Full wwPDB X-ray Structure Validation Report (i)

Oct 13, 2016 – 02:42 PM EDT

PDB ID	:	4JM0
Title	:	Structure of Human Cytomegalovirus Immune Modulator UL141
Authors	:	Nemcovicova, I.; Zajonc, D.M.
Deposited on	:	2013-03-13
Resolution	:	3.25 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:

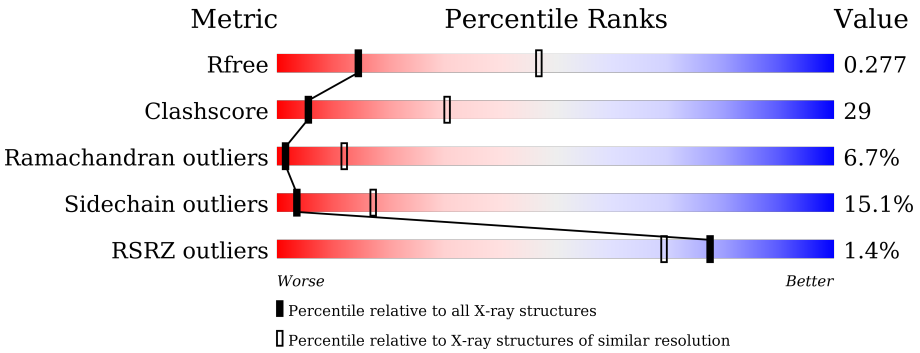
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	256	2% 40% 21% 7% 32%
1	B	256	38% 26% 5% 29%

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
2	NAG	A	501	-	-	-	X
3	NAG	A	504	X	-	-	-
3	NAG	A	505	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2863 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 Protein UL141.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1331	855	227	240	9			
1	B	183	Total	C	N	O	S	0	0	0
			1392	893	230	257	12			

There are 12 discrepancies between the modelled and reference sequences:

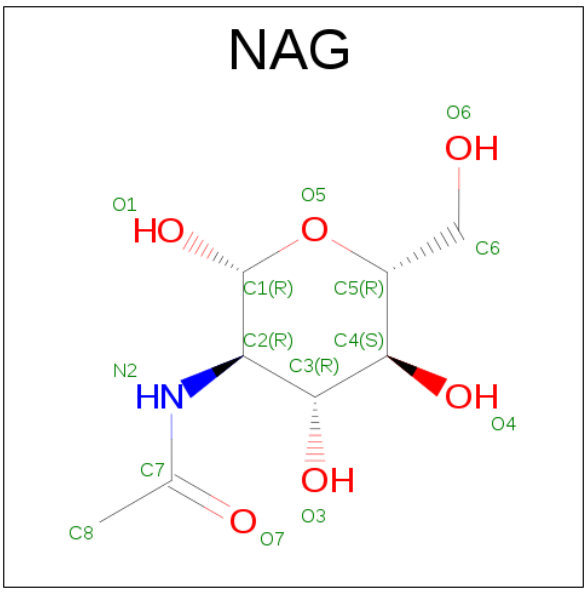
Chain	Residue	Modelled	Actual	Comment	Reference
A	280	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
A	281	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
A	282	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
A	283	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
A	284	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
A	285	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
B	280	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
B	281	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
B	282	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
B	283	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
B	284	HIS	-	EXPRESSION TAG	UNP Q6RJQ3
B	285	HIS	-	EXPRESSION TAG	UNP Q6RJQ3

