:G:100(C):PHE:HD1	1.99	0.45
3:F:128:ASP:O	3:F:170:ARG:NH1	2.50	0.45
3:B:38:LYS:HB2	3:B:38:LYS:HE2	1.72	0.45
4:G:82:LEU:HA	4:G:82:LEU:HD23	1.61	0.45
4:G:126:PRO:O	4:G:228:ARG:HG3	2.17	0.45
3:D:159:TYR:HB3	3:D:160:PRO:HD3	1.99	0.45
2:K:46:LEU:HD22	4:J:101:ASP:HA	1.98	0.45
2:K:3:VAL:HB	2:K:26:SER:HB3	1.98	0.45
1:E:28:THR:HG22	1:E:30:MET:H	1.82	0.45
4:J:37:MET:HG3	4:J:103:TRP:CZ3	2.52	0.45
2:K:4:LEU:HD22	2:K:23:CYS:SG	2.57	0.45
4:J:128:SER:HB2	4:J:228:ARG:O	2.17	0.45
1:A:299:PRO:HB3	1:A:308:TYR:CD2	2.52	0.45
2:I:14:SER:OG	2:I:17:GLN:HG3	2.17	0.45
2:I:49:TYR:CE1	2:I:53:ASN:HB2	2.52	0.45
2:I:155:ARG:HG2	2:I:155:ARG:NH1	2.32	0.44
2:L:34:HIS:O	2:L:88:CYS:HA	2.17	0.44
4:H:30:THR:HB	4:H:53:ASN:HB2	1.99	0.44
3:B:19:ASP:N	3:B:19:ASP:OD1	2.40	0.44
3:F:26:HIS:HB2	3:F:149:MET:SD	2.57	0.44
4:J:93:VAL:HG11	4:J:100(C):PHE:HB3	1.99	0.44
1:A:29:ILE:HD13	3:F:103:GLU:OE2	2.17	0.44
1:A:176:LEU:HD23	1:A:258:TYR:O	2.17	0.44
1:C:314:LEU:HD22	3:D:100:VAL:HG21	2.00	0.44
1:C:28:THR:HG22	1:C:31:GLU:H	1.83	0.44
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.99	0.44
1:E:117:HIS:ND1	1:E:260(A):VAL:HG11	2.31	0.44
3:F:80:LEU:O	3:F:80:LEU:HD12	2.16	0.44
2:I:89:GLN:NE2	4:G:100(C):PHE:HE1	2.16	0.44
1:E:114:ARG:NH2	1:E:264:ASP:OD1	2.50	0.44
4:H:142:CYS:HB2	4:H:157:TRP:CH2	2.52	0.44
4:J:176:ALA:HB2	4:J:187:LEU:HD23	2.00	0.44
2:K:89:GLN:NE2	4:J:100(C):PHE:HE1	2.16	0.44
2:K:124:GLN:HG3	4:J:122:TYR:CE2	2.53	0.44
4:G:60:ASN:OD1	4:G:61:GLN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:90:GLN:HE21	2:L:97:THR:HG22	1.82	0.44
1:E:214:VAL:HG13	1:E:215:PRO:HD2	2.00	0.44
4:H:52:PHE:CE2	4:H:53:ASN:HB3	2.53	0.44
1:E:176:LEU:HD23	1:E:178:VAL:HG22	2.00	0.44
2:I:59:PRO:HG2	2:I:62:PHE:HE2	1.82	0.44
1:E:88:VAL:HG22	1:E:268:MET:HE2	2.00	0.44
4:J:82:LEU:HD23	4:J:82:LEU:HA	1.77	0.43
3:F:119:TYR:CE2	3:F:136:GLY:HA2	2.53	0.43
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.84	0.43
4:G:153:THR:O	4:G:210:VAL:HA	2.19	0.43
2:L:148:TRP:CD2	2:L:179:LEU:HD13	2.53	0.43
1:A:117:HIS:ND1	1:A:260(A):VAL:HG11	2.33	0.43
1:C:14:CYS:O	3:D:24:TYR:HA	2.18	0.43
1:E:112:LEU:HD23	1:E:112:LEU:HA	1.82	0.43
4:G:2:VAL:HG12	4:G:27:TYR:HD1	1.82	0.43
1:A:236:ILE:HA	1:A:236:ILE:HD13	1.88	0.43
2:L:39:LYS:NZ	2:L:39:LYS:HB3	2.33	0.43
4:H:48:ILE:HG12	4:H:63:PHE:CE2	2.54	0.43
4:G:34:ILE:HG21	4:G:78:ALA:CB	2.49	0.43
3:F:107:THR:O	3:F:110:PHE:HB3	2.17	0.43
2:L:111:ALA:O	2:L:200:THR:HG21	2.17	0.43
1:A:73:ASN:HA	1:A:74:PRO:HD2	1.80	0.43
2:L:150:ILE:HG12	2:L:192:TYR:CD1	2.53	0.43
3:B:170:ARG:O	3:B:173:ILE:HG22	2.18	0.43
1:C:26:VAL:HB	3:D:104:ASN:ND2	2.34	0.43
4:G:93:VAL:HG11	4:G:100(C):PHE:HB3	2.00	0.43
2:I:140:TYR:CG	2:I:141:PRO:HA	2.53	0.43
4:H:137:MET:SD	4:H:194:PRO:HA	2.59	0.43
1:E:283:THR:HG23	1:E:284:PRO:HD2	2.01	0.43
2:L:98:PHE:CE1	4:H:37:MET:HE1	2.54	0.43
3:D:101:LEU:HA	3:D:101:LEU:HD23	1.80	0.43
4:J:93:VAL:HG21	4:J:103:TRP:CE3	2.53	0.43
4:G:48:ILE:HD12	4:G:80:MET:HE1	2.00	0.43
