Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:59 PM GMT

PDB ID	:	4YW7
Title	:	Structural Insight into Divalent Galactoside Binding to Pseudomonas aeruginosa lectin LecA
Authors	:	Visini, R.; Jin, X.; Michaud, G.; Bergmann, M.; Gillon, E.; Imberty, A.; Stocker, A.; Darbre, T.; Pieters, R.; Reymond, J.-L.
Deposited on	:	2015-03-20
Resolution	:	1.82 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:

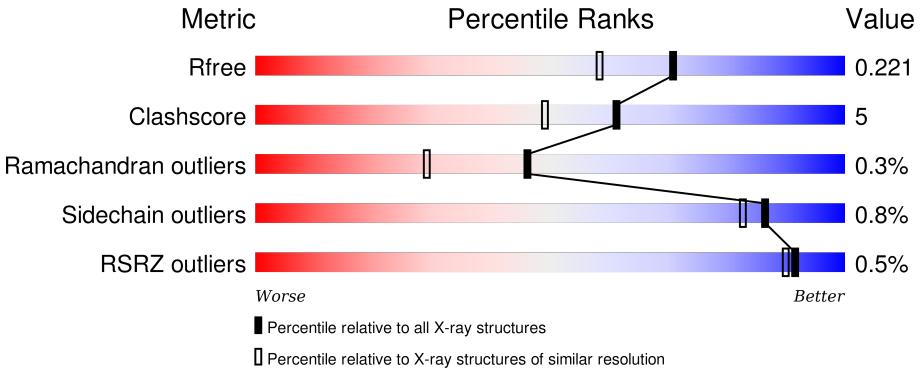
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.82 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	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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	121	93% 6% •
1	B	121	% 88% 12%
1	C	121	2% 86% 14%
1	D	121	92% 8%
1	E	121	% 83% 14% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	121	90% 9%
1	G	121	90% 10%
1	H	121	% 87% 10%
1	I	121	88% 11%
1	J	121	% 91% 8%
1	K	121	% 92% 8%
1	L	121	96%
1	M	121	94% 6%
1	N	121	% 83% 16%
1	O	121	92% 8%
1	P	121	% 85% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	4J0	C	201	-	-	-	X
4	4J0	I	202	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16634 atoms, of which 136 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.

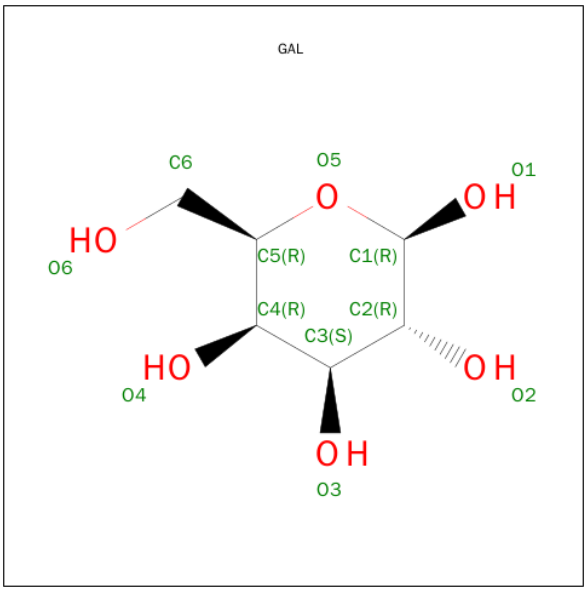
- Molecule 1 is a protein called PA-I galactophilic lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			896	566	154	173	3			
1	B	121	Total	C	N	O	S	0	0	0
			886	561	152	170	3			
1	C	121	Total	C	N	O	S	0	0	0
			893	565	153	172	3			
1	D	121	Total	C	N	O	S	0	0	0
			889	563	153	170	3			
1	E	121	Total	C	N	O	S	0	0	0
			898	566	155	174	3			
1	F	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	G	121	Total	C	N	O	S	0	0	0
			897	565	156	173	3			
1	H	119	Total	C	N	O	S	0	0	0
			886	558	153	172	3			
1	I	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	J	121	Total	C	N	O	S	0	0	0
			895	565	154	173	3			
1	K	121	Total	C	N	O	S	0	0	0
			888	562	154	169	3			
1	L	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	M	121	Total	C	N	O	S	0	0	0
			898	566	155	174	3			
1	N	119	Total	C	N	O	S	0	0	0
			883	557	152	171	3			
1	O	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	P	121	Total	C	N	O	S	0	0	0
			892	564	153	172	3			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	K	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	N	1	Total Ca 1 1	0	0
2	O	1	Total Ca 1 1	0	0
2	L	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	M	1	Total Ca 1 1	0	0

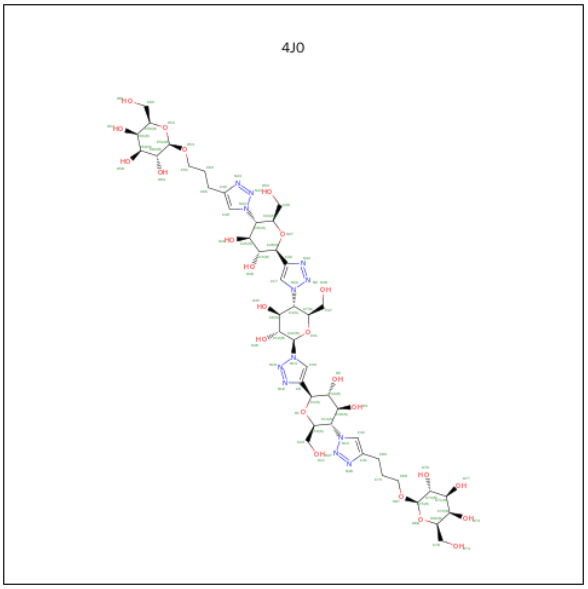
- Molecule 3 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	D	1	Total C O 12 6 6	0	0
3	E	1	Total C O 12 6 6	0	0
3	F	1	Total C O 12 6 6	0	0
3	G	1	Total C O 12 6 6	0	0
3	H	1	Total C O 12 6 6	0	0
3	J	1	Total C O 12 6 6	0	0
3	K	1	Total C O 12 6 6	0	0
3	L	1	Total C O 12 6 6	0	0
3	N	1	Total C O 12 6 6	0	0
3	O	1	Total C O 12 6 6	0	0