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

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



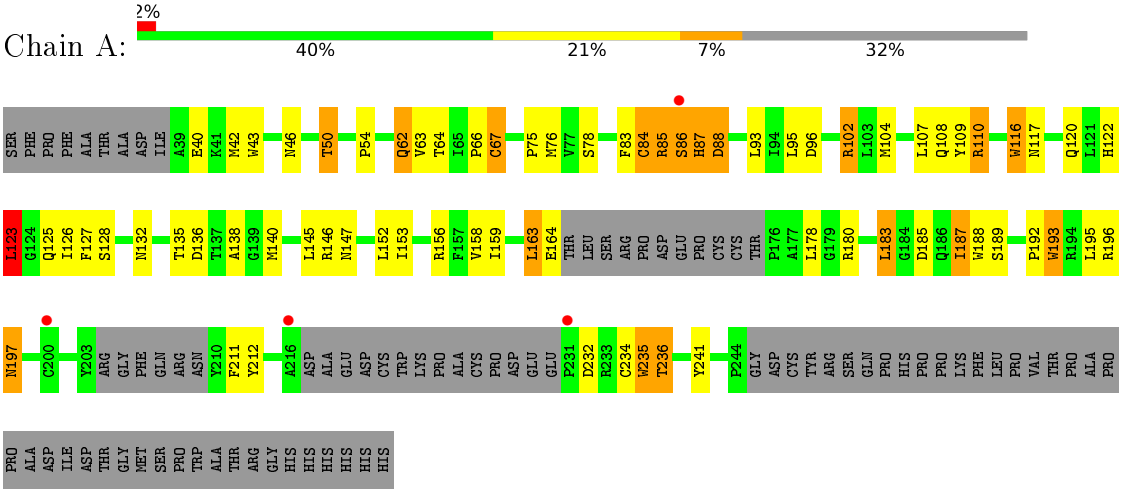
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 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.

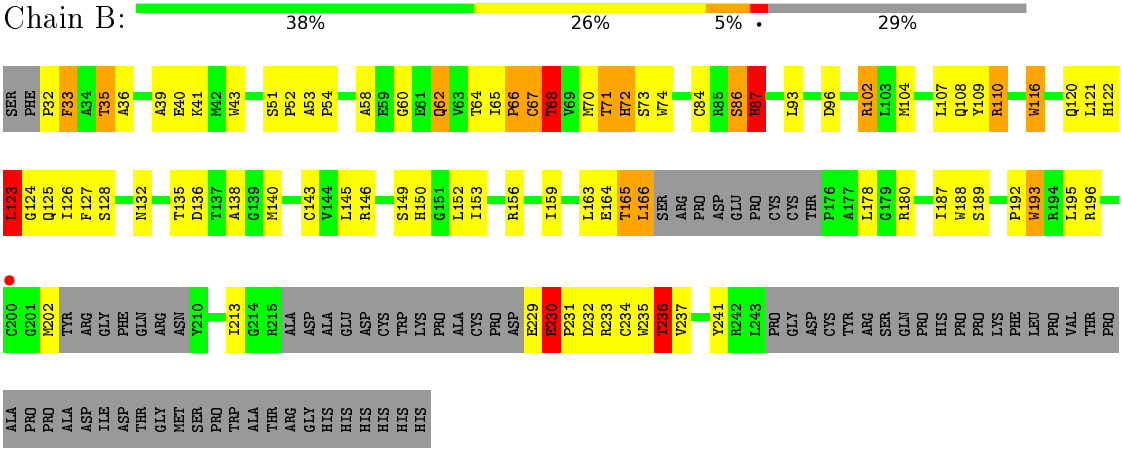
- Molecule 1: Protein UL141

Chain A:



- Molecule 1: Protein UL141

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	96.06Å 96.06Å 136.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	11.98 – 3.25 11.98 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.5 (11.98-3.25) 99.7 (11.98-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 3.28Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.201 , 0.279 0.210 , 0.277	Depositor DCC
R_{free} test set	930 reflections (8.72%)	DCC
Wilson B-factor (Å^2)	76.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2863	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.333 respectively for untwinned datasets, and 0.375, 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

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	1.07	5/1366 (0.4%)	1.10	7/1868 (0.4%)
1	B	1.09	4/1427 (0.3%)	1.04	4/1949 (0.2%)
All	All	1.08	9/2793 (0.3%)	1.07	11/3817 (0.3%)

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	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	TRP	CD2-CE2	6.91	1.49	1.41
1	A	116	TRP	CD2-CE2	6.26	1.48	1.41
1	A	188	TRP	CD2-CE2	5.98	1.48	1.41
1	B	116	TRP	CD2-CE2	5.73	1.48	1.41
1	A	193	TRP	CD2-CE2	5.61	1.48	1.41
1	B	193	TRP	CD2-CE2	5.53	1.48	1.41
1	A	235	TRP	CD2-CE2	5.46	1.47	1.41
1	A	43	TRP	CD2-CE2	5.24	1.47	1.41
1	B	84	CYS	CB-SG	5.14	1.91	1.82