3:B:57:ASP:O	3:B:60:ASN:HB2	2.19	0.43
2:K:164:THR:HG23	4:J:174:PHE:CD1	2.54	0.43
3:F:159:TYR:HB3	3:F:160:PRO:HD3	2.01	0.43
1:C:28:THR:CG2	1:C:30:MET:H	2.32	0.42
2:K:107:LYS:HA	2:K:140:TYR:OH	2.19	0.42
4:J:167:SER:O	4:J:171:VAL:HG23	2.19	0.42
4:H:73:ARG:HG2	4:H:73:ARG:H	1.49	0.42
2:K:47:LEU:HD23	2:K:58:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:200:TRP:CD1	4:G:202:PRO:HA	2.54	0.42
1:C:42:ILE:HB	1:C:293:PRO:HG2	2.01	0.42
2:L:62:PHE:CD1	2:L:75:ILE:HG12	2.55	0.42
1:C:189:ALA:O	1:C:192:THR:HG22	2.19	0.42
3:B:2:LEU:O	3:F:113:SER:OG	2.34	0.42
7:B:2002:NAG:H4	7:B:2003:MAN:H2	1.27	0.42
1:E:131:GLU:HB3	1:E:133(A):LEU:HG	2.01	0.42
2:K:186:TYR:HE1	2:K:192:TYR:CE2	2.37	0.42
4:G:66:ARG:HG3	4:G:66:ARG:H	1.59	0.42
1:A:118:PHE:CD1	1:A:258:TYR:HB3	2.55	0.42
2:K:27(C):ASP:OD2	2:K:31:SER:OG	2.23	0.42
4:G:148:PHE:HA	4:G:149:PRO:HA	1.75	0.42
2:L:186:TYR:CE1	2:L:192:TYR:CE2	3.07	0.42
2:L:59:PRO:HG2	2:L:62:PHE:CE2	2.55	0.42
1:A:37:THR:HB	1:A:38:HIS:ND1	2.33	0.42
4:J:2:VAL:HG13	4:J:27:TYR:HD1	1.84	0.42
4:H:93:VAL:CG1	4:H:100(C):PHE:HB3	2.50	0.42
6:C:3001:NAG:H61	6:C:3002:NAG:HN2	1.84	0.42
2:I:162:SER:OG	4:G:175:PRO:HG2	2.19	0.42
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.55	0.42
3:F:150:GLU:HG2	3:F:153:ARG:NH1	2.34	0.42
1:A:299:PRO:HB3	1:A:308:TYR:CE2	2.54	0.42
3:F:68:ARG:NH1	3:F:81:ASN:OD1	2.53	0.42
1:E:42:ILE:HB	1:E:293:PRO:HG2	2.01	0.42
2:K:113:PRO:HD3	2:K:198:HIS:HD2	1.82	0.42
4:J:148:PHE:HA	4:J:149:PRO:HA	1.76	0.42
1:C:44:GLU:HB2	1:C:292:MET:HG3	2.00	0.42
2:I:195:GLU:HG3	2:I:206:VAL:HG22	2.01	0.42
4:H:19:LYS:HE2	4:H:81:ASP:OD1	2.20	0.42
1:C:135:VAL:HG22	1:C:146:SER:CA	2.49	0.42
3:D:38:LYS:HG3	3:D:38:LYS:H	1.48	0.42
1:C:279:THR:CG2	1:C:287:ALA:HB1	2.47	0.42
2:I:27(B):VAL:O	2:I:27(B):VAL:HG22	2.19	0.42
4:G:37:MET:HE3	4:G:37:MET:HB3	1.80	0.41
1:A:127:TRP:CE2	1:A:154:LEU:HD11	2.55	0.41
3:D:85:GLU:O	3:D:89:LEU:HG	2.19	0.41
1:A:131:GLU:HG2	1:A:157:LYS:HG3	2.02	0.41
2:L:27(B):VAL:HG23	2:L:92:ASN:HB2	2.02	0.41
2:L:118:PHE:HA	2:L:119:PRO:HD3	1.87	0.41
2:L:119:PRO:HG3	2:L:209:PHE:CD2	2.55	0.41
1:E:200:THR:OG1	1:E:215:PRO:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2008:NAG:H62	6:A:2009:NAG:H82	2.01	0.41
4:J:33:THR:HG23	4:J:95:ASN:HD22	1.86	0.41
1:C:197:ASN:HA	1:C:198:PRO:HD3	1.93	0.41
1:E:18:HIS:HD2	1:E:37:THR:OG1	2.03	0.41
2:L:193:THR:HG22	2:L:194:CYS:N	2.34	0.41
2:L:87:PHE:CE1	2:L:101:GLY:HA3	2.56	0.41
2:L:18:ARG:O	2:L:18:ARG:HG3	2.20	0.41
1:A:28:THR:CG2	1:A:30:MET:H	2.29	0.41
1:A:20:ASN:HA	6:A:2010:NAG:H82	2.03	0.41
1:E:48:ASN:OD1	1:E:48:ASN:C	2.59	0.41
1:A:283:THR:CG2	1:A:285:MET:H	2.21	0.41
1:E:268:MET:HE3	1:E:268:MET:HB3	1.89	0.41
4:J:146:GLY:HA2	4:J:184:LEU:HB3	2.02	0.41
1:A:42:ILE:HB	1:A:293:PRO:CG	2.50	0.41
4:H:157:TRP:CZ2	4:H:191:VAL:HG12	2.56	0.41
1:E:28:THR:HG22	1:E:31:GLU:H	1.85	0.41
1:C:51:LEU:HD22	1:C:268:MET:HE1	2.02	0.41
1:E:183:HIS:HB2	1:E:252:ILE:HD11	2.02	0.41
4:H:36:TRP:CZ3	4:H:92:CYS:HB2	2.56	0.41
