Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:07 AM GMT

PDB ID	:	3O61
Title	:	Structure of the E100A E.coli GDP-mannose hydrolase (yffh) in complex with GDP-mannose and Mg++
Authors	:	Amzel, L.M.; Gabelli, S.B.; Boto, A.N.
Deposited on	:	2010-07-28
Resolution	:	2.45 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

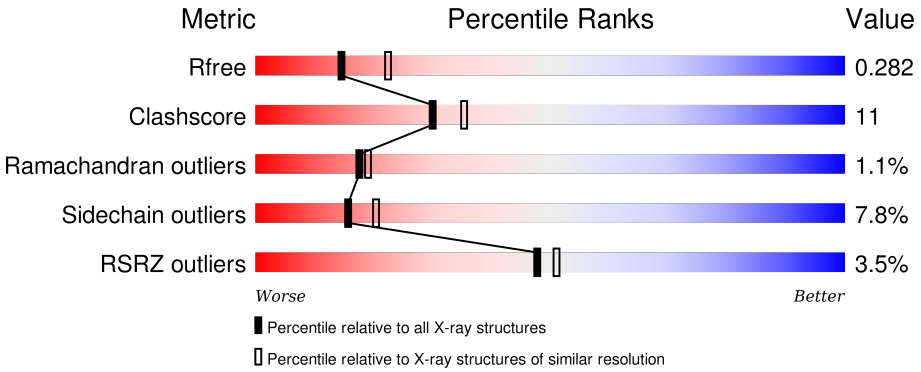
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	191	5% 74% 21%
1	B	191	4% 68% 28%
1	C	191	2% 70% 19% 6% 5%
1	D	191	3% 74% 23%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6246 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.

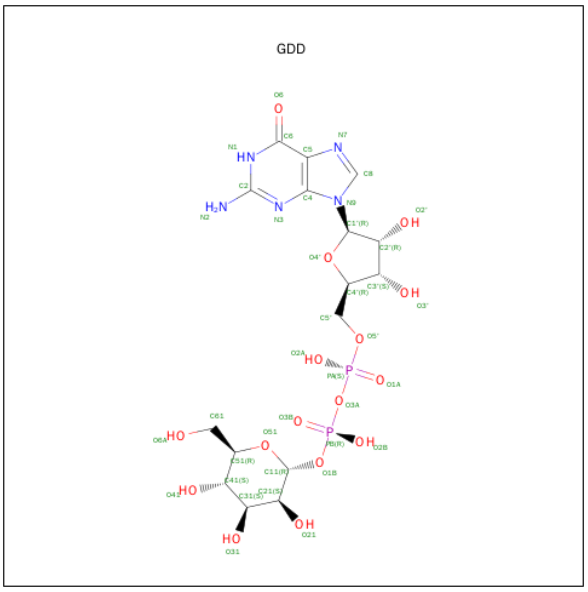
- Molecule 1 is a protein called GDP-mannose pyrophosphatase nudK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	0
			1496	945	254	291	6			
1	B	187	Total	C	N	O	S	0	0	0
			1492	943	254	290	5			
1	C	182	Total	C	N	O	S	0	0	0
			1467	929	248	285	5			
1	D	190	Total	C	N	O	S	0	0	0
			1516	956	257	298	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ALA	GLU	ENGINEERED MUTATION	UNP P37128
B	100	ALA	GLU	ENGINEERED MUTATION	UNP P37128
C	100	ALA	GLU	ENGINEERED MUTATION	UNP P37128
D	100	ALA	GLU	ENGINEERED MUTATION	UNP P37128

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (three-letter code: GDD) (formula: $C_{16}H_{25}N_5O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	B	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	C	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	D	1	Total	C	N	O	P	0	0
			39	16	5	16	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Na 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is water.