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	LEU	CA-CB-CG	7.85	133.36	115.30
1	B	123	LEU	CA-CB-CG	6.35	129.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	236	THR	N-CA-CB	5.80	121.32	110.30
1	B	93	LEU	CB-CG-CD2	-5.47	101.71	111.00
1	A	67	CYS	O-C-N	5.21	131.04	122.70
1	A	66	PRO	O-C-N	5.21	131.03	122.70
1	A	183	LEU	CB-CG-CD1	5.11	119.68	111.00
1	A	123	LEU	CB-CG-CD2	5.08	119.63	111.00
1	A	67	CYS	CA-C-N	-5.05	106.08	117.20
1	B	236	THR	N-CA-C	-5.04	97.39	111.00
1	A	123	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	GLU	Peptide

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	1331	0	1220	69	0
1	B	1392	0	1277	84	0
2	A	28	0	25	1	0
2	B	56	0	50	4	0
3	A	56	0	52	14	0
All	All	2863	0	2624	155	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 29.

All (155) 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:A:84:CYS:SG	1:A:234:CYS:CB	2.15	1.34
1:A:147:ASN:HD21	3:A:505:NAG:C1	1.55	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:THR:O	1:B:68:THR:HG22	1.56	1.05
1:A:180:ARG:HH21	1:B:73:SER:HA	1.16	1.04
1:B:67:CYS:SG	1:B:143:CYS:CB	2.48	1.00
1:A:86:SER:O	1:A:87:HIS:HB3	1.60	1.00
1:B:67:CYS:O	1:B:68:THR:HB	1.60	0.99
1:B:120:GLN:NE2	1:B:125:GLN:HE21	1.61	0.98
1:B:72:HIS:CE1	1:B:145:LEU:HD22	2.01	0.95
1:B:120:GLN:HE22	1:B:125:GLN:NE2	1.63	0.95
1:B:102:ARG:HG2	1:B:102:ARG:HH11	1.29	0.93
1:B:66:PRO:O	1:B:67:CYS:HB2	1.64	0.93
1:A:120:GLN:HE22	1:A:125:GLN:HE21	1.17	0.92
1:A:117:ASN:OD1	2:A:501:NAG:H2	1.69	0.91
1:A:147:ASN:ND2	3:A:505:NAG:C2	2.34	0.90
1:A:147:ASN:HD21	3:A:505:NAG:C2	1.84	0.90
3:A:505:NAG:O4	3:A:506:NAG:C2	2.20	0.89
1:B:62:GLN:HB2	1:B:132:ASN:OD1	1.73	0.87
1:B:120:GLN:HE22	1:B:125:GLN:HE21	0.87	0.85
3:A:505:NAG:C4	3:A:506:NAG:C1	2.56	0.83
3:A:505:NAG:HO4	3:A:506:NAG:C1	1.90	0.81
1:B:102:ARG:NH1	1:B:102:ARG:HG2	1.94	0.81
1:A:84:CYS:CB	1:A:234:CYS:SG	2.68	0.81
1:B:66:PRO:O	1:B:67:CYS:CB	2.29	0.80
1:B:86:SER:O	1:B:110:ARG:NH2	2.15	0.78
1:A:86:SER:O	1:A:87:HIS:CB	2.30	0.78
1:B:67:CYS:O	1:B:68:THR:CB	2.30	0.78
1:B:232:ASP:HB3	1:B:234:CYS:H	1.50	0.76
1:A:84:CYS:CB	1:A:234:CYS:HG	1.95	0.76
1:B:60:GLY:O	2:B:301:NAG:H82	1.86	0.75
1:B:72:HIS:HE1	1:B:145:LEU:HD22	1.51	0.74
1:B:102:ARG:CG	1:B:102:ARG:HH11	2.01	0.74
1:A:180:ARG:NH2	1:B:73:SER:HA	2.00	0.74
1:A:147:ASN:ND2	3:A:505:NAG:N2	2.36	0.74
1:A:102:ARG:HG2	1:A:102:ARG:HH11	1.53	0.73
1:A:185:ASP:HB2	1:A:241:TYR:HD1	1.52	0.73
1:B:87:HIS:HB3	1:B:110:ARG:HH21	1.56	0.70
1:B:107:LEU:O	1:B:109:TYR:N	2.25	0.70
1:A:84:CYS:SG	1:A:234:CYS:HB2	2.30	0.70
1:B:138:ALA:HB1	1:B:159:ILE:O	1.92	0.70
1:A:180:ARG:HD2	1:B:71:THR:CG2	2.22	0.69
1:A:120:GLN:NE2	1:A:125:GLN:HE21	1.91	0.69