- Molecule 4 is (2R,3R,4S,5R,6R,2'R,3'R,4'S,5'R,6'R)-2,2'-([(2R,3R,4S,5S,6S)-3,4-dihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2,5-diyl]bis{1H-1,2,3-triazole-1,4-diyl[(2S,3R,4S,5S,6S)-3,4-dihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2,5-diyl]-1H-1,2,3-triazole-1,4-di

ylpropane-3,1-diyloxy})bis[6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol] (three-letter code: 4J0) (formula: $C_{44}H_{68}N_{12}O_{24}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	H	N	O	0	0
			148	44	68	12	24		
4	I	1	Total	C	H	N	O	0	0
			148	44	68	12	24		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		
5	B	113	Total	O	0	0
			113	113		
5	C	107	Total	O	0	0
			107	107		
5	D	109	Total	O	0	0
			109	109		
5	E	103	Total	O	0	0
			103	103		
5	F	105	Total	O	0	0
			105	105		
5	G	119	Total	O	0	0
			119	119		
5	H	125	Total	O	0	0
			125	125		

Continued on next page...

Continued from previous page...

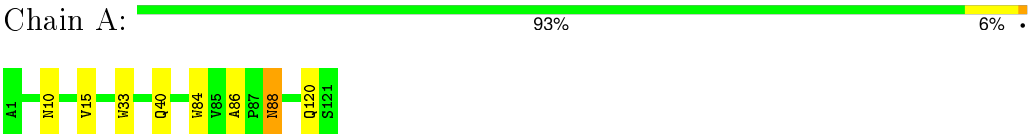
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	147	Total O 147 147	0	0
5	J	107	Total O 107 107	0	0
5	K	100	Total O 100 100	0	0
5	L	131	Total O 131 131	0	0
5	M	128	Total O 128 128	0	0
5	N	112	Total O 112 112	0	0
5	O	135	Total O 135 135	0	0
5	P	108	Total O 108 108	0	0

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.

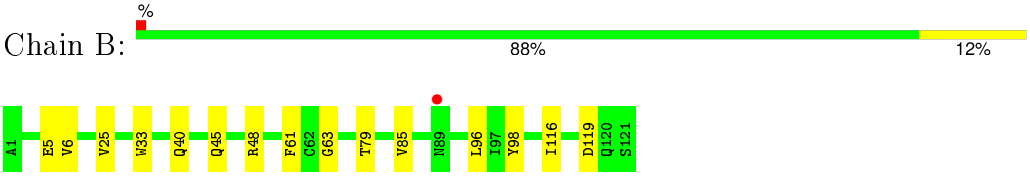
- Molecule 1: PA-I galactophilic lectin

Chain A:



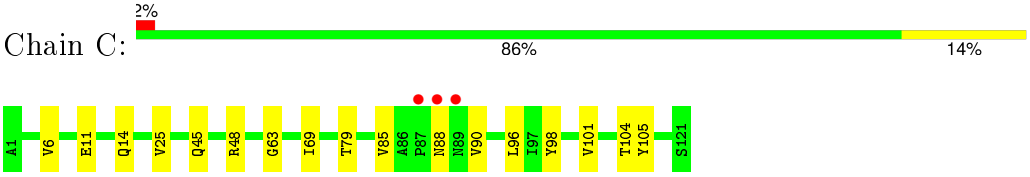
- Molecule 1: PA-I galactophilic lectin

Chain B:



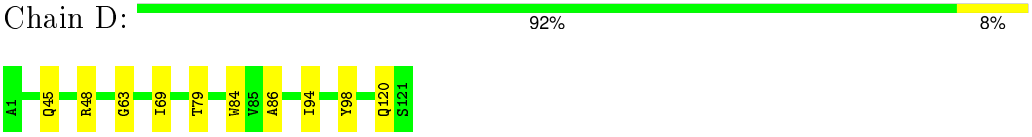
- Molecule 1: PA-I galactophilic lectin

Chain C:



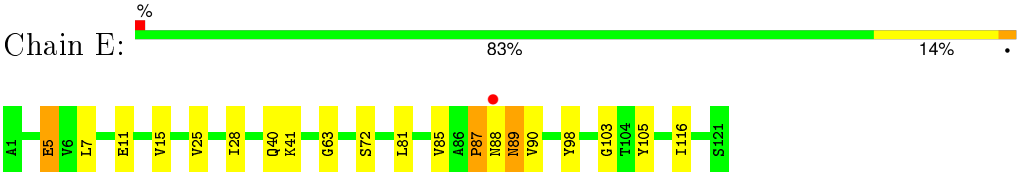
- Molecule 1: PA-I galactophilic lectin

Chain D:



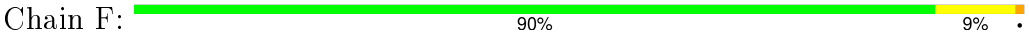
- Molecule 1: PA-I galactophilic lectin

Chain E:



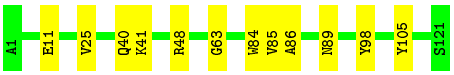
- Molecule 1: PA-I galactophilic lectin

Chain F:



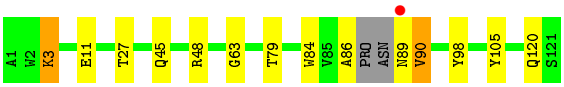
• Molecule 1: PA-I galactophilic lectin

Chain G:



• Molecule 1: PA-I galactophilic lectin

Chain H:

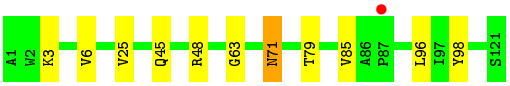


• Molecule 1: PA-I galactophilic lectin

Chain I:

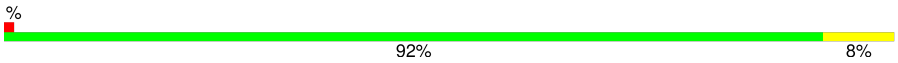
• Molecule 1: PA-I galactophilic lectin

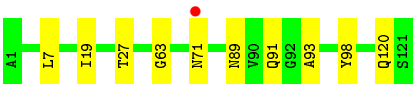
Chain J:



• Molecule 1: PA-I galactophilic lectin

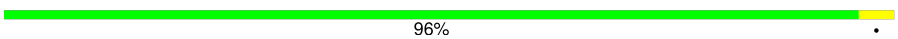
Chain K:





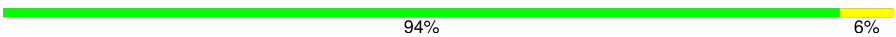
• Molecule 1: PA-I galactophilic lectin

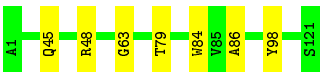
Chain L:



• Molecule 1: PA-I galactophilic lectin

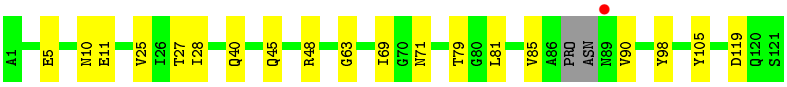
Chain M:





• Molecule 1: PA-I galactophilic lectin

Chain N:



• Molecule 1: PA-I galactophilic lectin

Chain O:

• Molecule 1: PA-I galactophilic lectin

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.57Å 89.31Å 100.01Å 90.04° 89.83° 79.61°	Depositor
Resolution (Å)	16.03 – 1.82 16.03 – 1.82	Depositor EDS
% Data completeness (in resolution range)	89.1 (16.03-1.82) 88.3 (16.03-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.221 0.184 , 0.221	Depositor DCC
R_{free} test set	6654 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	14.3	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 39.5	EDS
Estimated twinning fraction	0.459 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 134632 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16634	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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: 4J0, CA, GAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/919	0.46	0/1255
1	B	0.26	0/909	0.49	0/1243
1	C	0.26	0/916	0.47	0/1251
1	D	0.24	0/912	0.44	0/1246
1	E	0.27	0/921	0.46	0/1258
1	F	0.26	0/924	0.45	0/1262
1	G	0.25	0/920	0.45	0/1257
1	H	0.26	0/907	0.46	0/1236
1	I	0.26	0/924	0.45	0/1262
1	J	0.25	0/918	0.46	0/1254
1	K	0.24	0/911	0.45	0/1245
1	L	0.27	0/924	0.44	0/1262
1	M	0.26	0/921	0.45	0/1258
1	N	0.25	0/904	0.44	0/1232
1	O	0.26	0/924	0.44	0/1262
1	P	0.26	0/915	0.47	0/1252
All	All	0.26	0/14669	0.46	0/20035

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	896	0	855	8	0
1	B	886	0	838	11	0
1	C	893	0	851	17	0
1	D	889	0	847	5	0
1	E	898	0	857	14	0
1	F	901	0	861	9	0
1	G	897	0	857	9	0
1	H	886	0	847	12	0
1	I	901	0	861	13	0
1	J	895	0	853	11	0
1	K	888	0	847	10	0
1	L	901	0	861	4	0
1	M	898	0	857	4	0
1	N	883	0	843	17	0
1	O	901	0	861	10	0
1	P	892	0	846	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	12	0	10	1	0
3	B	12	0	10	0	0
3	D	12	0	10	0	0
3	E	12	0	10	0	0
3	F	12	0	10	0	0
3	G	12	0	10	0	0
3	H	12	0	10	0	0
3	J	12	0	10	0	0
3	K	12	0	10	0	0
3	L	12	0	10	0	0
3	N	12	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	12	0	10	0	0
4	C	80	68	66	0	0
4	I	80	68	64	0	0
5	A	124	0	0	6	0
5	B	113	0	0	1	0
5	C	107	0	0	2	0
5	D	109	0	0	1	1
5	E	103	0	0	2	0
5	F	105	0	0	2	0
5	G	119	0	0	3	2
5	H	125	0	0	4	1
5	I	147	0	0	6	1
5	J	107	0	0	2	2
5	K	100	0	0	1	0
5	L	131	0	0	1	0
5	M	128	0	0	0	1
5	N	112	0	0	3	0
5	O	135	0	0	0	1
5	P	108	0	0	3	1
All	All	16498	136	13892	156	5

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 5.