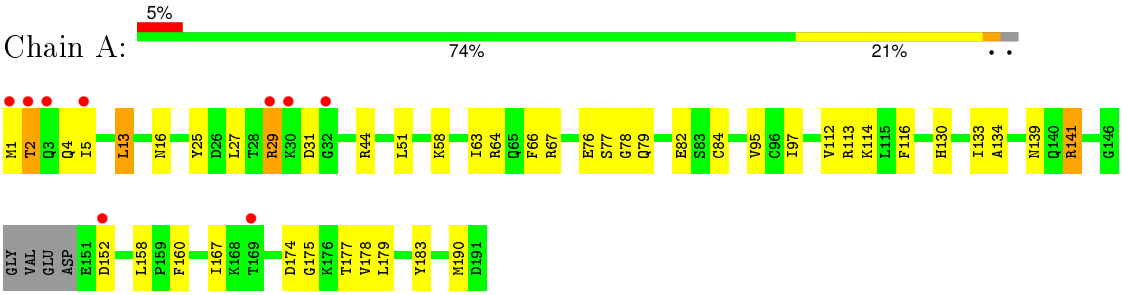
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	26	Total O 26 26	0	0
6	B	27	Total O 27 27	0	0
6	C	25	Total O 25 25	0	0
6	D	34	Total O 34 34	0	0

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.

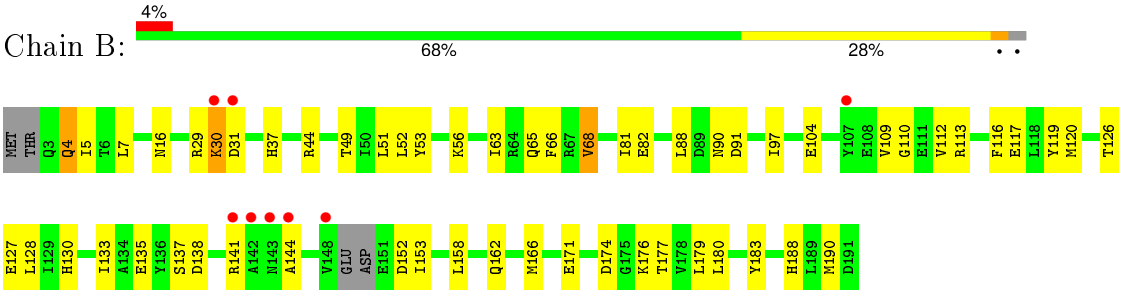
- Molecule 1: GDP-mannose pyrophosphatase nudK

Chain A:



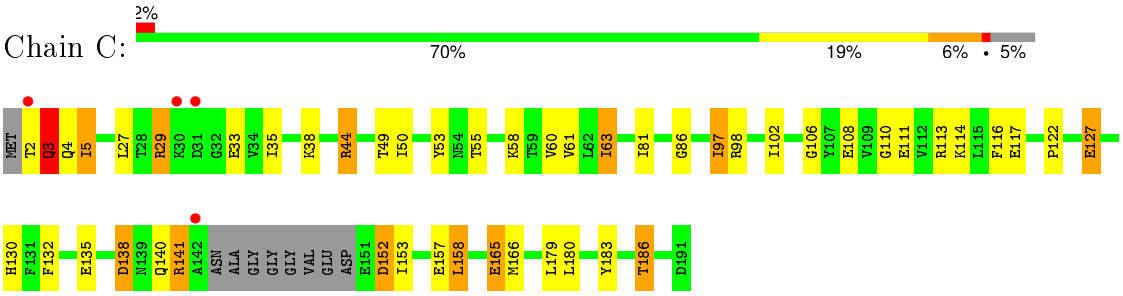
- Molecule 1: GDP-mannose pyrophosphatase nudK

Chain B:



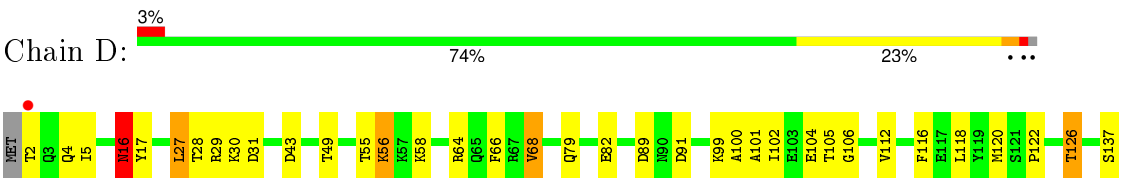
- Molecule 1: GDP-mannose pyrophosphatase nudK