4:H:95:ASN:HA	4:H:100(C):PHE:HA	2.02	0.41
4:G:24:THR:HG21	4:G:29:PHE:CD1	2.56	0.41
2:I:89:GLN:HG3	2:I:98:PHE:CE1	2.55	0.41
4:H:24:THR:HG22	4:H:76:SER:OG	2.21	0.41
3:D:62:GLN:HG3	3:D:92:TRP:CD2	2.56	0.41
1:A:96(A):LEU:HD23	1:A:96(A):LEU:HA	1.84	0.41
3:B:76:ARG:HH22	3:F:74:GLU:CD	2.22	0.41
1:E:29:ILE:HD12	3:F:105:GLU:OE2	2.21	0.41
4:H:33:THR:HG1	4:H:35:HIS:HE2	1.66	0.40
4:J:70:THR:OG1	4:J:79:TYR:HB2	2.21	0.40
4:H:19:LYS:HZ1	4:H:81:ASP:HB2	1.83	0.40
1:A:135:VAL:HG13	1:A:136:SER:N	2.37	0.40
2:I:27(D):ASN:O	2:I:28:PHE:HB2	2.22	0.40
1:C:53:ASP:OD2	4:G:98:SER:OG	2.32	0.40
1:E:44:GLU:HB2	1:E:292:MET:HG3	2.03	0.40
3:B:76:ARG:NH2	3:F:74:GLU:OE2	2.44	0.40
1:E:29:ILE:HG13	1:E:29:ILE:H	1.47	0.40
3:F:55:ILE:HG12	3:F:99:LEU:HD21	2.04	0.40
2:L:4:LEU:HD23	2:L:4:LEU:HA	1.73	0.40
4:H:11:LEU:HA	4:H:110:THR:O	2.21	0.40
4:H:33:THR:HG23	4:H:95:ASN:HD22	1.86	0.40
4:J:200:TRP:CD1	4:J:202:PRO:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:176:ALA:HA	4:H:187:LEU:HB3	2.03	0.40
4:H:212:HIS:HA	4:H:213:PRO:HD2	1.96	0.40
2:L:95:PRO:O	2:L:97:THR:HG22	2.21	0.40
2:K:167:ASP:HB3	2:K:170:ASP:OD1	2.21	0.40
1:E:138:ALA:HB2	1:E:226:GLN:HG2	2.04	0.40
4:H:66:ARG:H	4:H:66:ARG:HG3	1.53	0.40
1:A:134:GLY:HA3	1:A:153:TRP:HB3	2.04	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	322/334 (96%)	304 (94%)	17 (5%)	1 (0%)	46 83
1	C	322/334 (96%)	303 (94%)	18 (6%)	1 (0%)	46 83
1	E	322/334 (96%)	304 (94%)	16 (5%)	2 (1%)	30 74
2	I	215/218 (99%)	194 (90%)	19 (9%)	2 (1%)	21 67
2	K	215/218 (99%)	197 (92%)	18 (8%)	0	100 100
2	L	215/218 (99%)	197 (92%)	18 (8%)	0	100 100
3	B	175/181 (97%)	170 (97%)	5 (3%)	0	100 100
3	D	175/181 (97%)	171 (98%)	3 (2%)	1 (1%)	30 74
3	F	175/181 (97%)	170 (97%)	5 (3%)	0	100 100
4	G	220/222 (99%)	189 (86%)	28 (13%)	3 (1%)	14 59
4	H	220/222 (99%)	190 (86%)	26 (12%)	4 (2%)	11 54
4	J	220/222 (99%)	192 (87%)	23 (10%)	5 (2%)	8 50
All	All	2796/2865 (98%)	2581 (92%)	196 (7%)	19 (1%)	26 72

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	323	SER
4	H	135	ASN
4	J	129	ALA
4	H	229	ASP
4	G	96	TYR
4	J	96	TYR
4	J	168	SER
1	A	144	LYS
1	C	144	LYS
1	E	144	LYS
4	H	96	TYR
4	G	129	ALA
2	I	138	ASN
2	I	158	GLY
4	H	41	HIS
4	G	229	ASP
4	J	82(B)	SER
3	D	12	GLY
4	J	151	PRO

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	291/300 (97%)	279 (96%)	12 (4%)	37 76
1	C	291/300 (97%)	280 (96%)	11 (4%)	40 77
1	E	291/300 (97%)	282 (97%)	9 (3%)	47 81
2	I	190/191 (100%)	184 (97%)	6 (3%)	46 81
2	K	190/191 (100%)	179 (94%)	11 (6%)	25 66
2	L	190/191 (100%)	173 (91%)	17 (9%)	12 50
3	B	151/155 (97%)	148 (98%)	3 (2%)	63 87
3	D	151/155 (97%)	149 (99%)	2 (1%)	76 92
3	F	151/155 (97%)	149 (99%)	2 (1%)	76 92
4	G	193/193 (100%)	174 (90%)	19 (10%)	10 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	H	193/193 (100%)	177 (92%)	16 (8%)	14 52
4	J	193/193 (100%)	180 (93%)	13 (7%)	20 62
All	All	2475/2517 (98%)	2354 (95%)	121 (5%)	31 71

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	37	THR