All (156) 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:I:22:PRO:HD3	1:I:91:GLN:HG3	1.53	0.90
1:N:11:GLU:HG2	1:N:105:TYR:HB2	1.63	0.79
1:G:89:ASN:ND2	5:G:1022:HOH:O	2.17	0.78
1:N:11:GLU:CG	1:N:105:TYR:HB2	2.14	0.77
1:F:22:PRO:HD3	1:F:91:GLN:HG3	1.69	0.74
1:N:11:GLU:HG2	1:N:105:TYR:CG	2.22	0.74
1:N:71:ASN:ND2	5:N:1001:HOH:O	2.21	0.72
1:I:20:TYR:O	1:I:91:GLN:HG2	1.90	0.72
1:N:25:VAL:HG22	1:N:85:VAL:HG22	1.72	0.71
1:C:6:VAL:HG22	1:C:14:GLN:HB3	1.73	0.71
1:J:48:ARG:NH2	5:J:1002:HOH:O	2.25	0.69
1:C:6:VAL:HG21	1:C:96:LEU:CB	2.23	0.67
1:C:6:VAL:HG21	1:C:96:LEU:HB2	1.76	0.66
1:N:11:GLU:HG2	1:N:105:TYR:CB	2.24	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ASN:OD1	5:F:1002:HOH:O	2.13	0.66
1:A:10:ASN:OD1	5:A:1001:HOH:O	2.13	0.66
1:N:11:GLU:HG2	1:N:105:TYR:CD1	2.33	0.64
1:E:11:GLU:HG3	1:E:105:TYR:CD1	2.32	0.64
1:H:89:ASN:O	1:H:90:VAL:HG22	1.98	0.64
1:I:120:GLN:NE2	5:I:1002:HOH:O	2.31	0.63
1:H:89:ASN:O	5:H:1039:HOH:O	2.15	0.63
1:C:11:GLU:HG2	1:C:105:TYR:CD1	2.33	0.63
1:K:71:ASN:HB3	5:K:1016:HOH:O	1.97	0.63
1:J:6:VAL:HG21	1:J:96:LEU:CB	2.28	0.63
1:H:120:GLN:OE1	1:N:119:ASP:HB3	1.98	0.62
1:H:11:GLU:HG2	1:H:105:TYR:CD1	2.34	0.62
1:J:71:ASN:HB2	1:P:89:ASN:CB	2.29	0.62
1:P:11:GLU:HG2	1:P:105:TYR:CG	2.33	0.62
1:E:87:PRO:O	1:E:89:ASN:N	2.33	0.62
1:H:48:ARG:HD3	5:H:1013:HOH:O	2.00	0.62
1:E:25:VAL:HG22	1:E:85:VAL:CG2	2.30	0.62
1:P:11:GLU:HG2	1:P:105:TYR:CD1	2.35	0.60
1:C:11:GLU:HG2	1:C:105:TYR:CG	2.36	0.60
1:I:71:ASN:ND2	5:I:1003:HOH:O	2.32	0.60
1:J:6:VAL:HG21	1:J:96:LEU:HB3	1.84	0.60
1:G:11:GLU:HG2	1:G:105:TYR:CD1	2.37	0.59
1:P:15:VAL:HG13	5:P:352:HOH:O	2.02	0.58
1:B:45:GLN:HG3	1:B:79:THR:HG23	1.83	0.58
1:F:120:GLN:NE2	5:F:1001:HOH:O	2.01	0.58
1:P:6:VAL:HG21	1:P:96:LEU:CB	2.33	0.58
1:C:25:VAL:HG22	1:C:85:VAL:HG22	1.85	0.58
1:P:15:VAL:O	5:P:301:HOH:O	2.17	0.57
1:B:6:VAL:HG21	1:B:96:LEU:HB3	1.85	0.57
1:H:11:GLU:HG2	1:H:105:TYR:CG	2.38	0.57
3:A:901:GAL:O1	5:A:1002:HOH:O	2.16	0.57
1:P:25:VAL:HG22	1:P:85:VAL:HG22	1.85	0.57
1:E:90:VAL:HG23	5:E:1064:HOH:O	2.05	0.57
1:C:69:ILE:HB	1:C:90:VAL:CG1	2.35	0.56
1:A:88:ASN:ND2	5:A:1027:HOH:O	2.39	0.56
1:B:6:VAL:HG21	1:B:96:LEU:CB	2.36	0.55
1:F:22:PRO:HD3	1:F:91:GLN:CG	2.34	0.55
1:H:84:TRP:CH2	1:H:86:ALA:HA	2.42	0.55
1:N:69:ILE:HB	1:N:90:VAL:CG1	2.36	0.54
1:D:84:TRP:CH2	1:D:86:ALA:HA	2.42	0.54
1:P:69:ILE:HB	1:P:90:VAL:CG1	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:GLU:OE2	1:E:103:GLY:N	2.30	0.54
1:I:53:GLN:NE2	5:I:1006:HOH:O	2.41	0.54
1:P:45:GLN:HG3	1:P:79:THR:HG23	1.91	0.53
1:J:6:VAL:HG21	1:J:96:LEU:HB2	1.92	0.53
1:K:120:GLN:HE22	1:O:119:ASP:HB3	1.74	0.52
1:J:6:VAL:CG2	1:J:96:LEU:HB2	2.39	0.52
1:C:101:VAL:O	1:C:104:THR:OG1	2.22	0.52
1:E:72:SER:HB3	1:E:90:VAL:HG21	1.92	0.52
1:N:40:GLN:NE2	5:N:1030:HOH:O	2.35	0.51
1:G:84:TRP:CH2	1:G:86:ALA:HA	2.45	0.51
1:K:89:ASN:O	1:K:91:GLN:NE2	2.43	0.51
1:G:11:GLU:HG2	1:G:105:TYR:CG	2.46	0.51
1:E:25:VAL:HG22	1:E:85:VAL:HG22	1.93	0.51
1:C:6:VAL:HG21	1:C:96:LEU:HB3	1.92	0.50
1:D:45:GLN:HG3	1:D:79:THR:HG23	1.93	0.50
1:G:48:ARG:HD3	5:G:1001:HOH:O	2.11	0.50
1:N:28:ILE:HD12	1:N:81:LEU:HD12	1.95	0.49
1:I:89:ASN:OD1	5:I:1001:HOH:O	2.20	0.49
1:E:72:SER:HB3	1:E:90:VAL:CG2	2.42	0.49
1:A:88:ASN:ND2	5:A:1028:HOH:O	2.46	0.49
1:P:6:VAL:HG21	1:P:96:LEU:HB2	1.93	0.49
1:P:6:VAL:HG21	1:P:96:LEU:HB3	1.93	0.49
1:K:120:GLN:HE22	1:O:120:GLN:H	1.59	0.48
1:G:48:ARG:NH1	5:G:1001:HOH:O	2.46	0.48
1:J:63:GLY:HA2	1:J:98:TYR:CZ	2.48	0.48