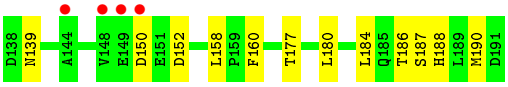
Chain C:



- Molecule 1: GDP-mannose pyrophosphatase nudK

Chain D:




D138
N139
A144
V148
E149
D150
E151
D152
L158
P159
F160
T177
L180
L184
Q185
T186
S187
H188
L189
M190
D191

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.28Å 55.82Å 158.12Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	32.40 – 2.45 32.40 – 2.45	Depositor EDS
% Data completeness (in resolution range)	92.7 (32.40-2.45) 92.7 (32.40-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.290 0.219 , 0.282	Depositor DCC
R_{free} test set	1644 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	1.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 29.2	EDS
Estimated twinning fraction	0.025 for -k,-h,-l 0.025 for k,h,-l 0.094 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 32616 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6246	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: NA, MG, GDD, CL

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	1/1517 (0.1%)	0.75	0/2046
1	B	0.65	0/1513	0.75	0/2041
1	C	0.72	0/1488	0.77	0/2008
1	D	0.71	0/1538	0.77	2/2077 (0.1%)
All	All	0.69	1/6056 (0.0%)	0.76	2/8172 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	SER	CB-OG	5.70	1.49	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	68	VAL	CB-CA-C	-6.82	98.44	111.40
1	D	91	ASP	CB-CG-OD1	5.28	123.06	118.30