2:B:301:NAG:H61	2:B:302:NAG:C1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLN:HE21	1:A:122:HIS:H	1.42	0.68
1:B:66:PRO:O	1:B:127:PHE:O	2.12	0.67
1:A:67:CYS:O	1:A:126:ILE:HA	1.95	0.67
1:B:68:THR:HA	1:B:125:GLN:O	1.95	0.67
1:A:232:ASP:HB3	1:A:234:CYS:H	1.60	0.66
1:A:178:LEU:O	1:A:192:PRO:HB3	1.96	0.66
3:A:505:NAG:H61	3:A:506:NAG:C1	2.26	0.65
1:A:102:ARG:NH1	1:A:102:ARG:HG2	2.10	0.65
1:A:196:ARG:HB2	1:A:212:TYR:CZ	2.32	0.65
1:A:180:ARG:HD2	1:B:71:THR:HG22	1.77	0.64
1:B:70:MET:O	1:B:71:THR:C	2.35	0.63
1:B:159:ILE:HD12	1:B:159:ILE:N	2.12	0.63
1:B:120:GLN:HE21	1:B:122:HIS:H	1.46	0.63
1:A:107:LEU:O	1:A:109:TYR:N	2.33	0.62
1:A:147:ASN:ND2	3:A:505:NAG:H2	2.14	0.61
1:A:138:ALA:HB1	1:A:159:ILE:O	2.03	0.59
1:A:120:GLN:HE22	1:A:125:GLN:NE2	1.93	0.59
1:A:54:PRO:HD3	1:A:241:TYR:CD2	2.38	0.59
3:A:503:NAG:O3	3:A:504:NAG:H5	2.04	0.58
1:B:110:ARG:HH11	1:B:110:ARG:CG	2.16	0.58
1:B:140:MET:SD	1:B:237:VAL:HG21	2.44	0.58
1:A:87:HIS:CD2	1:A:88:ASP:N	2.74	0.56
1:A:102:ARG:CG	1:A:102:ARG:HH11	2.19	0.56
1:B:166:LEU:HD13	1:B:166:LEU:N	2.22	0.56
1:A:178:LEU:O	1:A:192:PRO:CB	2.54	0.55
1:B:64:THR:CG2	1:B:65:ILE:N	2.69	0.55
1:A:62:GLN:HB2	1:A:132:ASN:OD1	2.06	0.55
2:B:301:NAG:C6	2:B:302:NAG:C1	2.84	0.55
1:B:32:PRO:N	1:B:33:PHE:HA	2.21	0.55
1:B:195:LEU:HD12	1:B:196:ARG:O	2.06	0.54
1:A:54:PRO:HD3	1:A:241:TYR:CE2	2.42	0.54
1:B:107:LEU:C	1:B:109:TYR:H	2.10	0.54
1:A:159:ILE:HD12	1:A:159:ILE:N	2.22	0.54
1:B:43:TRP:NE1	1:B:153:ILE:HD12	2.23	0.54
1:B:40:GLU:HB2	1:B:150:HIS:CD2	2.43	0.54
1:B:64:THR:HG22	1:B:65:ILE:N	2.22	0.54
1:B:62:GLN:CB	1:B:132:ASN:OD1	2.51	0.53
1:B:67:CYS:SG	1:B:143:CYS:HB3	2.46	0.52
1:A:116:TRP:HA	1:A:128:SER:O	2.10	0.52
1:A:232:ASP:C	1:A:234:CYS:H	2.11	0.52
1:A:83:PHE:CE2	1:A:110:ARG:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ARG:CG	1:B:110:ARG:NH1	2.72	0.52
1:A:107:LEU:C	1:A:109:TYR:H	2.13	0.52
1:B:166:LEU:HD13	1:B:166:LEU:H	1.75	0.51
1:B:54:PRO:HD3	1:B:241:TYR:CD2	2.45	0.51
1:B:72:HIS:ND1	1:B:145:LEU:HD22	2.24	0.50
1:B:70:MET:O	1:B:71:THR:O	2.29	0.50
1:A:185:ASP:HB2	1:A:241:TYR:CD1	2.40	0.50
3:A:505:NAG:O4	3:A:506:NAG:H2	2.10	0.50
1:B:43:TRP:CE2	1:B:153:ILE:HD12	2.47	0.50
1:B:67:CYS:O	1:B:68:THR:O	2.30	0.49
1:A:123:LEU:HD11	1:B:64:THR:O	2.13	0.49
1:A:85:ARG:O	1:A:86:SER:O	2.30	0.48
1:B:178:LEU:O	1:B:192:PRO:HB3	2.14	0.48
1:B:229:GLU:HA	1:B:230:GLU:HA	1.58	0.48
1:B:65:ILE:O	1:B:128:SER:HA	2.13	0.48
1:A:110:ARG:NH1	1:A:136:ASP:O	2.46	0.48
1:B:110:ARG:HH11	1:B:110:ARG:HG3	1.77	0.48
1:A:63:VAL:HB	1:B:123:LEU:CD1	2.44	0.47
1:B:145:LEU:HB2	1:B:152:LEU:HB3	1.96	0.47
1:A:180:ARG:HA	1:A:189:SER:O	2.15	0.47
1:A:85:ARG:O	1:A:86:SER:C	2.52	0.47
1:B:234:CYS:O	1:B:236:THR:N	2.48	0.47
1:B:180:ARG:HA	1:B:189:SER:O	2.14	0.46