1	A	83(A)	GLU
1	A	102	PHE
1	A	133(A)	LEU
1	A	135	VAL
1	A	174	GLU
1	A	176	LEU
1	A	192	THR
1	A	260(A)	VAL
1	A	261	LYS
1	A	291	SER
1	C	28	THR
1	C	37	THR
1	C	83(A)	GLU
1	C	102	PHE
1	C	133(A)	LEU
1	C	135	VAL
1	C	174	GLU
1	C	176	LEU
1	C	260(A)	VAL
1	C	261	LYS
1	C	291	SER
1	E	28	THR
1	E	29	ILE
1	E	83(A)	GLU
1	E	135	VAL
1	E	159	SER
1	E	174	GLU
1	E	176	LEU
1	E	261	LYS
1	E	291	SER
2	L	14	SER
2	L	24	ARG

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Mol	Chain	Res	Type
2	L	30	LYS
2	L	39	LYS
2	L	42	GLN
2	L	43	SER
2	L	53	ASN
2	L	69	THR
2	L	70	ASP
2	L	83	VAL
2	L	97	THR
2	L	116	SER
2	L	142	LYS
2	L	157	ASN
2	L	184	ASP
2	L	197	THR
2	L	202	THR
2	I	39	LYS
2	I	42	GLN
2	I	53	ASN
2	I	83	VAL
2	I	97	THR
2	I	199	LYS
2	K	15	LEU
2	K	24	ARG
2	K	39	LYS
2	K	42	GLN
2	K	53	ASN
2	K	83	VAL
2	K	105	GLU
2	K	165	ASP
2	K	178	THR
2	K	193	THR
2	K	207	LYS
3	B	22	TYR
3	B	38	LYS
3	B	80	LEU
3	D	38	LYS
3	D	80	LEU
3	F	22	TYR
3	F	80	LEU
4	H	1	GLU
4	H	2	VAL
4	H	11	LEU

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Mol	Chain	Res	Type
4	H	12	VAL
4	H	18	VAL
4	H	24	THR
4	H	30	THR
4	H	33	THR
4	H	58	THR
4	H	73	ARG
4	H	75	SER
4	H	190	SER
4	H	204	GLU
4	H	209	ASN
4	H	222	LYS
4	H	229	ASP
4	G	2	VAL
4	G	11	LEU
4	G	12	VAL
4	G	18	VAL
4	G	34	ILE
4	G	58	THR
4	G	62	LYS
4	G	64	LYS
4	G	66	ARG
4	G	70	THR
4	G	79	TYR
4	G	82(C)	LEU
4	G	92	CYS
4	G	108	THR
4	G	109	VAL
4	G	115	LYS
4	G	134	THR
4	G	177	VAL
4	G	228	ARG
4	J	5	GLN
4	J	12	VAL
4	J	18	VAL
4	J	23	LYS
4	J	41	HIS
4	J	58	THR
4	J	66	ARG
4	J	74	SER
4	J	108	THR
4	J	166	LEU

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Mol	Chain	Res	Type
4	J	209	ASN
4	J	218	LYS
4	J	229	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	276	ASN
3	B	146	ASN
4	H	95	ASN
4	G	95	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

48 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	$\#\|Z\| > 2$
5	NAG	A	2001	1,5	14,14,15	0.31	0	15,19,21	0.65	1 (6%)
5	NAG	A	2002	5	14,14,15	0.52	0	15,19,21	0.42	0
5	MAN	A	2003	5	11,11,12	2.05	3 (27%)	14,15,17	1.90	4 (28%)
5	MAN	A	2004	5	11,11,12	1.19	1 (9%)	14,15,17	1.55	2 (14%)
5	MAN	A	2005	5	11,11,12	1.02	1 (9%)	14,15,17	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	2006	1,6	14,14,15	0.20	0	15,19,21	0.34	0
6	NAG	A	2007	6	14,14,15	0.20	0	15,19,21	0.25	0
6	NAG	A	2008	1,6	14,14,15	0.64	1 (7%)	15,19,21	0.54	0
6	NAG	A	2009	6	14,14,15	0.54	0	15,19,21	0.36	0
6	NAG	A	2010	1,6	14,14,15	0.35	0	15,19,21	0.35	0
6	NAG	A	2011	6	14,14,15	0.55	0	15,19,21	0.28	0
7	NAG	A	2012	1,7	14,14,15	0.23	0	15,19,21	0.28	0
7	NAG	A	2013	7	14,14,15	0.40	0	15,19,21	0.34	0
7	MAN	A	2014	7	11,11,12	1.51	3 (27%)	14,15,17	1.70	3 (21%)
7	NAG	B	2001	3,7	14,14,15	0.35	0	15,19,21	0.53	0
7	NAG	B	2002	7	14,14,15	0.46	0	15,19,21	1.41	2 (13%)
7	MAN	B	2003	7	11,11,12	1.79	2 (18%)	14,15,17	2.05	3 (21%)
6	NAG	C	3001	1,6	14,14,15	0.22	0	15,19,21	0.48	0
6	NAG	C	3002	6	14,14,15	0.21	0	15,19,21	0.26	0
5	NAG	C	3003	1,5	14,14,15	0.47	0	15,19,21	0.34	0
