



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 11:29 PM EDT

PDB ID : 1NMM  
Title : beta-1,4-galactosyltransferase mutant Cys342Thr complex with alpha-lactalbumin and GlcNAc  
Authors : Ramakrishnan, B.; Shah, P.S.; Qasba, P.K.  
Deposited on : 2003-01-10  
Resolution : 2.00 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.23.2  
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) : 2.23.2

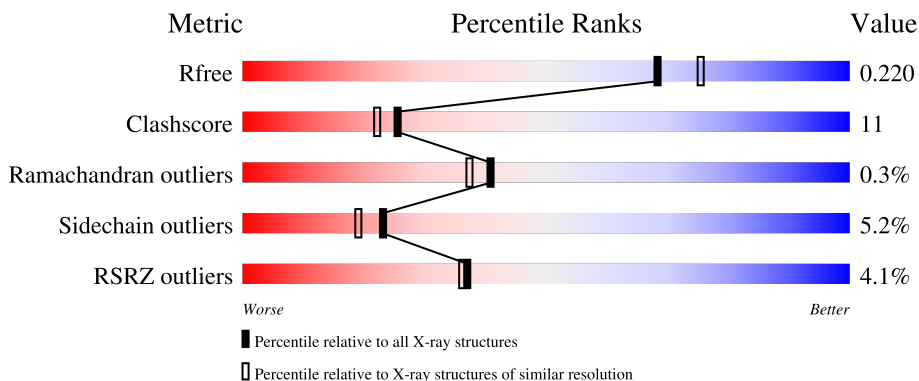
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	123	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0.5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0.5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">4%      82%      17%      •</p>
1	C	123	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0.5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0.5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">3%      79%      20%      •</p>
2	B	286	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0.5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">4%      76%      16%      • 5%</p>
2	D	286	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0.5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0.5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">4%      74%      19%      • 5%</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7232 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 ALPHA-LACTALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	123	980	620	156	195	9	0	0	0
1	C	123	980	620	156	195	9	0	0	0

- Molecule 2 is a protein called BETA-1,4-GALACTOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	272	2219	1425	382	399	13	0	0	0
2	D	272	2219	1425	382	399	13	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MET	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	UNP P08037
B	124	GLN	-	SEE REMARK 999	UNP P08037
B	125	MET	-	SEE REMARK 999	UNP P08037
B	126	GLY	-	SEE REMARK 999	UNP P08037
B	127	ARG	-	SEE REMARK 999	UNP P08037
B	128	GLY	-	SEE REMARK 999	UNP P08037
B	129	SER	-	SEE REMARK 999	UNP P08037
B	342	THR	CYS	engineered mutation	UNP P08037
D	117	ALA	-	SEE REMARK 999	UNP P08037
D	118	SER	-	SEE REMARK 999	UNP P08037

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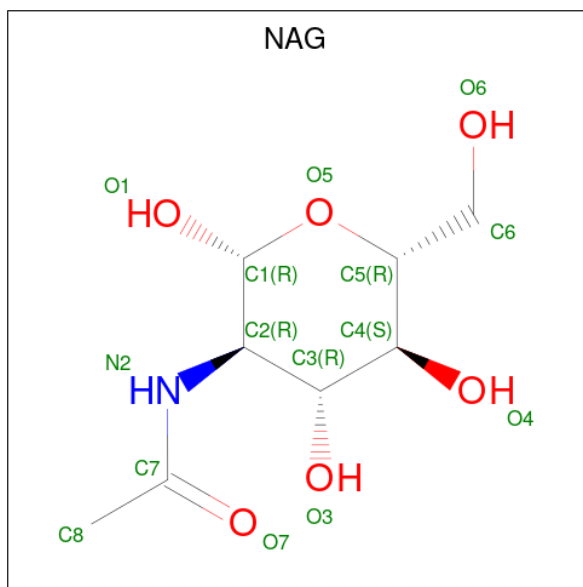
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Chain	Residue	Modelled	Actual	Comment	Reference
D	119	MET	-	SEE REMARK 999	UNP P08037
D	120	THR	-	SEE REMARK 999	UNP P08037
D	121	GLY	-	SEE REMARK 999	UNP P08037
D	122	GLY	-	SEE REMARK 999	UNP P08037
D	123	GLN	-	SEE REMARK 999	UNP P08037
D	124	GLN	-	SEE REMARK 999	UNP P08037
D	125	MET	-	SEE REMARK 999	UNP P08037
D	126	GLY	-	SEE REMARK 999	UNP P08037
D	127	ARG	-	SEE REMARK 999	UNP P08037
D	128	GLY	-	SEE REMARK 999	UNP P08037
D	129	SER	-	SEE REMARK 999	UNP P08037
D	342	THR	CYS	engineered mutation	UNP P08037

