Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 04:57 am GMT

PDB ID	:	3ZYB
Title	:	CRYSTAL STRUCTURE OF PA-IL LECTIN COMPLEXED WITH GALAG0 AT 2.3 A RESOLUTION
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Deposited on	:	2011-08-19
Resolution	:	2.29 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

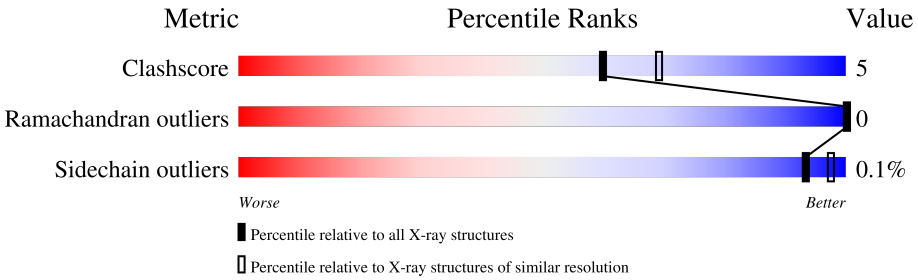
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.29 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	122	96%
1	B	122	86% 13%
1	C	122	88% 11%
1	D	122	91% 8%
1	E	122	90% 9%
1	F	122	84% 15%
1	G	122	89% 11%
1	H	122	88% 11%

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Mol	Chain	Length	Quality of chain
2	I	4	
2	J	4	
2	N	4	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8394 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 PA-I galactophilic lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	B	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	C	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	D	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	E	121	Total	C	N	O	S	0	0	0
			901	567	156	175	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
			901	567	156	175	3			
1	H	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			

- Molecule 2 is a protein called GALA-LYS-PRO-LEUNH2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	4	Total	C	N	O	0	0	1
			25	17	5	3			
2	J	4	Total	C	N	O	0	0	1
			25	17	5	3			
2	N	4	Total	C	N	O	0	0	1
			25	17	5	3			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

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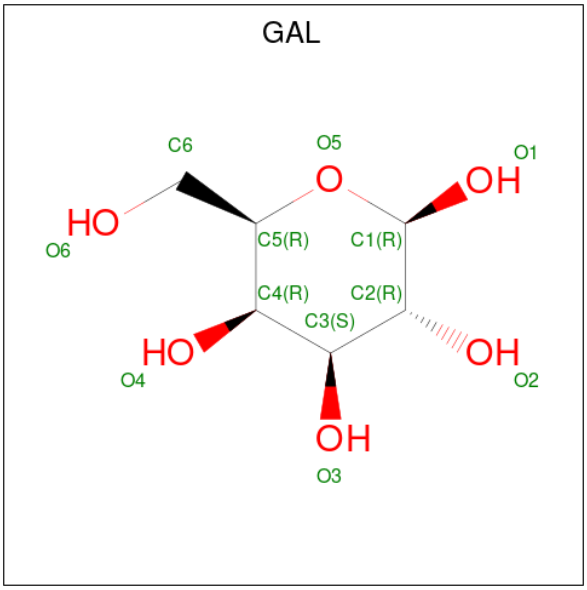
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0

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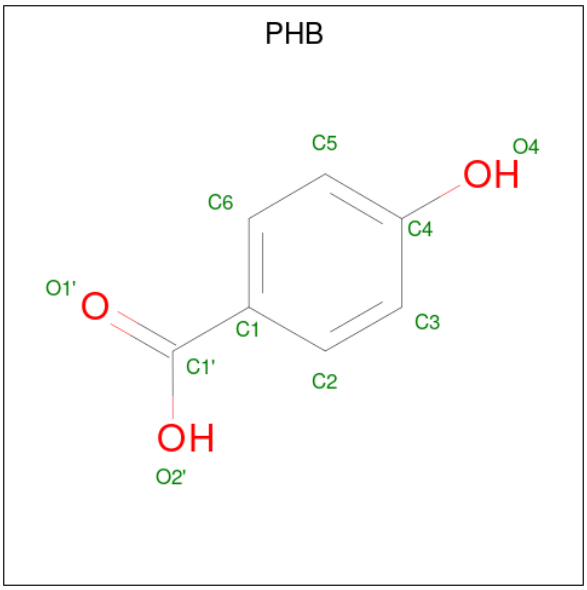
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 11 6 5	0	0
4	F	1	Total C O 11 6 5	0	0
4	G	1	Total C O 11 6 5	0	0
4	H	1	Total C O 11 6 5	0	0