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	1496	0	1496	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1492	0	1490	42	0
1	C	1467	0	1468	36	0
1	D	1516	0	1508	33	0
2	A	39	0	23	1	0
2	B	39	0	23	2	0
2	C	39	0	23	3	0
2	D	39	0	23	2	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
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	C	1	0	0	0	0
6	A	26	0	0	4	0
6	B	27	0	0	1	0
6	C	25	0	0	1	0
6	D	34	0	0	1	0
All	All	6246	0	6054	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:A:29:ARG:HG2	1:A:29:ARG:HH11	0.89	1.04
1:A:29:ARG:HG2	1:A:29:ARG:NH1	1.68	1.00
1:A:29:ARG:NH2	1:B:152:ASP:HB2	1.76	0.99
1:C:158:LEU:HD12	1:C:158:LEU:H	1.35	0.88
1:A:29:ARG:CG	1:A:29:ARG:HH11	1.82	0.87
1:C:152:ASP:HB2	1:D:2:THR:HG23	1.58	0.83
1:A:95:VAL:HG11	1:D:55:THR:HG21	1.63	0.81
1:A:1:MET:HG3	1:B:65:GLN:HB2	1.63	0.78
1:A:141:ARG:HH11	1:A:141:ARG:HG3	1.49	0.78
1:A:29:ARG:NH2	1:B:152:ASP:CB	2.47	0.78
1:B:66:PHE:HE2	1:B:68:VAL:HG13	1.48	0.77
1:A:141:ARG:NH1	1:A:141:ARG:HG3	2.01	0.75
1:B:141:ARG:HH21	1:B:144:ALA:HA	1.49	0.75
1:D:5:ILE:HD13	1:D:27:LEU:HD12	1.70	0.72
1:C:158:LEU:CD1	1:C:158:LEU:H	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:PHE:CE2	1:B:68:VAL:HG13	2.26	0.70
1:D:5:ILE:HD13	1:D:27:LEU:CD1	2.21	0.70
1:A:95:VAL:CG1	1:D:55:THR:HG21	2.23	0.67
1:C:122:PRO:HD2	2:D:3846:GDD:H611	1.76	0.67
1:A:175:GLY:HA3	1:B:120:MET:HE2	1.77	0.66
1:A:1:MET:HB3	1:B:66:PHE:H	1.61	0.65
1:A:179:LEU:HG	1:B:179:LEU:HG	1.79	0.65
1:C:108:GLU:O	1:C:140:GLN:HG2	1.98	0.64
1:C:127:GLU:OE2	2:C:3846:GDD:O41	2.08	0.64
1:A:141:ARG:HH11	1:A:141:ARG:CG	2.12	0.62
1:C:29:ARG:HD3	1:D:152:ASP:OD2	2.00	0.61
1:A:29:ARG:HH21	1:B:152:ASP:HB2	1.59	0.61
1:C:158:LEU:HD12	1:C:158:LEU:N	2.11	0.61
1:A:63:ILE:HD13	1:A:84:CYS:HA	1.83	0.60
1:B:113:ARG:NH2	1:B:183:TYR:OH	2.34	0.60
1:A:29:ARG:HH22	1:B:152:ASP:CB	2.12	0.60
1:A:5:ILE:HD13	1:A:27:LEU:HD23	1.84	0.59
1:A:113:ARG:NH2	1:A:183:TYR:OH	2.35	0.59
1:C:2:THR:N	1:C:27:LEU:HG	2.16	0.59
1:C:63:ILE:HG23	1:C:153:ILE:HG23	1.85	0.58
1:C:138:ASP:OD1	1:C:138:ASP:N	2.25	0.57
1:C:3:GLN:C	1:C:3:GLN:HE21	2.07	0.57
1:B:162:GLN:O	1:B:166:MET:HG3	2.04	0.57
1:A:58:LYS:HD3	1:A:58:LYS:N	2.20	0.56
1:D:100:ALA:O	1:D:104:GLU:HG3	2.06	0.56