1:B:165:THR:O	1:B:165:THR:CG2	2.63	0.46
1:B:110:ARG:NH1	1:B:136:ASP:O	2.48	0.46
1:B:72:HIS:ND1	1:B:145:LEU:HD13	2.30	0.46
1:A:195:LEU:HD12	1:A:196:ARG:O	2.15	0.46
2:B:301:NAG:O3	2:B:301:NAG:O7	2.30	0.46
1:B:58:ALA:HB2	1:B:213:ILE:CG2	2.47	0.45
1:A:163:LEU:HD23	1:A:211:PHE:HB2	1.97	0.45
1:A:46:ASN:O	1:A:50:THR:HG23	2.16	0.45
1:B:71:THR:H	1:B:124:GLY:HA2	1.82	0.45
1:A:42:MET:O	1:A:153:ILE:N	2.41	0.45
1:B:121:LEU:HD11	1:B:126:ILE:HG13	1.98	0.45
1:A:211:PHE:O	1:A:212:TYR:HB3	2.17	0.44
1:B:233:ARG:HG2	1:B:233:ARG:O	2.16	0.44
1:A:107:LEU:C	1:A:109:TYR:N	2.70	0.44
1:B:53:ALA:HB1	1:B:54:PRO:HD2	2.00	0.44
3:A:503:NAG:O3	3:A:504:NAG:C5	2.65	0.44
1:A:140:MET:HG2	1:A:158:VAL:HG22	2.00	0.43
1:B:116:TRP:HA	1:B:128:SER:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:PRO:HD3	1:B:241:TYR:CE2	2.53	0.43
1:B:74:TRP:CD1	1:B:74:TRP:N	2.86	0.43
1:A:145:LEU:HB2	1:A:152:LEU:HB3	2.00	0.43
1:A:87:HIS:CD2	1:A:87:HIS:C	2.91	0.43
1:B:62:GLN:HE21	1:B:62:GLN:HB2	1.53	0.43
1:A:64:THR:HB	1:B:121:LEU:HD22	2.01	0.43
1:A:63:VAL:HB	1:B:123:LEU:HD13	2.00	0.43
1:A:147:ASN:HD22	3:A:505:NAG:H2	1.81	0.43
1:B:102:ARG:HD3	1:B:116:TRP:CZ2	2.54	0.43
1:B:121:LEU:O	1:B:122:HIS:HB3	2.19	0.43
1:B:178:LEU:O	1:B:192:PRO:CB	2.67	0.43
1:A:180:ARG:NE	1:B:72:HIS:O	2.48	0.43
1:B:62:GLN:O	1:B:62:GLN:CG	2.68	0.42
1:B:39:ALA:HB3	1:B:149:SER:O	2.19	0.42
1:B:166:LEU:N	1:B:166:LEU:CD1	2.83	0.42
1:B:58:ALA:HA	1:B:213:ILE:HB	2.01	0.42
1:B:72:HIS:N	1:B:72:HIS:CD2	2.88	0.42
1:A:232:ASP:C	1:A:234:CYS:N	2.74	0.41
1:A:102:ARG:HD3	1:A:116:TRP:CZ2	2.55	0.41
1:A:187:ILE:HG12	1:A:187:ILE:H	1.63	0.41
3:A:505:NAG:C5	3:A:506:NAG:C1	2.98	0.41
1:A:195:LEU:HG	1:A:195:LEU:O	2.21	0.41
1:A:196:ARG:HB2	1:A:212:TYR:CE2	2.56	0.41
1:A:75:PRO:HG2	1:A:76:MET:HG3	2.03	0.41
1:A:102:ARG:HD3	1:A:116:TRP:HZ2	1.85	0.40
1:A:67:CYS:N	1:A:127:PHE:O	2.50	0.40
1:A:78:SER:HA	1:A:93:LEU:O	2.20	0.40
1:B:51:SER:HA	1:B:52:PRO:HD2	1.98	0.40
1:B:71:THR:N	1:B:124:GLY:HA2	2.36	0.40
1:B:102:ARG:HD3	1:B:116:TRP:HZ2	1.86	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	167/256 (65%)	139 (83%)	19 (11%)	9 (5%)	2 18
1	B	175/256 (68%)	145 (83%)	16 (9%)	14 (8%)	1 8
All	All	342/512 (67%)	284 (83%)	35 (10%)	23 (7%)	1 12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	236	THR
1	B	36	ALA
1	B	67	CYS
1	B	108	GLN
1	B	230	GLU
1	B	236	THR
1	B	66	PRO
1	B	87	HIS
1	B	235	TRP
1	A	85	ARG
1	A	86	SER
1	A	235	TRP
1	B	193	TRP
1	A	40	GLU
1	B	35	THR
1	A	108	GLN
1	A	193	TRP
1	A	197	ASN
1	B	68	THR
1	B	71	THR
1	B	86	SER
1	B	231	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	132/224 (59%)	113 (86%)	19 (14%)	4 19
1	B	140/224 (62%)	118 (84%)	22 (16%)	3 15
All	All	272/448 (61%)	231 (85%)	41 (15%)	3 17