1:K:120:GLN:NE2	1:O:120:GLN:H	2.11	0.48
1:B:25:VAL:HG22	1:B:85:VAL:HG22	1.95	0.48
1:C:6:VAL:HG22	1:C:14:GLN:CB	2.44	0.48
1:P:25:VAL:HG22	1:P:85:VAL:CG2	2.44	0.48
1:P:69:ILE:CG2	1:P:90:VAL:HG12	2.44	0.48
1:J:3:LYS:HE2	1:L:3:LYS:CE	2.44	0.48
1:E:28:ILE:HD12	1:E:81:LEU:HD12	1.96	0.48
1:K:19:ILE:HD13	1:K:93:ALA:HA	1.95	0.47
1:B:48:ARG:HG3	1:B:61:PHE:CZ	2.48	0.47
1:F:33:TRP:CE3	1:I:48:ARG:HD2	2.49	0.47
1:C:63:GLY:HA2	1:C:98:TYR:CZ	2.50	0.47
1:P:63:GLY:HA2	1:P:98:TYR:CZ	2.49	0.47
1:A:15:VAL:HG23	5:A:1069:HOH:O	2.13	0.47
1:I:63:GLY:HA2	1:I:98:TYR:CZ	2.50	0.47
1:D:63:GLY:HA2	1:D:98:TYR:CZ	2.50	0.47
1:N:45:GLN:HG3	1:N:79:THR:HG23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:GLY:HA2	1:G:98:TYR:CZ	2.50	0.47
1:B:40:GLN:NE2	5:B:312:HOH:O	2.32	0.47
1:B:63:GLY:HA2	1:B:98:TYR:CZ	2.50	0.47
1:L:63:GLY:HA2	1:L:98:TYR:CZ	2.50	0.46
1:O:63:GLY:HA2	1:O:98:TYR:CZ	2.51	0.46
1:D:120:GLN:HB2	5:D:301:HOH:O	2.14	0.46
1:A:120:GLN:HG3	1:B:119:ASP:HA	1.98	0.46
1:F:41:LYS:HB2	1:I:48:ARG:NH1	2.31	0.45
1:N:63:GLY:HA2	1:N:98:TYR:CZ	2.51	0.45
1:A:40:GLN:NE2	5:A:1026:HOH:O	2.36	0.45
1:C:6:VAL:CG2	1:C:96:LEU:HB2	2.45	0.45
1:L:41:LYS:HE3	5:L:1038:HOH:O	2.15	0.45
1:F:20:TYR:O	1:F:91:GLN:HG2	2.16	0.45
1:E:63:GLY:HA2	1:E:98:TYR:CZ	2.52	0.45
1:I:71:ASN:HB2	5:I:1046:HOH:O	2.16	0.45
1:I:71:ASN:HA	5:I:1086:HOH:O	2.15	0.45
1:K:120:GLN:HE21	1:O:120:GLN:HB3	1.82	0.45
1:H:3:LYS:NZ	5:H:1002:HOH:O	2.30	0.44
1:K:120:GLN:HE21	1:O:120:GLN:CB	2.30	0.44
1:F:84:TRP:CH2	1:F:86:ALA:HA	2.52	0.44
1:P:88:ASN:O	1:P:90:VAL:HG23	2.18	0.44
1:E:28:ILE:HG12	1:E:116:ILE:HG12	2.00	0.44
1:K:63:GLY:HA2	1:K:98:TYR:CZ	2.53	0.44
1:N:69:ILE:HB	1:N:90:VAL:HG11	2.00	0.43
1:M:84:TRP:CH2	1:M:86:ALA:HA	2.53	0.43
1:H:63:GLY:HA2	1:H:98:TYR:CZ	2.53	0.43
1:J:48:ARG:NH2	5:J:1005:HOH:O	2.50	0.43
1:H:45:GLN:HG3	1:H:79:THR:HG23	2.01	0.43
1:O:40:GLN:HG2	1:O:41:LYS:N	2.34	0.43
1:H:27:THR:HG21	1:K:27:THR:HG21	1.99	0.43
1:A:84:TRP:CH2	1:A:86:ALA:HA	2.54	0.43
1:A:33:TRP:CE3	1:M:48:ARG:HD2	2.53	0.43
1:I:84:TRP:CH2	1:I:86:ALA:HA	2.54	0.43
1:B:5:GLU:OE2	1:O:2:TRP:HA	2.19	0.42
1:P:84:TRP:CH2	1:P:86:ALA:HA	2.54	0.42
1:I:45:GLN:HG3	1:I:79:THR:HG23	2.01	0.42
1:N:27:THR:HG21	1:O:27:THR:HG21	2.01	0.42
1:P:48:ARG:HD3	5:P:302:HOH:O	2.19	0.42
1:E:40:GLN:HG2	1:E:41:LYS:N	2.34	0.42
1:C:25:VAL:HG22	1:C:85:VAL:CG2	2.48	0.41
1:M:63:GLY:HA2	1:M:98:TYR:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:10:ASN:ND2	5:N:1006:HOH:O	2.53	0.41
1:C:14:GLN:OE1	5:C:309:HOH:O	2.22	0.41
1:G:25:VAL:HG22	1:G:85:VAL:CG2	2.51	0.41
1:E:15:VAL:HG23	5:E:1052:HOH:O	2.20	0.41
1:P:6:VAL:CG2	1:P:96:LEU:HB2	2.51	0.41
1:C:69:ILE:HB	1:C:90:VAL:HG12	2.02	0.41
1:J:45:GLN:HG3	1:J:79:THR:HG23	2.03	0.41
5:C:373:HOH:O	1:E:5:GLU:HG3	2.21	0.41
1:F:63:GLY:HA2	1:F:98:TYR:CZ	2.56	0.41
1:L:40:GLN:HG2	1:L:41:LYS:N	2.36	0.41
1:M:45:GLN:HG3	1:M:79:THR:HG23	2.03	0.41
1:D:69:ILE:HG12	1:D:94:ILE:HG12	2.02	0.41
1:N:48:ARG:HD2	1:O:33:TRP:CE3	2.56	0.41
1:J:25:VAL:HG22	1:J:85:VAL:HG22	2.02	0.41
1:B:6:VAL:CG2	1:B:96:LEU:HB2	2.51	0.40
1:H:89:ASN:HA	5:H:1087:HOH:O	2.22	0.40
1:C:45:GLN:CG	1:C:79:THR:HG23	2.51	0.40
1:G:40:GLN:HG2	1:G:41:LYS:N	2.37	0.40
1:B:33:TRP:CE3	1:C:48:ARG:HD2	2.57	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:1031:HOH:O	5:P:330:HOH:O[1_655]	2.14	0.06
5:G:1013:HOH:O	5:M:1004:HOH:O[1_655]	2.15	0.05
5:J:1003:HOH:O	5:O:1029:HOH:O[1_556]	2.16	0.04
5:H:1018:HOH:O	5:I:1004:HOH:O[1_644]	2.17	0.03
5:D:323:HOH:O	5:G:1010:HOH:O[1_455]	2.17	0.03