1:C:63:ILE:HG23	1:C:153:ILE:CG2	2.37	0.55
1:C:122:PRO:HD2	2:D:3846:GDD:C61	2.36	0.55
6:A:200:HOH:O	1:D:56:LYS:HE2	2.07	0.55
1:B:127:GLU:OE1	2:B:3846:GDD:O41	2.25	0.54
1:D:58:LYS:HE3	1:D:190:MET:O	2.07	0.54
1:A:5:ILE:HD13	1:A:27:LEU:CD2	2.38	0.54
1:D:160:PHE:CE1	1:D:184:LEU:HD23	2.43	0.53
1:C:98:ARG:NH1	1:C:110:GLY:O	2.34	0.53
1:D:99:LYS:NZ	6:D:207:HOH:O	2.41	0.53
2:C:3846:GDD:C61	1:D:122:PRO:HD2	2.39	0.53
1:A:167:ILE:HD13	1:A:178:VAL:HG13	1.91	0.52
1:B:53:TYR:O	1:B:135:GLU:HA	2.10	0.52
1:A:174:ASP:O	1:A:178:VAL:HG23	2.10	0.52
1:A:112:VAL:HG12	1:A:134:ALA:HB2	1.91	0.52
1:A:114:LYS:NZ	1:A:130:HIS:HD2	2.08	0.52
1:A:29:ARG:NH2	6:A:214:HOH:O	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ASP:OD2	1:B:176:LYS:HG2	2.10	0.52
1:B:4:GLN:HE21	1:B:5:ILE:H	1.58	0.52
1:B:166:MET:HB3	1:B:171:GLU:HB3	1.92	0.51
1:C:50:ILE:HA	1:C:132:PHE:O	2.10	0.51
1:B:120:MET:HE2	1:B:120:MET:HA	1.92	0.51
1:D:56:LYS:HD2	1:D:56:LYS:H	1.76	0.51
1:A:64:ARG:HD3	1:A:79:GLN:HB3	1.93	0.50
1:D:49:THR:HG23	1:D:180:LEU:HD11	1.93	0.50
1:C:106:GLY:O	1:C:141:ARG:HA	2.11	0.50
1:A:51:LEU:HB3	1:A:133:ILE:HG22	1.92	0.50
1:B:29:ARG:C	1:B:31:ASP:H	2.15	0.50
1:B:82:GLU:OE1	1:B:176:LYS:NZ	2.33	0.50
1:A:82:GLU:HA	1:A:177:THR:OG1	2.12	0.49
1:C:53:TYR:O	1:C:135:GLU:HA	2.11	0.49
1:C:44:ARG:HG3	6:C:192:HOH:O	2.13	0.49
1:C:49:THR:HG23	1:C:180:LEU:HD11	1.93	0.49
1:A:29:ARG:HH22	1:B:152:ASP:HB3	1.78	0.49
1:C:5:ILE:HG12	1:D:66:PHE:CE1	2.47	0.49
1:A:25:TYR:CD1	1:B:68:VAL:HG11	2.48	0.48
1:D:64:ARG:HE	1:D:79:GLN:HB3	1.78	0.48
1:A:1:MET:CB	1:B:66:PHE:H	2.25	0.48
1:C:183:TYR:O	1:C:186:THR:HG22	2.14	0.48
1:D:139:ASN:OD1	1:D:139:ASN:N	2.40	0.48
1:D:2:THR:HG21	1:D:29:ARG:HD3	1.95	0.48
6:A:214:HOH:O	1:B:152:ASP:N	2.47	0.48
1:C:3:GLN:HG3	1:C:4:GLN:N	2.28	0.48
1:A:13:LEU:HD11	1:B:16:ASN:HD22	1.78	0.48
1:A:16:ASN:OD1	1:A:16:ASN:C	2.53	0.47
1:B:82:GLU:HA	1:B:177:THR:OG1	2.14	0.47
1:D:118:LEU:HB2	1:D:120:MET:CE	2.44	0.47
1:D:187:SER:O	1:D:188:HIS:HB2	2.14	0.47
1:A:29:ARG:CG	1:A:29:ARG:NH1	2.52	0.47
1:D:29:ARG:HB2	1:D:31:ASP:OD1	2.14	0.47
1:B:4:GLN:HE21	1:B:5:ILE:N	2.11	0.47
1:C:50:ILE:HG22	1:C:97:ILE:HD11	1.97	0.47
1:B:104:GLU:HG2	1:B:153:ILE:HD12	1.97	0.47
1:B:119:TYR:CE1	1:B:128:LEU:HD13	2.49	0.46