- Molecule 5 is P-HYDROXYBENZOIC ACID (three-letter code: PHB) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 7 2	0	0
5	B	1	Total C O 9 7 2	0	0
5	C	1	Total C O 9 7 2	0	0
5	D	1	Total C O 9 7 2	0	0
5	E	1	Total C O 9 7 2	0	0
5	F	1	Total C O 9 7 2	0	0
5	G	1	Total C O 9 7 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 9 7 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	128	Total O 128 128	0	0
6	B	115	Total O 115 115	0	0
6	C	136	Total O 136 136	0	0
6	D	149	Total O 149 149	0	0
6	E	108	Total O 108 108	0	0
6	F	98	Total O 98 98	0	0
6	G	96	Total O 96 96	0	0
6	H	105	Total O 105 105	0	0
6	I	3	Total O 3 3	0	0
6	J	4	Total O 4 4	0	0
6	N	1	Total O 1 1	0	0

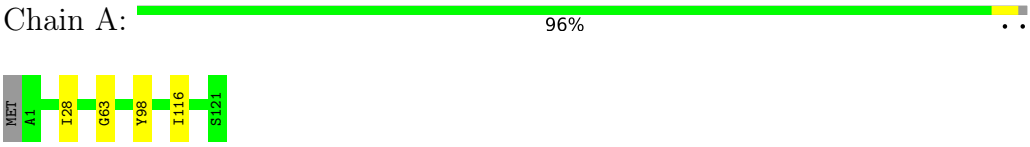
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS failed to run properly.

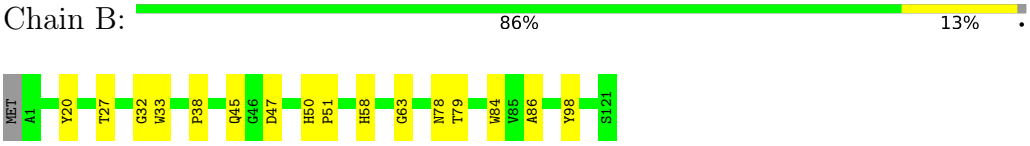
- Molecule 1: PA-I galactophilic lectin

Chain A:



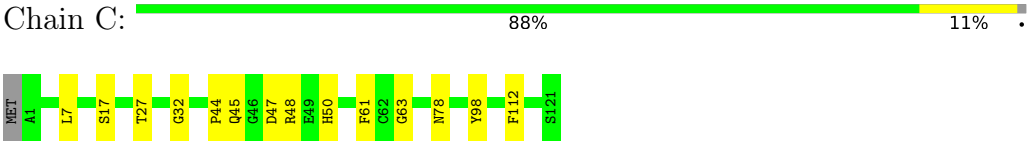
- Molecule 1: PA-I galactophilic lectin

Chain B:



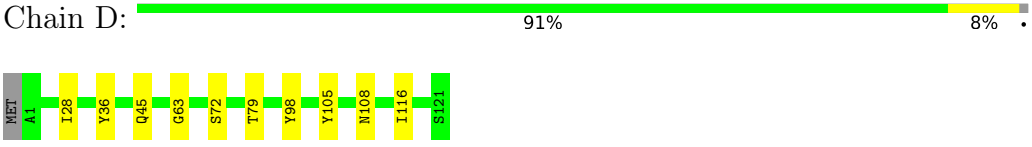
- Molecule 1: PA-I galactophilic lectin

Chain C:



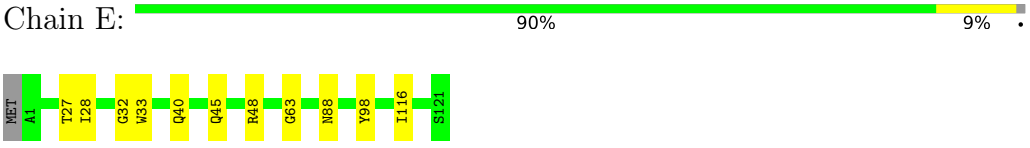
- Molecule 1: PA-I galactophilic lectin

Chain D:



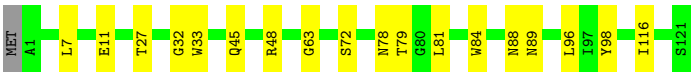
- Molecule 1: PA-I galactophilic lectin

Chain E:



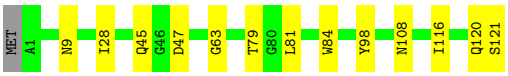
- Molecule 1: PA-I galactophilic lectin

Chain F:



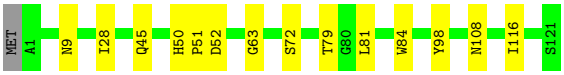
• Molecule 1: PA-I galactophilic lectin

Chain G:



• Molecule 1: PA-I galactophilic lectin

Chain H:



• Molecule 2: GALA-LYS-PRO-LEUNH2

Chain I:

• Molecule 2: GALA-LYS-PRO-LEUNH2

Chain J:

• Molecule 2: GALA-LYS-PRO-LEUNH2

Chain N:

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.33Å 128.56Å 146.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.29	Depositor
% Data completeness (in resolution range)	99.6 (49.26-2.29)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.07Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.214 , 0.240	Depositor
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.605	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8394	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0013e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GAL, NH2, PHB, CA

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	0.21	0/924	0.38	0/1262
1	B	0.21	0/924	0.39	0/1262
1	C	0.21	0/924	0.39	0/1262
1	D	0.21	0/924	0.38	0/1262
1	E	0.21	0/924	0.38	0/1262
1	F	0.21	0/924	0.39	0/1262
1	G	0.20	0/924	0.38	0/1262
1	H	0.20	0/924	0.38	0/1262
2	I	0.21	0/24	0.38	0/31
2	J	0.19	0/24	0.38	0/31
2	N	0.25	0/24	0.43	0/31
All	All	0.21	0/7464	0.39	0/10189

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	901	0	861	2	0
1	B	901	0	861	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	901	0	861	13	0
1	D	901	0	861	6	0
1	E	901	0	861	9	0
1	F	901	0	861	14	0
1	G	901	0	861	8	0
1	H	901	0	861	10	0
2	I	25	0	30	0	0
2	J	25	0	30	2	0
2	N	25	0	30	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	11	0	10	1	0
4	B	11	0	10	0	0
4	C	11	0	10	0	0
4	D	11	0	10	0	0
4	E	11	0	10	0	0
4	F	11	0	10	0	0
4	G	11	0	10	0	0
4	H	11	0	10	0	0
5	A	9	0	4	0	0
5	B	9	0	4	0	0
5	C	9	0	4	0	0
5	D	9	0	4	0	0
5	E	9	0	4	0	0
5	F	9	0	4	0	0
5	G	9	0	4	0	0
5	H	9	0	4	0	0
6	A	128	0	0	0	1
6	B	115	0	0	1	0
6	C	136	0	0	2	3
6	D	149	0	0	1	0
6	E	108	0	0	1	1
6	F	98	0	0	1	0
6	G	96	0	0	4	1
6	H	105	0	0	1	0
6	I	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	4	0	0	2	0
6	N	1	0	0	0	0
All	All	8394	0	7090	67	3