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	62	GLN
1	A	84	CYS
1	A	88	ASP
1	A	95	LEU
1	A	96	ASP
1	A	102	ARG
1	A	104	MET
1	A	110	ARG
1	A	123	LEU
1	A	135	THR
1	A	146	ARG
1	A	156	ARG
1	A	163	LEU
1	A	164	GLU
1	A	183	LEU
1	A	187	ILE
1	A	197	ASN
1	A	236	THR
1	B	33	PHE
1	B	35	THR
1	B	41	LYS
1	B	62	GLN
1	B	68	THR
1	B	72	HIS
1	B	87	HIS
1	B	96	ASP
1	B	102	ARG
1	B	104	MET
1	B	110	ARG
1	B	123	LEU
1	B	135	THR
1	B	146	ARG
1	B	156	ARG
1	B	163	LEU

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Mol	Chain	Res	Type
1	B	164	GLU
1	B	165	THR
1	B	166	LEU
1	B	187	ILE
1	B	202	MET
1	B	236	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	87	HIS
1	A	120	GLN
1	A	147	ASN
1	A	155	GLN
1	B	62	GLN
1	B	117	ASN
1	B	120	GLN
1	B	155	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

6 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	$\#\|Z\|>2$
2	NAG	A	501	2	14,14,15	0.86	0	15,19,21	2.02	5 (33%)
2	NAG	A	502	2	14,14,15	0.78	0	15,19,21	2.55	4 (26%)
2	NAG	B	301	1,2	14,14,15	0.54	0	15,19,21	0.60	0
2	NAG	B	302	2	14,14,15	0.54	0	15,19,21	0.59	0
2	NAG	B	303	1,2	14,14,15	0.76	0	15,19,21	2.04	4 (26%)
2	NAG	B	304	2	14,14,15	0.75	0	15,19,21	1.26	2 (13%)