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

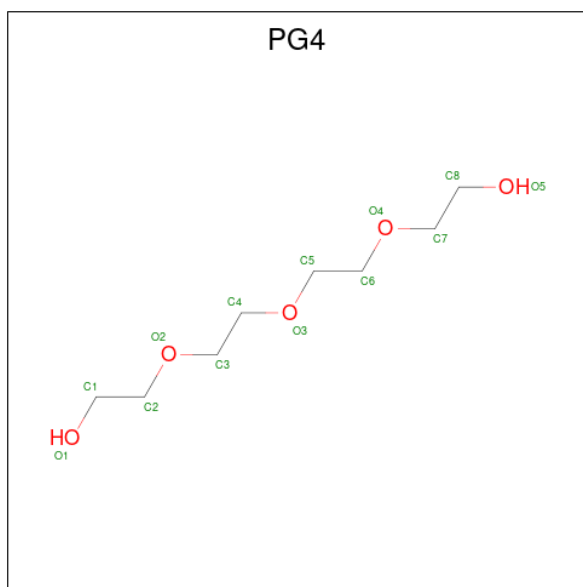
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

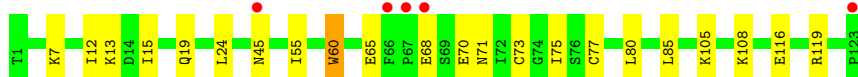
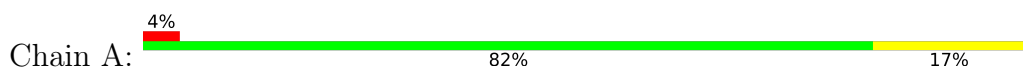
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		
6	B	265	Total	O	0	0
			265	265		
6	C	141	Total	O	0	0
			141	141		
6	D	253	Total	O	0	0
			253	253		

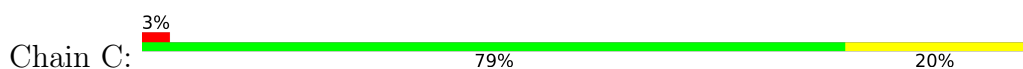
### 3 Residue-property plots [i](#)

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.

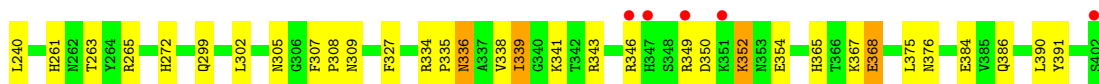
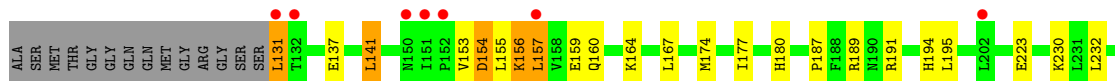
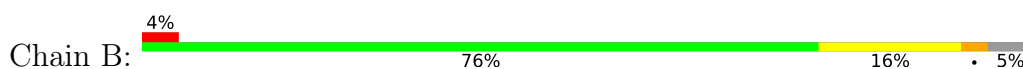
- Molecule 1: ALPHA-LACTALBUMIN