1:B:97:ILE:HD12	1:B:97:ILE:HA	1.81	0.46
1:C:102:ILE:HD11	1:C:108:GLU:HG3	1.97	0.46
1:C:61:VAL:HG22	1:C:157:GLU:HG3	1.97	0.46
1:A:175:GLY:HA3	1:B:120:MET:CE	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LYS:N	1:D:56:LYS:HD2	2.31	0.46
1:D:2:THR:OG1	1:D:27:LEU:HG	2.16	0.46
1:D:5:ILE:CD1	1:D:27:LEU:HD11	2.45	0.46
1:D:16:ASN:HB3	1:D:17:TYR:H	1.41	0.46
1:B:104:GLU:HG2	1:B:153:ILE:CD1	2.46	0.45
1:A:139:ASN:HA	1:C:165:GLU:HG2	1.98	0.45
1:A:160:PHE:HB2	1:A:190:MET:CE	2.47	0.45
1:A:5:ILE:HG21	1:B:66:PHE:CZ	2.52	0.45
1:C:114:LYS:NZ	1:C:130:HIS:HD2	2.14	0.45
1:D:5:ILE:CD1	1:D:27:LEU:CD1	2.94	0.44
1:B:37:HIS:HA	6:B:212:HOH:O	2.17	0.44
1:A:63:ILE:CD1	1:A:84:CYS:HA	2.48	0.44
1:B:88:LEU:O	1:B:91:ASP:HB2	2.18	0.44
1:C:55:THR:O	1:C:58:LYS:HE3	2.17	0.44
1:D:4:GLN:HB3	1:D:28:THR:HB	1.99	0.43
1:B:52:LEU:HD21	1:B:109:VAL:HG11	2.01	0.43
1:A:160:PHE:HB2	1:A:190:MET:HE2	2.01	0.43
1:A:95:VAL:HG11	1:D:55:THR:CG2	2.40	0.43
1:C:2:THR:O	1:C:2:THR:HG22	2.18	0.42
1:D:82:GLU:HA	1:D:177:THR:OG1	2.20	0.42
1:C:114:LYS:NZ	1:C:117:GLU:OE1	2.48	0.42
1:D:102:ILE:O	1:D:106:GLY:HA2	2.19	0.42
1:A:97:ILE:HD12	1:A:97:ILE:HA	1.81	0.42
1:D:43:ASP:OD1	1:D:126:THR:HG21	2.19	0.41
1:C:33:GLU:OE2	1:C:35:ILE:HD11	2.20	0.41
1:B:188:HIS:O	1:B:190:MET:N	2.53	0.41
1:C:29:ARG:NH2	1:D:150:ASP:O	2.53	0.41
1:A:66:PHE:CE1	1:A:78:GLY:HA3	2.55	0.41
1:B:51:LEU:HB3	1:B:133:ILE:HG22	2.03	0.41
1:C:81:ILE:HD13	1:C:166:MET:HE3	2.03	0.41
1:B:63:ILE:O	1:B:81:ILE:HA	2.21	0.40
1:B:117:GLU:HG2	1:B:130:HIS:ND1	2.37	0.40
1:D:101:ALA:O	1:D:105:THR:OG1	2.32	0.40
1:C:86:GLY:HA2	2:C:3846:GDD:PA	2.61	0.40
1:B:49:THR:HG23	1:B:180:LEU:HD11	2.03	0.40
1:C:60:VAL:HG23	1:C:158:LEU:HD13	2.03	0.40
6:A:199:HOH:O	2:B:3846:GDD:H611	2.21	0.40
1:A:67:ARG:NH1	2:A:3846:GDD:O3B	2.48	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	183/191 (96%)	170 (93%)	11 (6%)	2 (1%)	17	19
1	B	183/191 (96%)	164 (90%)	17 (9%)	2 (1%)	17	19
1	C	178/191 (93%)	168 (94%)	8 (4%)	2 (1%)	17	19
1	D	188/191 (98%)	173 (92%)	13 (7%)	2 (1%)	17	19
All	All	732/764 (96%)	675 (92%)	49 (7%)	8 (1%)	17	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	C	3	GLN
1	D	16	ASN
1	A	152	ASP
1	B	30	LYS
1	C	29	ARG
1	D	89	ASP
1	B	110	GLY

