Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 – 06:45 PM EDT

PDB ID	:	2Z48
Title	:	Crystal Structure of Hemolytic Lectin CEL-III Complexed with GalNac
Authors	:	Hatakeyama, T.; Unno, H.; Eto, S.; Hidemura, H.; Uchida, T.; Kouzuma, Y.
Deposited on	:	2007-06-13
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

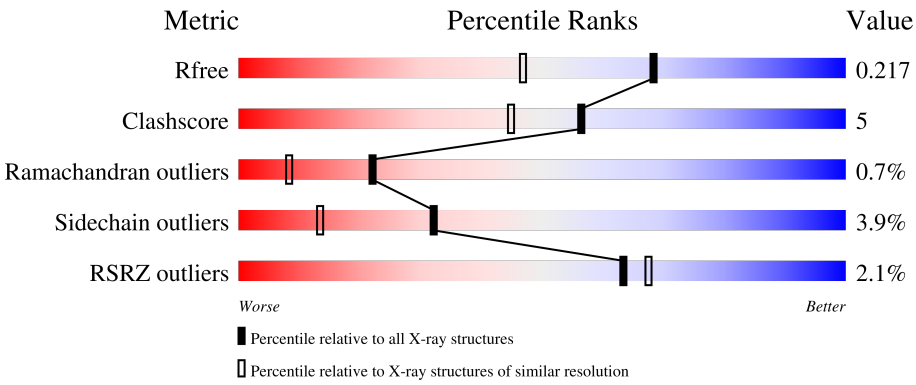
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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% 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	432	2% 90% 8% •
1	B	432	2% 88% 9% ••

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7642 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 Hemolytic lectin CEL-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	431	3305	2028	561	686	30	0	0	0
1	B	431	3305	2028	561	686	30	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	ASN	SEE REMARK 999	UNP Q868M7
A	16	PHE	TYR	SEE REMARK 999	UNP Q868M7
A	36	TYR	HIS	SEE REMARK 999	UNP Q868M7
A	48	ILE	MET	SEE REMARK 999	UNP Q868M7
A	92	GLN	LEU	SEE REMARK 999	UNP Q868M7
A	95	ARG	LYS	SEE REMARK 999	UNP Q868M7
A	97	THR	ALA	SEE REMARK 999	UNP Q868M7
A	122	ILE	VAL	SEE REMARK 999	UNP Q868M7
A	146	VAL	ILE	SEE REMARK 999	UNP Q868M7
A	173	ASP	GLU	SEE REMARK 999	UNP Q868M7
A	204	SER	GLN	SEE REMARK 999	UNP Q868M7
A	340	THR	SER	SEE REMARK 999	UNP Q868M7
A	404	VAL	ILE	SEE REMARK 999	UNP Q868M7
B	15	SER	ASN	SEE REMARK 999	UNP Q868M7
B	16	PHE	TYR	SEE REMARK 999	UNP Q868M7
B	36	TYR	HIS	SEE REMARK 999	UNP Q868M7
B	48	ILE	MET	SEE REMARK 999	UNP Q868M7
B	92	GLN	LEU	SEE REMARK 999	UNP Q868M7
B	95	ARG	LYS	SEE REMARK 999	UNP Q868M7
B	97	THR	ALA	SEE REMARK 999	UNP Q868M7
B	122	ILE	VAL	SEE REMARK 999	UNP Q868M7
B	146	VAL	ILE	SEE REMARK 999	UNP Q868M7
B	173	ASP	GLU	SEE REMARK 999	UNP Q868M7
B	204	SER	GLN	SEE REMARK 999	UNP Q868M7
B	340	THR	SER	SEE REMARK 999	UNP Q868M7