5	NAG	C	3004	5	14,14,15	0.77	1 (7%)	15,19,21	0.75	0
5	MAN	C	3005	5	11,11,12	1.90	4 (36%)	14,15,17	1.36	2 (14%)
5	MAN	C	3006	5	11,11,12	1.44	2 (18%)	14,15,17	1.63	2 (14%)
5	MAN	C	3007	5	11,11,12	1.65	2 (18%)	14,15,17	1.48	2 (14%)
6	NAG	C	3008	1,6	14,14,15	0.22	0	15,19,21	0.33	0
6	NAG	C	3009	6	14,14,15	0.19	0	15,19,21	0.22	0
6	NAG	C	3010	1,6	14,14,15	0.34	0	15,19,21	0.21	0
6	NAG	C	3011	6	14,14,15	0.63	0	15,19,21	0.47	0
6	NAG	C	3012	1,6	14,14,15	0.32	0	15,19,21	0.46	0
6	NAG	C	3013	6	14,14,15	0.25	0	15,19,21	0.22	0
9	NAG	D	2001	9,3	14,14,15	0.42	0	15,19,21	0.46	0
9	NAG	D	2002	9	14,14,15	0.45	0	15,19,21	1.08	1 (6%)
9	MAN	D	2003	9	11,11,12	2.03	3 (27%)	14,15,17	2.27	5 (35%)
9	MAN	D	2004	9	11,11,12	1.58	3 (27%)	14,15,17	1.15	1 (7%)
6	NAG	E	3001	1,6	14,14,15	0.34	0	15,19,21	0.17	0
6	NAG	E	3002	6	14,14,15	0.19	0	15,19,21	0.29	0
5	NAG	E	3003	1,5	14,14,15	0.31	0	15,19,21	0.37	0
5	NAG	E	3004	5	14,14,15	0.86	1 (7%)	15,19,21	0.69	0
5	MAN	E	3005	5	11,11,12	1.92	3 (27%)	14,15,17	1.86	3 (21%)
5	MAN	E	3006	5	11,11,12	1.35	2 (18%)	14,15,17	1.53	1 (7%)
5	MAN	E	3007	5	11,11,12	1.75	3 (27%)	14,15,17	1.82	4 (28%)
6	NAG	E	3008	1,6	14,14,15	0.68	1 (7%)	15,19,21	0.72	0
6	NAG	E	3009	6	14,14,15	1.17	1 (7%)	15,19,21	1.17	1 (6%)
7	NAG	E	3010	1,7	14,14,15	0.40	0	15,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	E	3011	7	14,14,15	0.35	0	15,19,21	0.40	0
7	MAN	E	3012	7	11,11,12	2.15	5 (45%)	14,15,17	2.27	3 (21%)
6	NAG	E	3013	1,6	14,14,15	0.19	0	15,19,21	0.46	0
6	NAG	E	3014	6	14,14,15	0.23	0	15,19,21	0.22	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
5	NAG	A	2001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2002	5	-	0/6/23/26	0/1/1/1
5	MAN	A	2003	5	-	0/2/19/22	0/1/1/1
5	MAN	A	2004	5	-	0/2/19/22	0/1/1/1
5	MAN	A	2005	5	-	0/2/19/22	0/1/1/1
6	NAG	A	2006	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	2007	6	-	0/6/23/26	0/1/1/1
6	NAG	A	2008	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	2009	6	-	0/6/23/26	0/1/1/1
6	NAG	A	2010	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	2011	6	-	0/6/23/26	0/1/1/1
7	NAG	A	2012	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	2013	7	-	0/6/23/26	0/1/1/1
7	MAN	A	2014	7	-	0/2/19/22	0/1/1/1
7	NAG	B	2001	3,7	-	0/6/23/26	0/1/1/1
7	NAG	B	2002	7	-	0/6/23/26	0/1/1/1
7	MAN	B	2003	7	-	0/2/19/22	0/1/1/1
6	NAG	C	3001	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	3002	6	-	0/6/23/26	0/1/1/1
5	NAG	C	3003	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	3004	5	-	0/6/23/26	0/1/1/1
5	MAN	C	3005	5	-	0/2/19/22	0/1/1/1
5	MAN	C	3006	5	-	0/2/19/22	0/1/1/1
5	MAN	C	3007	5	-	0/2/19/22	0/1/1/1
6	NAG	C	3008	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	3009	6	-	0/6/23/26	0/1/1/1
6	NAG	C	3010	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	3011	6	-	0/6/23/26	0/1/1/1
6	NAG	C	3012	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	3013	6	-	0/6/23/26	0/1/1/1