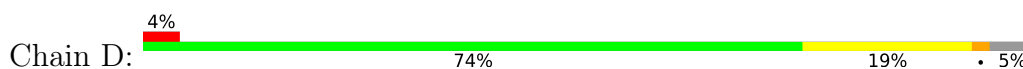
- Molecule 1: ALPHA-LACTALBUMIN



- Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE



- Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.02Å 95.63Å 100.21Å 90.00° 101.37° 90.00°	Depositor
Resolution (Å)	24.72 – 2.00 24.72 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.72-2.00) 98.5 (24.72-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.99Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.189 , 0.229 0.180 , 0.220	Depositor DCC
$R_{free}$ test set	7173 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtrriage
Anisotropy	0.209	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: PG4, CA, 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	0.49	0/1001	0.72	1/1350 (0.1%)
1	C	0.54	0/1001	0.77	0/1350
2	B	0.49	0/2279	0.71	0/3087
2	D	0.51	0/2279	0.73	0/3087
All	All	0.51	0/6560	0.73	1/8874 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	TRP	N-CA-C	5.05	124.63	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	980	0	936	14	0
1	C	980	0	936	21	0
2	B	2219	0	2187	49	0
2	D	2219	0	2187	52	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	15	0	0
4	D	15	0	15	1	0
5	D	20	0	26	5	0
6	A	123	0	0	5	0
6	B	265	0	0	6	0
6	C	141	0	0	1	0
6	D	253	0	0	7	0
All	All	7232	0	6302	135	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 11.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:LYS:HD3	1:C:123:PRO:HD2	1.26	1.14
1:A:71:ASN:HD21	1:A:75:ILE:H	1.15	0.94
1:C:122:LYS:HD3	1:C:123:PRO:CD	2.06	0.84
1:C:71:ASN:HD21	1:C:75:ILE:H	1.26	0.83
1:A:77:CYS:HB2	6:A:1002:HOH:O	1.80	0.81
2:D:305:ASN:HD21	2:D:376:ASN:H	1.32	0.76
2:B:299:GLN:HG3	6:B:982:HOH:O	1.84	0.76
2:B:336:ASN:HD22	2:B:338:VAL:H	1.33	0.75
1:C:10:HIS:HA	1:C:13:LYS:HE2	1.68	0.74
1:C:4:THR:HG23	1:C:7:LYS:HE2	1.71	0.73
2:D:268:SER:H	5:D:528:PG4:H31	1.53	0.72
2:B:305:ASN:HD21	2:B:376:ASN:H	1.36	0.72
1:A:45:ASN:HB2	6:B:1158:HOH:O	1.90	0.72
2:D:153:VAL:CG2	2:D:196:LYS:HB3	2.20	0.71
2:D:167:LEU:HD11	2:D:387:ARG:HB3	1.73	0.71
1:C:65:GLU:O	1:C:67:PRO:HD3	1.90	0.71
2:B:349:ARG:HG2	2:B:349:ARG:HH11	1.57	0.70
2:B:155:LEU:O	2:B:159:GLU:HG3	1.92	0.70
1:C:77:CYS:HB2	6:C:938:HOH:O	1.92	0.69
1:A:13:LYS:HE3	6:A:1063:HOH:O	1.91	0.69
1:C:122:LYS:CD	1:C:123:PRO:HD2	2.16	0.68
2:B:336:ASN:ND2	2:B:338:VAL:H	1.92	0.67
2:D:131:LEU:HD22	2:D:176:CYS:HA	1.76	0.67
1:C:4:THR:H	1:C:7:LYS:CE	2.08	0.67
2:D:132:THR:HG22	2:D:133:ALA:H	1.58	0.66
2:B:349:ARG:HD3	2:B:350:ASP:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:THR:H	1:C:7:LYS:HE3	1.62	0.64