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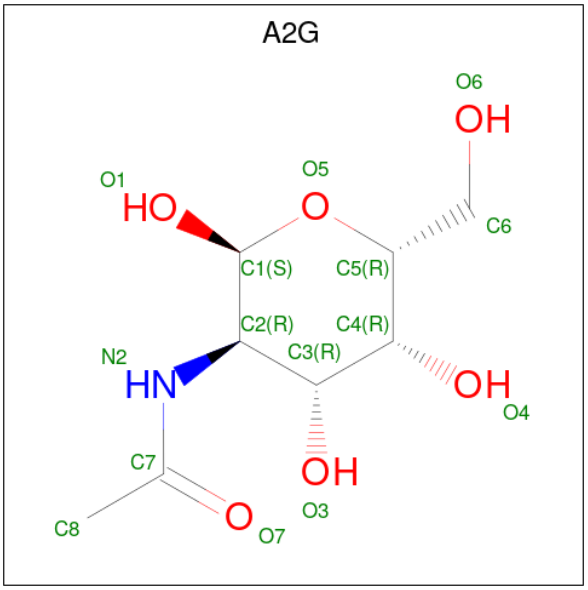
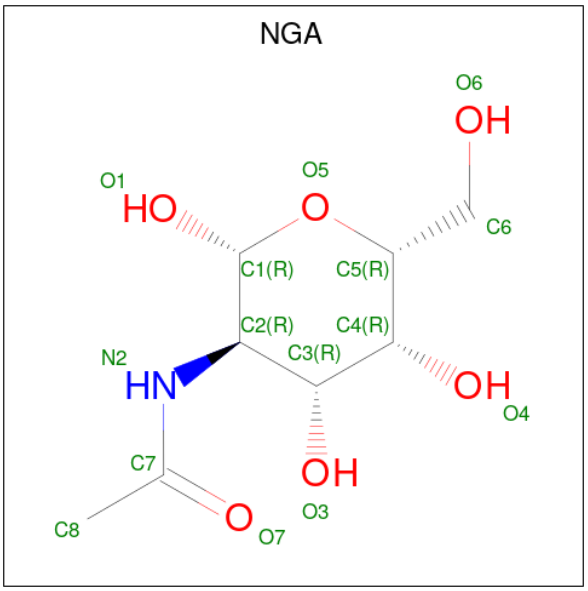
Chain	Residue	Modelled	Actual	Comment	Reference
B	404	VAL	ILE	SEE REMARK 999	UNP Q868M7

- Molecule 2 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-galactopyranose (three-letter code: NGA) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	8	1	6	0	0
			Total	C	N	O		
3	A	1	15	8	1	6	0	0
			Total	C	N	O		
3	A	1	15	8	1	6	0	0
			Total	C	N	O		
3	A	1	15	8	1	6	0	0
			Total	C	N	O		
3	B	1	15	8	1	6	0	0
			Total	C	N	O		
3	B	1	15	8	1	6	0	0
			Total	C	N	O		
3	B	1	15	8	1	6	0	0
			Total	C	N	O		
3	B	1	15	8	1	6	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	5	5	5	0	0
			Total	Ca		
4	B	5	5	5	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	2	2	2	0	0
			Total	Mg		
5	B	2	2	2	0	0

- Molecule 6 is water.

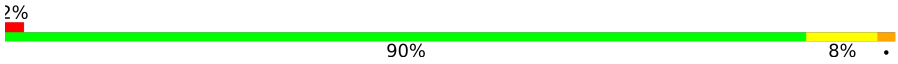
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	424	424	424	0	0
			Total	O		
6	B	414	414	414	0	0

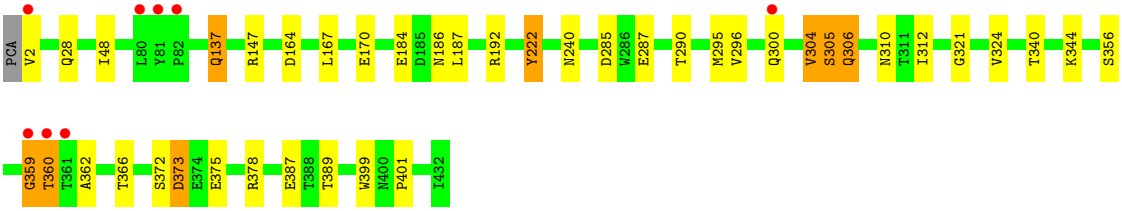
3 Residue-property plots (i)

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 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: Hemolytic lectin CEL-III