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
2	NAG	A	501	2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	NAG	B	301	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	302	2	-	0/6/23/26	0/1/1/1
2	NAG	B	303	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	304	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	304	NAG	O3-C3-C2	-2.49	104.05	109.37
2	B	304	NAG	O6-C6-C5	-2.41	103.24	111.30
2	A	501	NAG	O4-C4-C5	-2.15	103.57	109.23
2	A	502	NAG	C3-C4-C5	2.11	114.00	110.23
2	B	303	NAG	C1-O5-C5	2.26	115.46	112.14
2	A	501	NAG	C3-C4-C5	2.37	114.46	110.23
2	A	501	NAG	O5-C5-C4	2.41	114.13	110.13
2	B	303	NAG	C4-C3-C2	2.44	115.12	111.34
2	B	303	NAG	O5-C5-C6	2.74	113.22	107.34
2	A	502	NAG	O5-C5-C4	2.78	114.74	110.13
2	A	501	NAG	C2-N2-C7	3.85	128.11	123.11
2	A	501	NAG	C4-C3-C2	4.35	118.09	111.34
2	A	502	NAG	C1-O5-C5	5.21	119.81	112.14
2	B	303	NAG	C2-N2-C7	6.09	131.03	123.11
2	A	502	NAG	C2-N2-C7	7.00	132.21	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
2	B	301	NAG	4	0
2	B	302	NAG	2	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	$\#\|Z\| > 2$
3	NAG	A	503	1,3	14,14,15	0.55	0	15,19,21	0.61	0
3	NAG	A	504	3	14,14,15	0.54	0	15,19,21	0.59	0
3	NAG	A	505	1,3	14,14,15	1.02	1 (7%)	15,19,21	1.98	5 (33%)
3	NAG	A	506	3	14,14,15	0.66	0	15,19,21	1.55	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	503	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	504	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	506	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	NAG	C4-C3	2.20	1.58	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	506	NAG	C4-C3-C2	-3.10	106.53	111.34
3	A	505	NAG	O4-C4-C5	-2.50	102.64	109.23
3	A	505	NAG	O3-C3-C2	-2.09	104.91	109.37
3	A	506	NAG	O5-C5-C4	2.12	113.64	110.13
3	A	505	NAG	C2-N2-C7	3.18	127.24	123.11
3	A	505	NAG	C4-C3-C2	3.42	116.64	111.34
3	A	506	NAG	C1-O5-C5	4.13	118.22	112.14
3	A	505	NAG	C3-C4-C5	4.59	118.41	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	504	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAG	2	0
3	A	504	NAG	2	0
3	A	505	NAG	12	0
3	A	506	NAG	6	0

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	175/256 (68%)	-0.38	4 (2%)	64	54	44, 70, 130, 153	0
1	B	183/256 (71%)	-0.50	1 (0%)	91	88	42, 66, 125, 155	0
All	All	358/512 (69%)	-0.44	5 (1%)	78	69	42, 68, 129, 155	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	CYS	4.3
1	B	200	CYS	3.6
1	A	216	ALA	3.5
1	A	231	PRO	3.1
1	A	86	SER	2.0

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

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

6.3 Carbohydrates

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
2	NAG	A	501	14/15	0.81	0.39	16.37	103,125,133,163	0
2	NAG	B	303	14/15	0.94	0.17	0.30	62,75,91,111	0
2	NAG	B	302	14/15	0.62	0.56	-	109,128,140,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	502	14/15	0.51	0.39	-	111,179,192,192	0
2	NAG	B	301	14/15	0.76	0.33	-	81,102,112,113	0
2	NAG	B	304	14/15	0.90	0.26	-	76,83,103,110	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	505	14/15	0.82	0.30	2.23	81,102,112,113	0
3	NAG	A	504	14/15	0.65	0.56	-	109,128,140,149	0
3	NAG	A	503	14/15	0.74	0.37	-	81,102,112,113	0
3	NAG	A	506	14/15	0.77	0.36	-	109,128,140,149	0

6.5 Other polymers (i)

There are no such residues in this entry.