9	NAG	D	2001	9,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	D	2002	9	-	0/6/23/26	0/1/1/1
9	MAN	D	2003	9	-	0/2/19/22	0/1/1/1
9	MAN	D	2004	9	-	0/2/19/22	0/1/1/1
6	NAG	E	3001	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	3002	6	-	0/6/23/26	0/1/1/1
5	NAG	E	3003	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	3004	5	-	0/6/23/26	0/1/1/1
5	MAN	E	3005	5	-	0/2/19/22	0/1/1/1
5	MAN	E	3006	5	-	0/2/19/22	0/1/1/1
5	MAN	E	3007	5	-	0/2/19/22	0/1/1/1
6	NAG	E	3008	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	3009	6	-	0/6/23/26	0/1/1/1
7	NAG	E	3010	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	3011	7	-	0/6/23/26	0/1/1/1
7	MAN	E	3012	7	-	0/2/19/22	1/1/1/1
6	NAG	E	3013	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	3014	6	-	0/6/23/26	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3004	NAG	O5-C1	-3.04	1.38	1.43
5	C	3005	MAN	O5-C1	-2.76	1.39	1.43
5	E	3005	MAN	O5-C1	-2.67	1.39	1.43
5	C	3004	NAG	O5-C1	-2.67	1.39	1.43
7	A	2014	MAN	O5-C1	-2.63	1.39	1.43
6	E	3008	NAG	O5-C1	-2.43	1.39	1.43
6	A	2008	NAG	C1-C2	2.03	1.55	1.52
9	D	2004	MAN	O5-C5	2.03	1.47	1.43
7	A	2014	MAN	C4-C3	2.04	1.57	1.52
5	A	2004	MAN	O5-C5	2.05	1.47	1.43
5	A	2005	MAN	C4-C3	2.08	1.57	1.52
9	D	2003	MAN	O5-C5	2.15	1.48	1.43
7	E	3012	MAN	C4-C3	2.22	1.58	1.52
5	C	3005	MAN	C2-C3	2.26	1.55	1.52
5	C	3006	MAN	O5-C5	2.33	1.48	1.43
5	E	3006	MAN	C1-C2	2.34	1.57	1.52
5	A	2003	MAN	O5-C5	2.40	1.48	1.43
7	E	3012	MAN	C1-C2	2.44	1.58	1.52
5	E	3007	MAN	C4-C3	2.44	1.58	1.52
5	E	3005	MAN	C4-C3	2.46	1.58	1.52
5	E	3006	MAN	O5-C5	2.48	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3007	MAN	C1-C2	2.50	1.58	1.52
5	C	3005	MAN	C4-C3	2.60	1.59	1.52
9	D	2004	MAN	C4-C3	2.66	1.59	1.52
5	C	3006	MAN	C1-C2	2.73	1.58	1.52
7	E	3012	MAN	O5-C5	2.99	1.50	1.43
7	B	2003	MAN	O5-C5	3.08	1.50	1.43
7	E	3012	MAN	C4-C5	3.09	1.59	1.53
5	A	2003	MAN	C4-C3	3.11	1.60	1.52
7	A	2014	MAN	C4-C5	3.11	1.59	1.53
7	E	3012	MAN	C2-C3	3.13	1.56	1.52
9	D	2004	MAN	C4-C5	3.23	1.59	1.53
5	E	3007	MAN	C2-C3	3.27	1.57	1.52
5	E	3007	MAN	C1-C2	3.34	1.60	1.52
7	B	2003	MAN	C1-C2	3.54	1.60	1.52
5	C	3005	MAN	C4-C5	3.61	1.60	1.53
9	D	2003	MAN	C1-C2	3.86	1.61	1.52
5	C	3007	MAN	C2-C3	3.88	1.57	1.52
6	E	3009	NAG	O5-C1	3.99	1.50	1.43
9	D	2003	MAN	C2-C3	4.20	1.58	1.52
5	E	3005	MAN	C2-C3	4.34	1.58	1.52
5	A	2003	MAN	C2-C3	4.74	1.59	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2004	MAN	O2-C2-C3	-2.43	105.22	110.12
7	A	2014	MAN	O2-C2-C3	-2.30	105.50	110.12
5	E	3007	MAN	C1-C2-C3	2.02	111.94	109.54
5	C	3006	MAN	O2-C2-C1	2.03	113.27	109.21
7	B	2003	MAN	O2-C2-C1	2.09	113.40	109.21
7	E	3012	MAN	O3-C3-C2	2.11	113.82	110.00
5	A	2001	NAG	C1-O5-C5	2.21	115.05	112.25
5	C	3007	MAN	O5-C1-C2	2.22	114.46	110.86
9	D	2004	MAN	C1-O5-C5	2.24	115.09	112.25
9	D	2003	MAN	O3-C3-C2	2.30	114.16	110.00
9	D	2003	MAN	O2-C2-C1	2.36	113.94	109.21
5	C	3005	MAN	C1-O5-C5	2.57	115.51	112.25
7	E	3012	MAN	O5-C1-C2	2.58	115.05	110.86