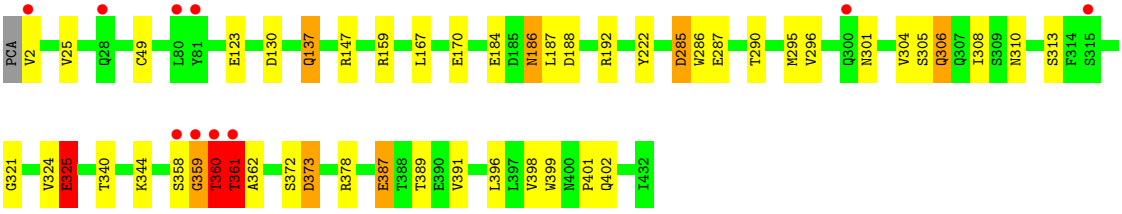
Chain A:





• Molecule 1: Hemolytic lectin CEL-III

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	52.64Å 65.17Å 66.67Å 85.30° 73.55° 89.94°	Depositor
Resolution (Å)	64.96 – 1.70 64.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (64.96-1.70) 96.4 (64.93-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.185 , 0.218 0.184 , 0.217	Depositor DCC
R_{free} test set	4489 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7642	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NGA, MG, A2G, 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	0.67	8/3365 (0.2%)	0.74	5/4563 (0.1%)
1	B	0.68	7/3365 (0.2%)	0.78	8/4563 (0.2%)
All	All	0.67	15/6730 (0.2%)	0.76	13/9126 (0.1%)

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	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	VAL	CB-CG1	-7.87	1.36	1.52
1	B	304	VAL	CB-CG2	-7.53	1.37	1.52
1	B	304	VAL	CB-CG1	-7.36	1.37	1.52
1	A	222	TYR	CE1-CZ	-6.57	1.30	1.38
1	B	222	TYR	CE1-CZ	-6.39	1.30	1.38
1	B	222	TYR	CE2-CZ	-6.30	1.30	1.38
1	A	222	TYR	CE2-CZ	-6.07	1.30	1.38
1	B	222	TYR	CG-CD2	-5.87	1.31	1.39
1	B	184	GLU	CD-OE2	-5.85	1.19	1.25
1	A	222	TYR	CG-CD2	-5.75	1.31	1.39
1	A	304	VAL	CB-CG2	-5.70	1.40	1.52
1	B	387	GLU	CD-OE1	-5.58	1.19	1.25
1	A	184	GLU	CD-OE2	-5.56	1.19	1.25
1	A	184	GLU	CD-OE1	-5.30	1.19	1.25
1	A	222	TYR	CG-CD1	-5.24	1.32	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	378	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	A	378	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	B	360	THR	C-N-CA	8.31	142.48	121.70
1	B	304	VAL	CG1-CB-CG2	-8.23	97.74	110.90
1	A	378	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	B	378	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	184	GLU	OE1-CD-OE2	-6.73	115.23	123.30
1	A	184	GLU	OE1-CD-OE2	-6.62	115.36	123.30
1	B	325	GLU	CA-CB-CG	6.59	127.90	113.40
1	B	359	GLY	N-CA-C	-5.60	99.11	113.10
1	A	304	VAL	CG1-CB-CG2	-5.38	102.28	110.90
1	B	387	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	A	387	GLU	OE1-CD-OE2	-5.06	117.22	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	358	SER	Peptide
1	B	361	THR	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	3305	0	3075	30	0
1	B	3305	0	3075	35	1
2	A	30	0	20	0	0
2	B	30	0	21	0	0
3	A	60	0	54	3	0
3	B	60	0	54	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	424	0	0	13	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	414	0	0	13	0
All	All	7642	0	6299	65	1