2:D:336:ASN:HD22	2:D:338:VAL:H	1.47	0.63
2:B:327:PHE:CZ	2:B:367:LYS:HB2	2.36	0.61
2:D:265:ARG:HH22	5:D:528:PG4:H21	1.66	0.60
2:D:154:ASP:OD1	2:D:156:LYS:HB2	2.01	0.60
2:D:268:SER:N	5:D:528:PG4:H31	2.16	0.59
2:D:132:THR:HG22	2:D:133:ALA:N	2.16	0.59
2:D:131:LEU:HD21	2:D:175:ASP:O	2.04	0.58
2:D:167:LEU:C	2:D:167:LEU:HD13	2.24	0.58
2:B:349:ARG:HD3	2:B:350:ASP:H	1.68	0.58
1:C:10:HIS:O	1:C:13:LYS:HG2	2.04	0.57
2:D:347:HIS:CD2	2:D:348:SER:N	2.72	0.57
1:A:68:GLU:HG2	1:A:68:GLU:O	2.05	0.56
1:A:65:GLU:HB2	6:A:1264:HOH:O	2.05	0.56
2:B:336:ASN:HD22	2:B:336:ASN:C	2.08	0.56
2:B:154:ASP:OD1	2:B:156:LYS:HB2	2.06	0.55
2:B:272:HIS:HB3	2:B:334:ARG:HG2	1.89	0.55
2:D:358:GLN:OE1	2:D:362:ARG:NH1	2.39	0.55
1:A:105:LYS:HD3	6:A:1326:HOH:O	2.07	0.54
2:B:336:ASN:HD22	2:B:338:VAL:N	2.03	0.54
2:D:349:ARG:HD2	6:D:1032:HOH:O	2.06	0.54
2:D:349:ARG:HG3	6:D:1581:HOH:O	2.09	0.53
2:D:180:HIS:CE1	2:D:265:ARG:HD2	2.44	0.53
2:B:187:PRO:HD3	2:B:232:LEU:HD21	1.91	0.53
2:D:295:ALA:C	2:D:296:LEU:HD12	2.30	0.52
2:B:223:GLU:OE2	2:B:352:LYS:NZ	2.41	0.52
2:D:167:LEU:CD1	2:D:387:ARG:HB3	2.37	0.52
2:D:187:PRO:HD3	2:D:232:LEU:CD2	2.40	0.51
2:B:174:MET:HG2	6:B:1180:HOH:O	2.11	0.51
2:D:187:PRO:HD3	2:D:232:LEU:HD21	1.93	0.50
2:B:180:HIS:CE1	2:B:265:ARG:HD3	2.47	0.50
2:B:191:ARG:HG2	2:B:191:ARG:HH11	1.77	0.49
1:C:116:GLU:OE2	1:C:119:ARG:HD2	2.12	0.49
2:D:195:LEU:HD22	2:D:199:LEU:HG	1.94	0.49
2:D:131:LEU:CD2	2:D:176:CYS:HA	2.43	0.49
1:C:32:HIS:HD2	4:D:527:NAG:O1	1.96	0.49
2:B:335:PRO:HB2	2:B:339:ILE:HG12	1.94	0.48
2:D:347:HIS:HD2	2:D:348:SER:N	2.11	0.48
2:B:141:LEU:HD23	2:B:261:HIS:CD2	2.48	0.48
2:B:153:VAL:HG12	2:B:154:ASP:N	2.28	0.48
2:B:336:ASN:ND2	2:B:339:ILE:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ASN:ND2	2:B:339:ILE:HG23	2.28	0.48
2:D:347:HIS:CD2	2:D:348:SER:H	2.32	0.48
1:C:121:GLU:O	1:C:122:LYS:C	2.53	0.47
2:B:154:ASP:OD1	2:B:157:LEU:N	2.44	0.47
1:C:116:GLU:OE1	1:C:119:ARG:NH2	2.47	0.47
2:B:131:LEU:HA	6:B:1482:HOH:O	2.14	0.47
2:D:365:HIS:O	2:D:368:GLU:HG3	2.15	0.47
2:B:131:LEU:HG	2:B:177:ILE:HG13	1.96	0.46
1:C:12:ILE:O	1:C:15:ILE:HG22	2.15	0.46
1:C:55:ILE:HD13	1:C:91:CYS:SG	2.56	0.46
2:B:137:GLU:OE2	2:D:351:LYS:NZ	2.40	0.46
2:B:338:VAL:O	2:B:341:LYS:HG3	2.16	0.46
2:D:339:ILE:HD11	6:D:1009:HOH:O	2.14	0.46
2:B:156:LYS:HA	2:B:156:LYS:HE3	1.98	0.46
1:C:4:THR:H	1:C:7:LYS:HE2	1.77	0.46
2:B:349:ARG:HG2	2:B:349:ARG:NH1	2.27	0.45
1:A:55:ILE:HB	1:A:80:LEU:HD13	1.99	0.45
2:D:272:HIS:HB3	2:D:334:ARG:HG2	1.99	0.45