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	164/167 (98%)	154 (94%)	10 (6%)	23	32
1	B	163/167 (98%)	150 (92%)	13 (8%)	15	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	162/167 (97%)	145 (90%)	17 (10%)	8 9
1	D	166/167 (99%)	155 (93%)	11 (7%)	21 28
All	All	655/668 (98%)	604 (92%)	51 (8%)	16 20

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	GLN
1	A	13	LEU
1	A	29	ARG
1	A	31	ASP
1	A	44	ARG
1	A	76	GLU
1	A	116	PHE
1	A	141	ARG
1	A	158	LEU
1	B	4	GLN
1	B	7	LEU
1	B	30	LYS
1	B	44	ARG
1	B	56	LYS
1	B	68	VAL
1	B	90	ASN
1	B	112	VAL
1	B	116	PHE
1	B	126	THR
1	B	137	SER
1	B	138	ASP
1	B	158	LEU
1	C	3	GLN
1	C	5	ILE
1	C	38	LYS
1	C	44	ARG
1	C	63	ILE
1	C	97	ILE
1	C	111	GLU
1	C	113	ARG
1	C	116	PHE
1	C	127	GLU
1	C	138	ASP

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Mol	Chain	Res	Type
1	C	141	ARG
1	C	152	ASP
1	C	158	LEU
1	C	165	GLU
1	C	179	LEU
1	C	186	THR
1	D	16	ASN
1	D	27	LEU
1	D	30	LYS
1	D	56	LYS
1	D	68	VAL
1	D	112	VAL
1	D	116	PHE
1	D	126	THR
1	D	137	SER
1	D	158	LEU
1	D	186	THR

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	130	HIS
1	B	4	GLN
1	B	16	ASN
1	B	182	ASN
1	C	3	GLN
1	C	22	ASN
1	C	130	HIS
1	C	140	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
2	GDD	A	3846	3	34,42,42	1.26	2 (5%)	47,65,65	1.64	8 (17%)
2	GDD	B	3846	3	34,42,42	1.28	4 (11%)	47,65,65	1.75	10 (21%)
2	GDD	C	3846	3	34,42,42	1.24	4 (11%)	47,65,65	1.96	14 (29%)
2	GDD	D	3846	3	34,42,42	1.24	3 (8%)	47,65,65	1.63	9 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDD	A	3846	3	-	0/19/59/59	0/4/4/4
2	GDD	B	3846	3	-	0/19/59/59	0/4/4/4
2	GDD	C	3846	3	-	0/19/59/59	0/4/4/4
2	GDD	D	3846	3	-	0/19/59/59	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3846	GDD	C6-N1	2.09	1.37	1.33
2	B	3846	GDD	O4'-C1'	2.48	1.44	1.41
2	C	3846	GDD	C6-N1	2.51	1.37	1.33
2	D	3846	GDD	C5-C4	2.80	1.46	1.40
2	C	3846	GDD	C5-C4	3.11	1.47	1.40
2	D	3846	GDD	O4'-C1'	3.18	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3846	GDD	O4'-C1'	3.22	1.45	1.41
2	A	3846	GDD	C5-C4	3.50	1.48	1.40
2	C	3846	GDD	C6-C5	3.58	1.48	1.41
2	B	3846	GDD	C5-C4	3.69	1.48	1.40
2	D	3846	GDD	C6-C5	4.30	1.49	1.41
2	B	3846	GDD	C6-C5	4.46	1.50	1.41
2	A	3846	GDD	C6-C5	4.53	1.50	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3846	GDD	C2'-C1'-N9	-5.28	106.23	114.29
2	C	3846	GDD	PB-O3A-PA	-5.08	118.46	132.73
2	B	3846	GDD	C5-C6-N1	-4.61	117.28	123.59
2	A	3846	GDD	C5-C6-N1	-4.20	117.84	123.59
2	B	3846	GDD	C4-C5-N7	-4.19	105.62	109.48
2	A	3846	GDD	C4-C5-N7	-4.15	105.67	109.48
2	D	3846	GDD	C2'-C1'-N9	-4.12	107.99	114.29
2	A	3846	GDD	N3-C2-N1	-3.94	121.45	127.44
2	D	3846	GDD	O3A-PB-O1B	-3.86	92.51	103.63
2	B	3846	GDD	C2'-C1'-N9	-3.86	108.39	114.29
2	C	3846	GDD	N3-C2-N1	-3.84	121.60	127.44
2	D	3846	GDD	C4-C5-N7	-3.63	106.14	109.48
2	D	3846	GDD	C5-C6-N1	-3.34	119.02	123.59