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 (65) 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:49:CYS:HB2	6:B:2141:HOH:O	1.56	1.04
1:A:310:ASN:HB3	1:A:360:THR:HG21	1.43	0.97
1:A:310:ASN:CB	1:A:360:THR:HG21	1.96	0.95
1:A:240:ASN:HB2	6:A:1622:HOH:O	1.68	0.92
1:A:192:ARG:CZ	6:A:1356:HOH:O	2.23	0.86
1:A:296:VAL:HG12	1:A:306:GLN:HG3	1.58	0.86
1:B:387:GLU:HG2	1:B:396:LEU:HD11	1.60	0.83
1:B:310:ASN:CB	1:B:360:THR:HG21	2.09	0.82
1:B:310:ASN:HB3	1:B:360:THR:HG21	1.62	0.80
1:A:312:ILE:HD11	6:A:1572:HOH:O	1.82	0.79
1:A:164:ASP:OD1	6:A:1576:HOH:O	2.06	0.72
1:B:295:MET:HG2	6:B:2155:HOH:O	1.87	0.72
1:B:362:ALA:HB1	6:B:2347:HOH:O	1.90	0.70
1:B:387:GLU:HG3	1:B:398:VAL:HG22	1.73	0.70
1:B:287:GLU:HG3	1:B:389:THR:HB	1.72	0.69
1:B:137:GLN:NE2	3:B:2002:NGA:O3	2.26	0.69
1:A:295:MET:HG2	6:A:1452:HOH:O	1.93	0.68
1:B:285:ASP:OD2	6:B:2305:HOH:O	2.11	0.67
1:B:290:THR:CG2	6:B:2416:HOH:O	2.44	0.66
1:A:359:GLY:HA2	1:A:360:THR:OG1	1.95	0.66
1:B:159:ARG:NH2	6:B:2365:HOH:O	2.29	0.66
1:A:310:ASN:HB2	1:A:360:THR:HG21	1.78	0.64
1:B:362:ALA:CB	6:B:2347:HOH:O	2.46	0.63
1:A:137:GLN:NE2	3:A:1002:NGA:O3	2.32	0.63
1:B:296:VAL:HG12	1:B:306:GLN:HG2	1.81	0.62
1:A:2:VAL:HB	6:A:1527:HOH:O	1.98	0.62
1:B:310:ASN:HB2	1:B:360:THR:HG21	1.82	0.61
1:B:290:THR:HG22	6:B:2416:HOH:O	2.01	0.61
1:A:340:THR:HG22	6:A:1562:HOH:O	2.01	0.60
1:B:301:ASN:HB2	6:B:2417:HOH:O	2.03	0.56
1:B:192:ARG:NH1	6:B:2295:HOH:O	2.38	0.56
1:A:192:ARG:NH1	6:A:1341:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASN:HB3	1:A:360:THR:CG2	2.27	0.55
1:A:287:GLU:HG3	1:A:389:THR:HB	1.88	0.55
1:A:305:SER:OG	1:A:366:THR:OG1	2.23	0.52
1:B:308:ILE:HG22	1:B:402:GLN:HG2	1.91	0.51
1:B:130:ASP:HB3	6:B:2286:HOH:O	2.12	0.50
1:A:192:ARG:NH2	6:A:1356:HOH:O	2.41	0.50
1:B:286:TRP:HE1	1:B:325:GLU:HG3	1.78	0.48
1:B:123:GLU:HG2	1:B:130:ASP:N	2.28	0.48
1:A:360:THR:HG22	6:A:1440:HOH:O	2.13	0.48
1:B:147:ARG:HD2	1:B:147:ARG:C	2.34	0.47
1:A:375:GLU:HG3	6:A:1603:HOH:O	2.14	0.47
1:B:372:SER:O	1:B:373:ASP:HB2	2.15	0.47
1:B:285:ASP:HB3	1:B:391:VAL:HB	1.96	0.47
1:A:399:TRP:CZ2	1:A:401:PRO:HB3	2.50	0.46
1:B:340:THR:HG22	6:B:2118:HOH:O	2.16	0.46
1:B:296:VAL:HG12	1:B:306:GLN:CG	2.46	0.46
1:B:310:ASN:HB3	1:B:360:THR:CG2	2.40	0.46
1:A:48:ILE:HG13	3:A:1006:NGA:H81	1.99	0.45
1:A:295:MET:CG	6:A:1452:HOH:O	2.58	0.45
1:A:356:SER:HB3	6:A:1572:HOH:O	2.16	0.45
1:A:296:VAL:CG1	1:A:306:GLN:HG3	2.37	0.45
1:B:399:TRP:CZ2	1:B:401:PRO:HB3	2.52	0.44
1:A:147:ARG:HD2	1:A:147:ARG:C	2.38	0.44
1:A:222:TYR:CD2	3:A:1004:NGA:H4	2.53	0.44
1:A:372:SER:O	1:A:373:ASP:HB2	2.18	0.43
1:B:321:GLY:O	1:B:324:VAL:HG12	2.18	0.43
1:A:192:ARG:HH21	1:A:324:VAL:HG23	1.83	0.42
1:B:359:GLY:CA	1:B:360:THR:OG1	2.66	0.42
1:B:372:SER:O	1:B:373:ASP:CB	2.68	0.42
1:B:186:ASN:HB3	1:B:188:ASP:OD1	2.20	0.41
1:B:387:GLU:CG	1:B:396:LEU:HD11	2.42	0.41
1:B:295:MET:CG	6:B:2155:HOH:O	2.53	0.41
1:A:321:GLY:O	1:A:324:VAL:HG12	2.21	0.40