2:B:155:LEU:HD22	2:B:390:LEU:HD12	1.99	0.45
2:D:155:LEU:O	2:D:159:GLU:HB2	2.17	0.44
2:D:174:MET:HG2	6:D:1134:HOH:O	2.17	0.44
2:D:253:VAL:HG22	2:D:253:VAL:O	2.18	0.44
2:D:336:ASN:HD21	2:D:338:VAL:HB	1.83	0.44
2:B:349:ARG:NH1	6:B:1332:HOH:O	2.49	0.44
1:A:108:LYS:HG2	6:A:1367:HOH:O	2.16	0.44
1:C:58:ARG:HD2	1:C:59:PHE:CE2	2.53	0.44
2:D:268:SER:OG	5:D:528:PG4:H42	2.18	0.43
1:A:45:ASN:O	1:A:45:ASN:CG	2.57	0.43
2:B:230:LYS:HD2	2:B:309:ASN:HB3	2.00	0.43
2:B:336:ASN:HD21	2:B:339:ILE:H	1.66	0.43
2:D:167:LEU:HD11	2:D:387:ARG:CB	2.45	0.43
1:A:12:ILE:O	1:A:15:ILE:HG22	2.18	0.43
1:C:4:THR:OG1	1:C:7:LYS:HG3	2.19	0.43
2:B:263:THR:CG2	2:B:265:ARG:HG2	2.49	0.43
1:A:60:TRP:O	1:A:73:CYS:HB2	2.19	0.43
1:A:116:GLU:OE1	1:A:119:ARG:NH2	2.52	0.43
2:B:157:LEU:HD22	2:B:157:LEU:HA	1.89	0.43
2:D:187:PRO:HG2	6:D:869:HOH:O	2.19	0.43
2:D:268:SER:H	5:D:528:PG4:C3	2.29	0.42
2:D:157:LEU:HD22	2:D:157:LEU:HA	1.80	0.42
2:B:336:ASN:ND2	2:B:336:ASN:C	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:ALA:O	2:D:296:LEU:HD12	2.19	0.42
2:B:307:PHE:HB3	2:B:308:PRO:HD2	2.00	0.42
2:D:261:HIS:HE1	6:D:1008:HOH:O	2.03	0.42
2:B:346:ARG:HD3	2:B:346:ARG:HA	1.67	0.42
2:D:277:MET:HE3	2:D:344:MET:HE3	2.02	0.41
2:D:401:PRO:O	2:D:402:SER:CB	2.68	0.41
2:B:191:ARG:NH2	2:B:350:ASP:OD2	2.53	0.41
2:D:194:HIS:HD2	6:D:1200:HOH:O	2.03	0.41
2:B:305:ASN:ND2	6:B:1159:HOH:O	2.53	0.41
2:B:365:HIS:O	2:B:368:GLU:HG2	2.21	0.41
2:B:131:LEU:N	2:B:131:LEU:HD23	2.36	0.41
2:B:153:VAL:CG1	2:B:154:ASP:N	2.84	0.41
1:C:65:GLU:O	1:C:67:PRO:CD	2.63	0.41
2:B:160:GLN:HE21	2:B:160:GLN:HB2	1.73	0.41
2:B:384:GLU:OE2	2:B:386:GLN:HG2	2.20	0.41
2:D:131:LEU:CD2	2:D:175:ASP:O	2.68	0.41
2:D:394:ILE:HG22	2:D:396:VAL:HG13	2.03	0.41
2:B:336:ASN:ND2	2:B:338:VAL:N	2.66	0.40
2:B:390:LEU:O	2:B:391:TYR:HB3	2.20	0.40
2:D:247:CYS:SG	2:D:266:CYS:N	2.94	0.40
2:D:131:LEU:HD22	2:D:176:CYS:CA	2.48	0.40
1:A:24:LEU:CD2	1:A:119:ARG:HA	2.51	0.40
2:B:263:THR:HG22	2:B:265:ARG:HG2	2.03	0.40
2:D:327:PHE:CZ	2:D:367:LYS:HB2	2.56	0.40
2:D:189:ARG:NH2	2:D:352:LYS:HB3	2.37	0.40
2:D:277:MET:CE	2:D:344:MET:HE3	2.52	0.40
2:D:336:ASN:ND2	2:D:339:ILE:H	2.20	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	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
1	C	121/123 (98%)	117 (97%)	2 (2%)	2 (2%)	9	4
2	B	270/286 (94%)	260 (96%)	10 (4%)	0	100	100
2	D	270/286 (94%)	264 (98%)	6 (2%)	0	100	100
All	All	782/818 (96%)	756 (97%)	24 (3%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	65	GLU
1	C	66	PHE