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 (67) 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:B:32:GLY:H	1:C:45:GLN:HE22	1.10	0.99
1:B:45:GLN:HE22	1:C:32:GLY:H	1.12	0.97
1:E:32:GLY:H	1:F:45:GLN:HE22	1.17	0.92
1:E:45:GLN:HE22	1:F:32:GLY:H	1.24	0.85
2:J:301:LYS:HG2	6:J:402:HOH:O	1.89	0.71
1:H:52:ASP:HB3	2:N:301:LYS:NZ	2.13	0.63
1:F:63:GLY:HA2	1:F:98:TYR:CZ	2.36	0.60
1:C:63:GLY:HA2	1:C:98:TYR:CZ	2.38	0.58
1:B:63:GLY:HA2	1:B:98:TYR:CZ	2.38	0.58
1:D:63:GLY:HA2	1:D:98:TYR:CZ	2.39	0.57
1:D:36:TYR:HA	1:D:108:ASN:OD1	2.04	0.57
1:C:7:LEU:HD22	6:C:422:HOH:O	2.04	0.56
1:E:63:GLY:HA2	1:E:98:TYR:CZ	2.40	0.56
1:G:28:ILE:HG12	1:G:116:ILE:HG12	1.88	0.56
1:C:45:GLN:HA	1:C:78:ASN:HD22	1.71	0.55
1:H:63:GLY:HA2	1:H:98:TYR:CZ	2.43	0.53
1:H:45:GLN:HG3	1:H:79:THR:HG23	1.90	0.53
1:A:63:GLY:HA2	1:A:98:TYR:CZ	2.43	0.53
1:H:72:SER:HB3	6:H:361:HOH:O	2.09	0.53
2:J:302:PRO:HA	6:J:401:HOH:O	2.09	0.53
1:E:28:ILE:HG12	1:E:116:ILE:HG12	1.92	0.52
1:B:58:HIS:O	1:F:7:LEU:HD21	2.10	0.51
1:E:48:ARG:HD2	1:F:33:TRP:CE3	2.46	0.51
1:B:47:ASP:HA	6:B:329:HOH:O	2.10	0.51
1:H:28:ILE:HG12	1:H:116:ILE:HG12	1.93	0.50
1:B:33:TRP:CE3	1:C:48:ARG:HD2	2.48	0.48
1:C:17:SER:HB3	1:E:88:ASN:HD21	1.79	0.47
1:B:45:GLN:HA	1:B:78:ASN:HD22	1.80	0.47
1:G:63:GLY:HA2	1:G:98:TYR:CZ	2.49	0.47
1:B:45:GLN:HG3	1:B:79:THR:HG23	1.97	0.47
1:H:52:ASP:HB3	2:N:301:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:GLN:HG3	1:G:79:THR:HG23	1.97	0.47
1:G:121:SER:HB2	6:G:361:HOH:O	2.15	0.46
1:B:32:GLY:H	1:C:45:GLN:NE2	1.94	0.46
1:D:105:TYR:HA	1:D:108:ASN:ND2	2.31	0.46
1:B:38:PRO:HB3	6:G:372:HOH:O	2.17	0.45
1:B:84:TRP:CH2	1:B:86:ALA:HA	2.51	0.45
1:E:27:THR:HG21	1:F:27:THR:HG21	1.98	0.45
1:F:81:LEU:HB3	1:F:84:TRP:HB2	2.00	0.44
1:B:45:GLN:NE2	1:C:32:GLY:H	1.96	0.44
1:D:28:ILE:HG12	1:D:116:ILE:HG12	2.00	0.44
1:E:40:GLN:HG3	6:E:347:HOH:O	2.17	0.44
1:F:88:ASN:O	1:F:89:ASN:HB2	2.18	0.43
1:G:47:ASP:HA	6:G:318:HOH:O	2.17	0.43
1:F:96:LEU:HD11	1:F:116:ILE:HD11	2.01	0.43
1:B:50:HIS:HA	1:B:51:PRO:HD3	1.88	0.43
1:F:45:GLN:HG3	1:F:79:THR:HG23	2.01	0.43
1:G:9:ASN:HA	1:G:108:ASN:HB2	2.01	0.43
1:H:52:ASP:HB3	2:N:301:LYS:HZ1	1.83	0.43
1:H:50:HIS:ND1	1:H:51:PRO:HD2	2.34	0.43
1:H:9:ASN:HA	1:H:108:ASN:HB2	2.01	0.42
1:H:81:LEU:HB3	1:H:84:TRP:HB2	2.00	0.42
1:F:45:GLN:HA	1:F:78:ASN:HD22	1.84	0.42
1:D:45:GLN:HG3	1:D:79:THR:HG23	2.01	0.42
1:G:120:GLN:NE2	6:G:305:HOH:O	2.52	0.42
1:B:27:THR:HG21	1:C:27:THR:HG21	2.01	0.42
1:A:28:ILE:HG12	1:A:116:ILE:HG12	2.02	0.42
1:C:47:ASP:OD2	1:C:50:HIS:HB2	2.19	0.42
1:D:72:SER:HA	6:D:304:HOH:O	2.20	0.42
1:G:81:LEU:HB3	1:G:84:TRP:HB2	2.02	0.41
2:N:301:LYS:HE2	2:N:301:LYS:HB2	1.88	0.41
1:C:44:PRO:HA	1:C:112:PHE:CE2	2.55	0.41
1:E:33:TRP:CE3	1:F:48:ARG:HD2	2.55	0.41
1:F:72:SER:HB2	6:F:361:HOH:O	2.21	0.41
4:A:202:GAL:H3	1:F:11:GLU:OE2	2.20	0.40
1:C:61:PHE:HA	6:C:302:HOH:O	2.21	0.40
1:B:20:TYR:CE1	1:B:86:ALA:HB3	2.56	0.40