All (1) 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)
1:B:306:GLN:NE2	6:A:1322:HOH:O[1_665]	2.12	0.08

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	429/432 (99%)	415 (97%)	11 (3%)	3 (1%)	22	8
1	B	429/432 (99%)	417 (97%)	9 (2%)	3 (1%)	22	8
All	All	858/864 (99%)	832 (97%)	20 (2%)	6 (1%)	22	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	GLY
1	B	361	THR
1	A	373	ASP
1	B	373	ASP
1	B	360	THR
1	A	362	ALA

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	370/370 (100%)	356 (96%)	14 (4%)	33	14
1	B	370/370 (100%)	355 (96%)	15 (4%)	30	12
All	All	740/740 (100%)	711 (96%)	29 (4%)	32	13

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	137	GLN
1	A	167	LEU
1	A	170	GLU
1	A	186	ASN
1	A	187	LEU
1	A	285	ASP
1	A	290	THR
1	A	300	GLN
1	A	304	VAL
1	A	305	SER
1	A	306	GLN
1	A	344	LYS
1	A	360	THR
1	B	2	VAL
1	B	25	VAL
1	B	137	GLN
1	B	167	LEU
1	B	170	GLU
1	B	186	ASN
1	B	187	LEU
1	B	285	ASP
1	B	305	SER
1	B	306	GLN
1	B	313	SER
1	B	325	GLU
1	B	344	LYS
1	B	360	THR
1	B	361	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	186	ASN
1	A	355	ASN
1	A	383	GLN
1	B	28	GLN
1	B	186	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 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	NGA	B	2004	-	15,15,15	0.57	0	21,21,21	1.29	1 (4%)
3	NGA	A	1004	-	15,15,15	0.62	0	21,21,21	1.08	2 (9%)
2	A2G	A	1001	-	15,15,15	0.54	0	21,21,21	0.96	1 (4%)
2	A2G	A	1005	-	15,15,15	0.82	0	21,21,21	1.02	0
3	NGA	B	2002	-	15,15,15	0.52	0	21,21,21	0.96	1 (4%)
3	NGA	A	1006	-	15,15,15	0.71	0	21,21,21	0.98	1 (4%)
2	A2G	B	2005	-	15,15,15	0.73	0	21,21,21	0.95	1 (4%)
3	NGA	B	2006	-	15,15,15	0.57	0	21,21,21	0.98	0
2	A2G	B	2001	-	15,15,15	0.61	0	21,21,21	0.74	0
3	NGA	A	1002	-	15,15,15	0.48	0	21,21,21	1.05	3 (14%)
3	NGA	B	2003	-	15,15,15	0.45	0	21,21,21	1.29	1 (4%)
3	NGA	A	1003	-	15,15,15	0.55	0	21,21,21	1.15	2 (9%)