7	B	2002	NAG	C3-C4-C5	2.67	114.84	110.20
5	E	3007	MAN	O2-C2-C1	2.79	114.79	109.21
5	A	2003	MAN	C3-C4-C5	2.86	115.17	110.20
5	A	2003	MAN	C2-C3-C4	3.02	116.17	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2003	MAN	C1-O5-C5	3.05	116.12	112.25
9	D	2002	NAG	C1-O5-C5	3.29	116.42	112.25
7	B	2003	MAN	O5-C1-C2	3.29	116.20	110.86
5	C	3005	MAN	C3-C4-C5	3.33	116.00	110.20
9	D	2003	MAN	O5-C1-C2	3.34	116.28	110.86
5	E	3005	MAN	C3-C4-C5	3.49	116.29	110.20
5	E	3005	MAN	C2-C3-C4	3.61	117.17	111.04
7	A	2014	MAN	C1-O5-C5	3.64	116.86	112.25
5	E	3007	MAN	O5-C1-C2	3.64	116.77	110.86
5	C	3007	MAN	C1-O5-C5	3.67	116.91	112.25
5	E	3005	MAN	C1-C2-C3	3.67	113.88	109.54
5	A	2003	MAN	C1-C2-C3	3.70	113.92	109.54
9	D	2003	MAN	C1-C2-C3	3.82	114.06	109.54
7	A	2014	MAN	C3-C4-C5	3.85	116.91	110.20
5	E	3007	MAN	C1-O5-C5	4.03	117.37	112.25
6	E	3009	NAG	C1-O5-C5	4.08	117.43	112.25
5	E	3006	MAN	C1-O5-C5	4.29	117.69	112.25
5	A	2004	MAN	C1-O5-C5	4.41	117.84	112.25
7	B	2002	NAG	C1-O5-C5	4.58	118.06	112.25
5	C	3006	MAN	C1-O5-C5	4.95	118.53	112.25
9	D	2003	MAN	C1-O5-C5	5.12	118.75	112.25
7	B	2003	MAN	C1-O5-C5	5.67	119.45	112.25
7	E	3012	MAN	C1-O5-C5	7.08	121.23	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	3012	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2008	NAG	1	0
6	A	2009	NAG	1	0
6	A	2010	NAG	2	0
7	B	2001	NAG	1	0
7	B	2002	NAG	1	0
7	B	2003	MAN	1	0
6	C	3001	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3002	NAG	1	0
9	D	2002	NAG	1	0
9	D	2003	MAN	1	0
5	E	3003	NAG	1	0
5	E	3004	NAG	1	0

5.6 Ligand geometry

4 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	$\#\|Z\|>2$
8	NAG	F	2001	3	14,14,15	0.23	0	15,19,21	0.33	0
8	NAG	I	701	2	14,14,15	0.46	0	15,19,21	0.26	0
8	NAG	K	701	2	14,14,15	0.32	0	15,19,21	0.31	0
8	NAG	L	701	2	14,14,15	0.50	0	15,19,21	0.28	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
8	NAG	F	2001	3	-	0/6/23/26	0/1/1/1
8	NAG	I	701	2	-	0/6/23/26	0/1/1/1
8	NAG	K	701	2	-	0/6/23/26	0/1/1/1
8	NAG	L	701	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	324/334 (97%)	-0.22	0 100 100	104, 135, 164, 210	0
1	C	324/334 (97%)	-0.20	0 100 100	107, 138, 165, 200	0
1	E	324/334 (97%)	-0.18	0 100 100	97, 124, 151, 184	0
2	I	217/218 (99%)	-0.21	0 100 100	119, 148, 175, 191	0
2	K	217/218 (99%)	-0.13	1 (0%) 91 88	130, 166, 184, 211	0
2	L	217/218 (99%)	-0.27	0 100 100	96, 126, 150, 182	0
3	B	177/181 (97%)	-0.08	2 (1%) 82 74	99, 149, 207, 218	0
3	D	177/181 (97%)	-0.05	1 (0%) 90 85	101, 150, 192, 218	0
3	F	177/181 (97%)	-0.15	2 (1%) 82 74	103, 135, 172, 189	0
4	G	222/222 (100%)	-0.09	1 (0%) 91 88	104, 142, 186, 217	1 (0%)
4	H	222/222 (100%)	-0.20	1 (0%) 91 88	96, 126, 167, 203	1 (0%)
4	J	222/222 (100%)	0.00	3 (1%) 78 69	131, 162, 212, 235	1 (0%)
All	All	2820/2865 (98%)	-0.16	11 (0%) 93 90	96, 140, 189, 235	3 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1	GLY	4.4
4	J	134	THR	4.3
4	H	134	THR	3.6
3	B	1	GLY	3.2
3	D	1	GLY	2.9