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	119/121 (98%)	117 (98%)	2 (2%)	0	100 100
1	B	119/121 (98%)	113 (95%)	5 (4%)	1 (1%)	24 8
1	C	119/121 (98%)	116 (98%)	2 (2%)	1 (1%)	24 8
1	D	119/121 (98%)	117 (98%)	2 (2%)	0	100 100
1	E	119/121 (98%)	112 (94%)	4 (3%)	3 (2%)	7 1
1	F	119/121 (98%)	116 (98%)	3 (2%)	0	100 100
1	G	119/121 (98%)	116 (98%)	3 (2%)	0	100 100
1	H	115/121 (95%)	111 (96%)	3 (3%)	1 (1%)	21 7
1	I	119/121 (98%)	114 (96%)	5 (4%)	0	100 100
1	J	119/121 (98%)	115 (97%)	4 (3%)	0	100 100
1	K	119/121 (98%)	117 (98%)	2 (2%)	0	100 100
1	L	119/121 (98%)	116 (98%)	3 (2%)	0	100 100
1	M	119/121 (98%)	115 (97%)	4 (3%)	0	100 100
1	N	115/121 (95%)	112 (97%)	3 (3%)	0	100 100
1	O	119/121 (98%)	116 (98%)	3 (2%)	0	100 100
1	P	119/121 (98%)	116 (98%)	3 (2%)	0	100 100
All	All	1896/1936 (98%)	1839 (97%)	51 (3%)	6 (0%)	46 29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	ILE
1	E	88	ASN
1	H	90	VAL
1	E	89	ASN
1	C	88	ASN
1	E	87	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	92/94 (98%)	91 (99%)	1 (1%)	80 74
1	B	89/94 (95%)	89 (100%)	0	100 100
1	C	91/94 (97%)	91 (100%)	0	100 100
1	D	90/94 (96%)	89 (99%)	1 (1%)	80 74
1	E	93/94 (99%)	91 (98%)	2 (2%)	60 45
1	F	94/94 (100%)	92 (98%)	2 (2%)	61 47
1	G	93/94 (99%)	93 (100%)	0	100 100
1	H	92/94 (98%)	91 (99%)	1 (1%)	80 74
1	I	94/94 (100%)	93 (99%)	1 (1%)	80 74
1	J	92/94 (98%)	91 (99%)	1 (1%)	80 74
1	K	90/94 (96%)	89 (99%)	1 (1%)	80 74
1	L	94/94 (100%)	94 (100%)	0	100 100
1	M	93/94 (99%)	93 (100%)	0	100 100
1	N	91/94 (97%)	90 (99%)	1 (1%)	80 74
1	O	94/94 (100%)	93 (99%)	1 (1%)	80 74
1	P	91/94 (97%)	91 (100%)	0	100 100
All	All	1473/1504 (98%)	1461 (99%)	12 (1%)	86 83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	D	48	ARG
1	E	5	GLU
1	E	7	LEU
1	F	88	ASN
1	F	120	GLN
1	H	3	LYS
1	I	91	GLN
1	J	71	ASN
1	K	7	LEU
1	N	5	GLU
1	O	91	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	10	ASN
1	G	89	ASN
1	I	53	GLN
1	K	120	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 16 are monoatomic - leaving 14 for Mogul analysis.