All (3) 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)
6:C:330:HOH:O	6:E:377:HOH:O[1_455]	1.99	0.21
6:A:369:HOH:O	6:C:419:HOH:O[3_544]	2.03	0.17
6:C:374:HOH:O	6:G:305:HOH:O[2_454]	2.18	0.02

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	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
1	B	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
1	C	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
1	D	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
1	E	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
1	F	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
1	G	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
1	H	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
2	I	2/4 (50%)	2 (100%)	0	0	100	100
2	J	2/4 (50%)	2 (100%)	0	0	100	100
2	N	2/4 (50%)	2 (100%)	0	0	100	100
All	All	958/988 (97%)	929 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	94/95 (99%)	94 (100%)	0	100 100
1	B	94/95 (99%)	94 (100%)	0	100 100
1	C	94/95 (99%)	94 (100%)	0	100 100
1	D	94/95 (99%)	94 (100%)	0	100 100
1	E	94/95 (99%)	94 (100%)	0	100 100
1	F	94/95 (99%)	94 (100%)	0	100 100
1	G	94/95 (99%)	94 (100%)	0	100 100
1	H	94/95 (99%)	94 (100%)	0	100 100
2	I	3/3 (100%)	2 (67%)	1 (33%)	0 0
2	J	3/3 (100%)	3 (100%)	0	100 100
2	N	3/3 (100%)	3 (100%)	0	100 100
All	All	761/769 (99%)	760 (100%)	1 (0%)	93 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	115	ASN
1	B	45	GLN
1	B	53	GLN
1	B	78	ASN
1	C	45	GLN
1	C	78	ASN
1	E	45	GLN
1	E	78	ASN
1	E	88	ASN
1	F	45	GLN
1	F	78	ASN
1	G	78	ASN
1	G	120	GLN
1	H	40	GLN

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Mol	Chain	Res	Type
1	H	78	ASN
1	H	115	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.