2	B	3846	GDD	O3A-PB-O1B	-3.28	94.19	103.63
2	C	3846	GDD	O21-C21-C31	-3.25	103.02	110.34
2	C	3846	GDD	C5-C6-N1	-3.17	119.25	123.59
2	C	3846	GDD	O31-C31-C21	-3.14	103.26	110.34
2	D	3846	GDD	N3-C2-N1	-3.03	122.83	127.44
2	C	3846	GDD	O3A-PB-O1B	-2.95	95.15	103.63
2	A	3846	GDD	C6-C5-C4	-2.93	117.39	120.90
2	B	3846	GDD	N3-C2-N1	-2.85	123.11	127.44
2	C	3846	GDD	C6-C5-C4	-2.69	117.68	120.90
2	B	3846	GDD	O51-C11-O1B	-2.69	107.82	111.36
2	D	3846	GDD	O51-C11-C21	-2.58	104.99	110.28
2	C	3846	GDD	C4-C5-N7	-2.48	107.19	109.48
2	C	3846	GDD	O41-C41-C51	-2.42	102.83	109.24
2	B	3846	GDD	PB-O3A-PA	-2.26	126.37	132.73
2	D	3846	GDD	C6-C5-C4	-2.07	118.43	120.90
2	C	3846	GDD	C61-C51-C41	-2.06	107.94	113.02
2	B	3846	GDD	C6-C5-C4	-2.04	118.46	120.90
2	A	3846	GDD	N2-C2-N1	2.02	120.55	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3846	GDD	O3A-PA-O5'	2.02	108.31	102.94
2	B	3846	GDD	O2B-PB-O3B	2.05	123.62	112.53
2	A	3846	GDD	O51-C51-C61	2.22	111.96	106.36
2	A	3846	GDD	O2B-PB-O3A	2.25	115.29	105.09
2	D	3846	GDD	C4'-O4'-C1'	2.46	112.42	109.72
2	C	3846	GDD	O51-C51-C61	2.92	113.73	106.36
2	D	3846	GDD	C6-N1-C2	3.04	120.16	115.94
2	C	3846	GDD	C6-N1-C2	3.51	120.81	115.94
2	B	3846	GDD	C6-N1-C2	4.32	121.93	115.94
2	A	3846	GDD	C6-N1-C2	4.83	122.65	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3846	GDD	1	0
2	B	3846	GDD	2	0
2	C	3846	GDD	3	0
2	D	3846	GDD	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	187/191 (97%)	-0.03	9 (4%) 34 37	34, 54, 81, 93	0
1	B	187/191 (97%)	0.02	8 (4%) 39 43	35, 53, 91, 104	0
1	C	182/191 (95%)	-0.12	4 (2%) 65 68	35, 48, 77, 90	0
1	D	190/191 (99%)	-0.07	5 (2%) 59 62	33, 49, 75, 92	0
All	All	746/764 (97%)	-0.05	26 (3%) 48 51	33, 51, 81, 104	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	5.8
1	D	2	THR	5.4
1	B	148	VAL	5.1
1	C	142	ALA	5.0
1	A	1	MET	4.9
1	D	148	VAL	4.4
1	B	30	LYS	3.9
1	B	144	ALA	3.8
1	A	2	THR	3.7
1	A	152	ASP	3.6
1	D	150	ASP	3.4
1	A	169	THR	3.3
1	C	31	ASP	3.2
1	B	142	ALA	2.7
1	C	30	LYS	2.6
1	A	30	LYS	2.5
1	A	29	ARG	2.4
1	A	32	GLY	2.4
1	B	107	TYR	2.4
1	B	141	ARG	2.3
1	B	31	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	143	ASN	2.1
1	D	149	GLU	2.1
1	D	144	ALA	2.0
1	A	5	ILE	2.0
1	A	3	GLN	2.0

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
2	GDD	A	3846	39/39	0.86	0.19	0.69	48,52,57,60	0
3	MG	D	202	1/1	0.92	0.16	-0.06	39,39,39,39	0
2	GDD	B	3846	39/39	0.93	0.14	-0.25	45,52,56,57	0
2	GDD	D	3846	39/39	0.91	0.15	-0.35	46,53,57,59	0
2	GDD	C	3846	39/39	0.93	0.13	-0.42	44,51,54,55	0
3	MG	B	202	1/1	0.90	0.11	-0.91	42,42,42,42	0
3	MG	A	202	1/1	0.93	0.13	-1.12	44,44,44,44	0
4	NA	C	230	1/1	0.96	0.07	-1.93	51,51,51,51	0
5	CL	C	240	1/1	0.73	0.11	-	62,62,62,62	0
4	NA	A	204	1/1	0.90	0.18	-	51,51,51,51	0
3	MG	C	202	1/1	0.97	0.12	-	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.