2	K	149	LYS	2.8
4	J	140	LEU	2.4
4	G	43	LYS	2.2
3	B	141	TYR	2.1
4	J	221	LYS	2.0
3	F	177	ARG	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
5	NAG	A	2001	14/15	0.92	0.20	0.41	142,165,185,186	0
5	NAG	C	3003	14/15	0.94	0.16	-0.74	137,158,177,194	0
5	NAG	E	3003	14/15	0.90	0.16	-0.79	140,152,166,170	0
9	NAG	D	2001	14/15	0.87	0.35	-	180,205,219,225	0
7	NAG	E	3010	14/15	0.93	0.24	-	163,190,203,209	0
6	NAG	E	3002	14/15	0.78	0.43	-	197,212,219,219	0
6	NAG	C	3009	14/15	0.86	0.33	-	193,205,210,211	0
7	MAN	B	2003	11/12	0.45	0.48	-	209,241,248,248	0
5	MAN	A	2003	11/12	0.72	0.34	-	227,235,241,241	0
7	NAG	B	2002	14/15	0.80	0.59	-	222,239,247,247	0
7	NAG	E	3011	14/15	0.81	0.34	-	171,207,213,213	0
6	NAG	E	3013	14/15	0.88	0.37	-	159,190,199,208	0
5	MAN	C	3006	11/12	0.81	0.40	-	211,234,241,242	0
6	NAG	A	2011	14/15	0.82	0.58	-	170,186,192,195	0
7	NAG	B	2001	14/15	0.83	0.52	-	204,228,239,243	0
9	MAN	D	2004	11/12	0.82	0.36	-	212,240,244,244	0
5	MAN	C	3005	11/12	0.65	0.33	-	219,234,242,243	0
6	NAG	A	2008	14/15	0.80	0.36	-	195,214,225,228	0
9	MAN	D	2003	11/12	0.75	0.37	-	211,229,240,243	0
6	NAG	E	3009	14/15	0.88	0.29	-	180,202,209,209	0
7	NAG	A	2013	14/15	0.67	0.35	-	194,213,228,237	0
5	MAN	C	3007	11/12	0.69	0.43	-	223,235,246,246	0
5	MAN	E	3006	11/12	0.87	0.45	-	200,226,233,233	0
6	NAG	A	2006	14/15	0.83	0.18	-	159,181,194,208	0
6	NAG	A	2009	14/15	0.68	0.64	-	203,224,230,231	0
9	NAG	D	2002	14/15	0.88	0.45	-	209,229,235,236	0
7	MAN	A	2014	11/12	0.40	0.36	-	223,230,239,242	0
5	NAG	C	3004	14/15	0.86	0.21	-	194,204,221,226	0
6	NAG	E	3001	14/15	0.93	0.17	-	158,173,186,201	0
7	MAN	E	3012	11/12	0.70	0.31	-	184,206,217,217	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	C	3001	14/15	0.90	0.13	-	160,170,187,197	0
6	NAG	C	3011	14/15	0.72	0.54	-	151,188,191,192	0
5	MAN	E	3007	11/12	0.74	0.52	-	204,228,234,234	0
5	MAN	A	2004	11/12	0.82	0.38	-	224,237,243,246	0
6	NAG	C	3002	14/15	0.84	0.37	-	188,204,214,217	0
6	NAG	C	3008	14/15	0.85	0.23	-	160,180,198,204	0
5	NAG	A	2002	14/15	0.88	0.26	-	191,201,220,229	0
5	MAN	E	3005	11/12	0.68	0.31	-	211,224,230,230	0
5	NAG	E	3004	14/15	0.88	0.21	-	178,190,204,214	0
7	NAG	A	2012	14/15	0.94	0.09	-	158,173,189,199	0
6	NAG	E	3014	14/15	0.51	0.67	-	193,218,224,224	0
6	NAG	E	3008	14/15	0.94	0.18	-	155,174,183,197	0
5	MAN	A	2005	11/12	0.72	0.53	-	222,237,239,240	0
6	NAG	A	2010	14/15	0.88	0.40	-	165,179,188,191	0
6	NAG	A	2007	14/15	0.82	0.30	-	187,212,219,220	0
6	NAG	C	3013	14/15	0.73	0.50	-	195,215,220,220	0
6	NAG	C	3010	14/15	0.76	0.40	-	162,185,195,196	0
6	NAG	C	3012	14/15	0.86	0.37	-	174,190,204,213	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
8	NAG	I	701	14/15	0.73	0.26	-	144,169,178,178	0
8	NAG	L	701	14/15	0.85	0.14	-	137,155,163,171	0
8	NAG	K	701	14/15	0.87	0.19	-	158,172,178,179	0
8	NAG	F	2001	14/15	0.74	0.49	-	156,174,183,184	0

6.5 Other polymers

There are no such residues in this entry.