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	NGA	B	2004	-	-	0/6/26/26	0/1/1/1
3	NGA	A	1004	-	-	0/6/26/26	0/1/1/1
2	A2G	A	1001	-	-	0/6/26/26	0/1/1/1
2	A2G	A	1005	-	-	0/6/26/26	0/1/1/1
3	NGA	B	2002	-	-	0/6/26/26	0/1/1/1
3	NGA	A	1006	-	-	1/6/26/26	0/1/1/1
2	A2G	B	2005	-	-	0/6/26/26	0/1/1/1
3	NGA	B	2006	-	-	1/6/26/26	0/1/1/1
2	A2G	B	2001	-	-	0/6/26/26	0/1/1/1
3	NGA	A	1002	-	-	0/6/26/26	0/1/1/1
3	NGA	B	2003	-	-	0/6/26/26	0/1/1/1
3	NGA	A	1003	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2004	NGA	C1-C2-N2	-4.15	105.92	110.73
3	B	2003	NGA	C3-C2-N2	-4.07	102.93	110.62
3	A	1003	NGA	C3-C2-N2	-3.38	104.23	110.62
2	A	1001	A2G	C1-C2-N2	-2.89	107.39	110.73
3	B	2002	NGA	C3-C2-N2	-2.80	105.34	110.62
2	B	2005	A2G	C1-C2-N2	-2.42	107.93	110.73
3	A	1004	NGA	C3-C2-N2	-2.29	106.28	110.62
3	A	1003	NGA	C1-O5-C5	-2.16	109.59	113.66
3	A	1006	NGA	O5-C1-C2	2.16	111.68	109.52
3	A	1002	NGA	C3-C2-N2	-2.12	106.62	110.62
3	A	1004	NGA	C1-C2-N2	-2.12	108.28	110.73
3	A	1002	NGA	C1-C2-N2	-2.10	108.29	110.73
3	A	1002	NGA	O5-C1-C2	-2.07	107.44	109.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1006	NGA	C3-C2-N2-C7
3	B	2006	NGA	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1004	NGA	1	0
3	B	2002	NGA	1	0
3	A	1006	NGA	1	0
3	A	1002	NGA	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	431/432 (99%)	-0.16	8 (1%)	66	70	11, 18, 30, 44	0
1	B	431/432 (99%)	-0.14	10 (2%)	60	65	12, 18, 30, 42	0
All	All	862/864 (99%)	-0.15	18 (2%)	63	67	11, 18, 30, 44	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	GLY	7.5
1	A	359	GLY	7.2
1	A	81	TYR	5.0
1	B	361	THR	4.1
1	B	315	SER	4.0
1	B	300	GLN	3.9
1	B	2	VAL	3.8
1	B	360	THR	3.7
1	A	82	PRO	3.3
1	B	358	SER	3.3
1	A	2	VAL	3.3
1	B	81	TYR	3.2
1	A	360	THR	2.8
1	B	80	LEU	2.7
1	A	361	THR	2.5
1	A	80	LEU	2.5
1	A	300	GLN	2.5
1	B	28	GLN	2.2

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
3	NGA	B	2006	15/15	0.88	0.14	15,20,25,28	0
2	A2G	B	2001	15/15	0.89	0.10	23,28,31,36	0
3	NGA	A	1004	15/15	0.91	0.11	14,20,23,26	0
3	NGA	A	1006	15/15	0.92	0.13	14,19,23,26	0
3	NGA	B	2004	15/15	0.92	0.11	15,23,27,28	0
2	A2G	A	1001	15/15	0.92	0.09	22,28,32,32	0
2	A2G	B	2005	15/15	0.93	0.08	18,21,22,27	0
3	NGA	B	2002	15/15	0.95	0.08	18,20,23,24	0
3	NGA	B	2003	15/15	0.95	0.07	18,21,27,30	0
2	A2G	A	1005	15/15	0.95	0.08	14,18,23,25	0
3	NGA	A	1002	15/15	0.95	0.08	19,21,24,24	0
5	MG	B	1211	1/1	0.95	0.12	28,28,28,28	0
3	NGA	A	1003	15/15	0.96	0.07	16,19,22,26	0
5	MG	A	1111	1/1	0.98	0.07	23,23,23,23	0
4	CA	A	1102	1/1	0.98	0.05	19,19,19,19	0
4	CA	B	1202	1/1	0.99	0.04	19,19,19,19	0
4	CA	A	1007	1/1	0.99	0.06	21,21,21,21	0
5	MG	A	1112	1/1	0.99	0.05	14,14,14,14	0
4	CA	B	1201	1/1	0.99	0.06	20,20,20,20	0
5	MG	B	1212	1/1	0.99	0.07	16,16,16,16	0
4	CA	B	1204	1/1	1.00	0.09	15,15,15,15	0
4	CA	B	1205	1/1	1.00	0.07	14,14,14,14	0
4	CA	A	1205	1/1	1.00	0.06	12,12,12,12	0
4	CA	A	1103	1/1	1.00	0.06	16,16,16,16	0
4	CA	A	1104	1/1	1.00	0.07	14,14,14,14	0
4	CA	B	1203	1/1	1.00	0.08	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.