### 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	109/109 (100%)	105 (96%)	4 (4%)	34	32
1	C	109/109 (100%)	105 (96%)	4 (4%)	34	32
2	B	245/254 (96%)	226 (92%)	19 (8%)	12	8
2	D	245/254 (96%)	235 (96%)	10 (4%)	30	28
All	All	708/726 (98%)	671 (95%)	37 (5%)	23	19

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	19	GLN
1	A	70	GLU
1	A	85	LEU
2	B	131	LEU
2	B	141	LEU
2	B	154	ASP
2	B	156	LYS
2	B	157	LEU

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Mol	Chain	Res	Type
2	B	164	LYS
2	B	167	LEU
2	B	189	ARG
2	B	194	HIS
2	B	195	LEU
2	B	240	LEU
2	B	302	LEU
2	B	336	ASN
2	B	339	ILE
2	B	343	ARG
2	B	352	LYS
2	B	354	GLU
2	B	368	GLU
2	B	375	LEU
1	C	84	GLU
1	C	85	LEU
1	C	88	ASP
1	C	110	MET
2	D	131	LEU
2	D	141	LEU
2	D	157	LEU
2	D	195	LEU
2	D	240	LEU
2	D	263	THR
2	D	287	VAL
2	D	302	LEU
2	D	336	ASN
2	D	368	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	71	ASN
2	B	160	GLN
2	B	207	GLN
2	B	305	ASN
2	B	310	ASN
2	B	336	ASN
1	C	32	HIS
1	C	71	ASN
2	D	160	GLN

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Mol	Chain	Res	Type
2	D	161	GLN
2	D	162	ASN
2	D	194	HIS
2	D	261	HIS
2	D	305	ASN
2	D	310	ASN
2	D	336	ASN
2	D	347	HIS
2	D	365	HIS

### 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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
5	PG4	D	528	-	9,9,12	0.52	0	8,8,11	0.33	0
4	NAG	B	403	-	15,15,15	0.81	0	21,21,21	0.82	0
5	PG4	D	529	-	9,9,12	0.44	0	8,8,11	0.31	0
4	NAG	D	527	-	15,15,15	1.06	2 (13%)	21,21,21	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	D	528	-	-	5/7/7/10	-
4	NAG	B	403	-	-	0/6/26/26	0/1/1/1
5	PG4	D	529	-	-	5/7/7/10	-
4	NAG	D	527	-	-	0/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	527	NAG	C2-N2	2.93	1.50	1.45
4	D	527	NAG	C4-C5	2.08	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	529	PG4	O2-C3-C4-O3
5	D	529	PG4	O3-C5-C6-O4
5	D	528	PG4	O2-C3-C4-O3
5	D	529	PG4	O1-C1-C2-O2
5	D	528	PG4	O1-C1-C2-O2
5	D	528	PG4	O3-C5-C6-O4
5	D	529	PG4	C1-C2-O2-C3
5	D	529	PG4	C3-C4-O3-C5
5	D	528	PG4	C3-C4-O3-C5
5	D	528	PG4	C6-C5-O3-C4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	528	PG4	5	0
4	D	527	NAG	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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	123/123 (100%)	-0.20	5 (4%) 37 36	17, 27, 50, 62	0
1	C	123/123 (100%)	-0.16	4 (3%) 46 45	15, 24, 45, 74	0
2	B	272/286 (95%)	-0.20	12 (4%) 34 33	16, 26, 50, 67	0
2	D	272/286 (95%)	-0.21	11 (4%) 38 37	18, 26, 47, 60	0
All	All	790/818 (96%)	-0.20	32 (4%) 37 36	15, 26, 50, 74	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	PRO	9.8
2	D	402	SER	6.3
1	C	122	LYS	5.8
2	B	402	SER	5.0
2	D	152	PRO	4.5
2	B	152	PRO	4.2
2	B	349	ARG	4.0
1	A	123	PRO	3.4
2	B	131	LEU	3.3
1	A	66	PHE	3.1
2	D	132	THR	2.9
2	B	132	THR	2.9
2	D	131	LEU	2.9
2	B	157	LEU	2.8
1	C	45	ASN	2.8
2	B	150	ASN	2.7
2	B	151	ILE	2.7
2	B	346	ARG	2.7
2	D	160	GLN	2.6
2	B	347	HIS	2.5
1	A	68	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	67	PRO	2.4
2	D	136	GLU	2.3
2	D	151	ILE	2.3
2	B	351	LYS	2.3
2	D	157	LEU	2.3
2	D	349	ARG	2.3
2	D	150	ASN	2.3
1	A	45	ASN	2.2
2	D	156	LYS	2.1
2	B	202	LEU	2.1
1	C	14	ASP	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	PG4	D	528	10/13	0.73	0.28	56,59,62,64	0
5	PG4	D	529	10/13	0.82	0.14	58,59,61,61	0
4	NAG	D	527	15/15	0.98	0.10	16,18,19,21	0
3	CA	A	124	1/1	0.98	0.06	25,25,25,25	0
4	NAG	B	403	15/15	0.98	0.10	18,19,22,22	0
3	CA	C	526	1/1	1.00	0.06	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.