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	GAL	A	901	2	12,12,12	0.45	0	17,17,17	0.72	0
3	GAL	B	202	2	12,12,12	0.55	0	17,17,17	0.72	0
4	4J0	C	201	2	78,88,88	2.07	13 (16%)	91,129,129	1.76	10 (10%)
3	GAL	D	202	2	12,12,12	0.40	0	17,17,17	0.76	0
3	GAL	E	901	2	12,12,12	0.42	0	17,17,17	0.77	1 (5%)
3	GAL	F	901	2	12,12,12	0.51	0	17,17,17	0.81	0
3	GAL	G	901	2	12,12,12	0.46	0	17,17,17	0.81	0
3	GAL	H	901	2	12,12,12	0.44	0	17,17,17	0.74	0
4	4J0	I	202	2	78,88,88	2.00	13 (16%)	91,129,129	1.75	10 (10%)
3	GAL	J	901	2	12,12,12	0.51	0	17,17,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GAL	K	901	2	12,12,12	0.53	0	17,17,17	0.81	0
3	GAL	L	901	2	12,12,12	0.43	0	17,17,17	0.67	0
3	GAL	N	901	2	12,12,12	0.40	0	17,17,17	0.77	0
3	GAL	O	901	2	12,12,12	0.45	0	17,17,17	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	A	901	2	-	0/2/22/22	0/1/1/1
3	GAL	B	202	2	-	0/2/22/22	0/1/1/1
4	4J0	C	201	2	-	0/24/148/148	0/9/9/9
3	GAL	D	202	2	-	0/2/22/22	0/1/1/1
3	GAL	E	901	2	-	0/2/22/22	0/1/1/1
3	GAL	F	901	2	-	0/2/22/22	0/1/1/1
3	GAL	G	901	2	-	0/2/22/22	0/1/1/1
3	GAL	H	901	2	-	0/2/22/22	0/1/1/1
4	4J0	I	202	2	-	0/24/148/148	0/9/9/9
3	GAL	J	901	2	-	0/2/22/22	0/1/1/1
3	GAL	K	901	2	-	0/2/22/22	0/1/1/1
3	GAL	L	901	2	-	0/2/22/22	0/1/1/1
3	GAL	N	901	2	-	0/2/22/22	0/1/1/1
3	GAL	O	901	2	-	0/2/22/22	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	4J0	N16-N18	-9.52	1.20	1.34
4	I	202	4J0	N16-N18	-9.22	1.21	1.34
4	C	201	4J0	N43-N44	-7.42	1.23	1.34
4	I	202	4J0	N43-N44	-6.77	1.24	1.34
4	I	202	4J0	N32-N9	-6.49	1.25	1.34
4	C	201	4J0	N32-N9	-6.45	1.25	1.34
4	I	202	4J0	N18-N13	-5.28	1.25	1.34
4	C	201	4J0	N18-N13	-5.16	1.25	1.34
4	C	201	4J0	N44-N33	-4.60	1.26	1.34
4	I	202	4J0	N44-N33	-4.44	1.26	1.34
4	C	201	4J0	N37-N10	-4.41	1.26	1.34
4	C	201	4J0	N9-N20	-4.29	1.26	1.34
4	I	202	4J0	N37-N10	-4.14	1.27	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	202	4J0	N9-N20	-3.92	1.27	1.34
4	C	201	4J0	C17-N20	-3.00	1.32	1.35
4	I	202	4J0	C17-N20	-2.98	1.32	1.35
4	I	202	4J0	N38-N37	-2.96	1.30	1.34
4	C	201	4J0	N38-N37	-2.82	1.30	1.34
4	I	202	4J0	C42-N10	-2.55	1.33	1.35
4	C	201	4J0	C42-N10	-2.51	1.33	1.35
4	I	202	4J0	C39-N33	-2.37	1.33	1.35
4	C	201	4J0	C39-N33	-2.27	1.33	1.35
4	I	202	4J0	C29-N13	-2.13	1.33	1.35
4	C	201	4J0	C29-N13	-2.09	1.33	1.35
4	I	202	4J0	O67-C75	2.63	1.44	1.40
4	C	201	4J0	O67-C75	3.16	1.45	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	201	4J0	C42-N10-C14	-11.35	113.94	125.55
4	I	202	4J0	C42-N10-C14	-11.09	114.20	125.55
4	C	201	4J0	C17-N20-C4	-6.30	119.10	125.55
4	I	202	4J0	C17-N20-C4	-6.18	119.23	125.55
4	I	202	4J0	C80-C41-C42	-3.83	123.63	129.55
4	C	201	4J0	C80-C41-C42	-3.70	123.82	129.55
4	C	201	4J0	C8-C2-C34	-2.94	104.66	112.02
4	I	202	4J0	C8-C2-C34	-2.91	104.74	112.02
4	I	202	4J0	C65-C40-C39	-2.80	125.22	129.55
4	C	201	4J0	C51-O53-C52	-2.66	109.35	114.00
4	C	201	4J0	C65-C40-C39	-2.39	125.85	129.55
4	C	201	4J0	C8-C29-N13	-2.36	103.03	106.99
4	I	202	4J0	C51-O53-C52	-2.35	109.89	114.00
4	C	201	4J0	C52-O54-C56	-2.21	109.41	113.74
4	I	202	4J0	C8-C29-N13	-2.19	103.33	106.99
4	I	202	4J0	C52-O54-C56	-2.18	109.47	113.74
4	C	201	4J0	C42-C41-N38	-2.03	108.16	111.42
3	E	901	GAL	O5-C5-C4	2.00	113.49	109.67
4	I	202	4J0	C2-C8-N16	2.03	123.95	120.09
4	C	201	4J0	C28-C30-N32	3.38	126.52	120.09
4	I	202	4J0	C28-C30-N32	3.49	126.73	120.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	GAL	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	121/121 (100%)	-0.41	0 100 100	10, 15, 25, 43	0
1	B	121/121 (100%)	-0.39	1 (0%) 87 85	11, 18, 27, 39	0
1	C	121/121 (100%)	-0.41	3 (2%) 61 56	11, 15, 27, 48	0
1	D	121/121 (100%)	-0.36	0 100 100	12, 19, 29, 39	0
1	E	121/121 (100%)	-0.37	1 (0%) 87 85	11, 17, 28, 58	0
1	F	121/121 (100%)	-0.40	0 100 100	10, 16, 25, 41	0
1	G	121/121 (100%)	-0.41	0 100 100	11, 15, 27, 34	0
1	H	119/121 (98%)	-0.40	1 (0%) 87 85	11, 15, 28, 43	0
1	I	121/121 (100%)	-0.46	0 100 100	10, 16, 25, 31	0
1	J	121/121 (100%)	-0.34	1 (0%) 87 85	11, 17, 29, 42	0
1	K	121/121 (100%)	-0.32	1 (0%) 87 85	11, 19, 30, 37	0
1	L	121/121 (100%)	-0.41	0 100 100	10, 15, 25, 32	0
1	M	121/121 (100%)	-0.46	0 100 100	10, 16, 24, 30	0
1	N	119/121 (98%)	-0.41	1 (0%) 87 85	11, 17, 30, 50	0
1	O	121/121 (100%)	-0.46	0 100 100	9, 15, 25, 31	0
1	P	121/121 (100%)	-0.44	1 (0%) 87 85	10, 16, 27, 49	0
All	All	1932/1936 (99%)	-0.40	10 (0%) 91 90	9, 16, 28, 58	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	ASN	3.0
1	H	89	ASN	3.0
1	J	87	PRO	2.6
1	E	88	ASN	2.5
1	P	88	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	88	ASN	2.4
1	C	87	PRO	2.4
1	C	89	ASN	2.1
1	K	71	ASN	2.1
1	N	89	ASN	2.1

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
4	4J0	I	202	80/80	0.90	0.14	2.26	12,31,61,74	0
4	4J0	C	201	80/80	0.91	0.13	2.18	13,28,61,71	0
3	GAL	J	901	12/12	0.94	0.09	0.41	14,19,21,23	0
3	GAL	E	901	12/12	0.93	0.10	0.21	15,19,23,23	0
3	GAL	H	901	12/12	0.96	0.09	0.05	14,17,21,22	0
3	GAL	D	202	12/12	0.95	0.09	0.03	16,20,23,23	0
3	GAL	G	901	12/12	0.94	0.09	-0.28	15,19,22,24	0
3	GAL	O	901	12/12	0.95	0.07	-0.29	13,19,21,25	0
3	GAL	L	901	12/12	0.95	0.08	-0.69	14,18,20,22	0
3	GAL	A	901	12/12	0.94	0.07	-0.73	15,17,21,21	0
3	GAL	F	901	12/12	0.95	0.07	-0.75	15,19,21,24	0
3	GAL	N	901	12/12	0.96	0.07	-0.83	16,20,22,22	0
2	CA	C	202	1/1	1.00	0.07	-0.85	15,15,15,15	0
3	GAL	K	901	12/12	0.97	0.06	-0.88	14,20,21,22	0
2	CA	L	900	1/1	1.00	0.07	-1.28	15,15,15,15	0
3	GAL	B	202	12/12	0.98	0.07	-1.39	15,18,19,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	O	900	1/1	0.99	0.06	-1.41	22,22,22,22	0
2	CA	F	900	1/1	0.99	0.05	-1.57	14,14,14,14	0
2	CA	B	201	1/1	1.00	0.07	-1.74	18,18,18,18	0
2	CA	M	900	1/1	0.99	0.05	-1.81	19,19,19,19	0
2	CA	K	900	1/1	0.98	0.05	-2.15	17,17,17,17	0
2	CA	G	900	1/1	0.99	0.06	-2.31	16,16,16,16	0
2	CA	H	900	1/1	1.00	0.04	-2.38	15,15,15,15	0
2	CA	J	900	1/1	0.99	0.06	-2.73	19,19,19,19	0
2	CA	D	201	1/1	0.98	0.05	-2.89	16,16,16,16	0
2	CA	P	201	1/1	1.00	0.06	-2.90	13,13,13,13	0
2	CA	I	201	1/1	0.99	0.04	-2.94	17,17,17,17	0
2	CA	E	900	1/1	0.99	0.04	-3.19	15,15,15,15	0
2	CA	N	900	1/1	1.00	0.04	-3.45	18,18,18,18	0
2	CA	A	900	1/1	0.99	0.05	-4.88	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.