



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YRO
Title : Crystal structure of beta14,-galactosyltransferase mutant ARG228Lys in complex with alpha-lactalbumin in the presence of UDP-galactose and Mn
Authors : Ramakrishnan, B.; Boeggeman, E.; Qasba, P.K.
Deposited on : 2005-02-04
Resolution : 1.90 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 ⓘ](#)) 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

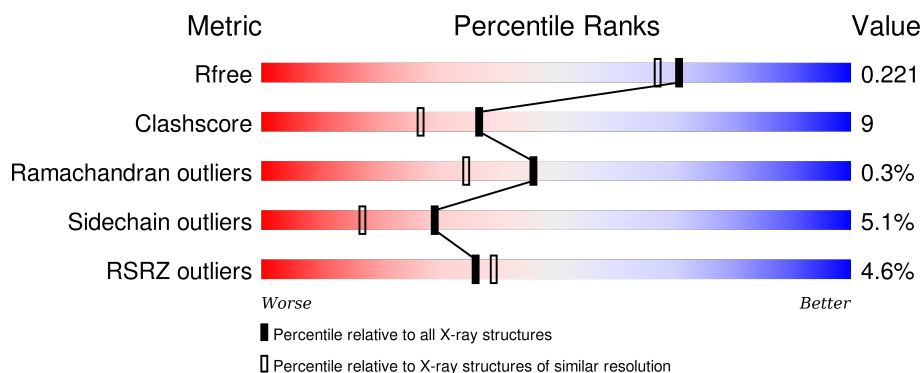
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 $\leq 5\%$. 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> <div>6%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>•</div> </div> </div>
1	C	123	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>
2	B	286	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 5%</div> </div> </div>
2	D	286	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	UDP	B	405	-	-	-	X
6	UDP	D	530	-	-	-	X
8	PG4	A	806	-	-	-	X
8	PG4	C	807	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7388 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
1	A	123	Total	C	N	O	S	0	0	0
			980	620	156	195	9			
1	C	123	Total	C	N	O	S	0	0	0
			980	620	156	195	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	272	Total	C	N	O	S	0	0	0
			2217	1425	380	399	13			
2	D	272	Total	C	N	O	S	0	0	0
			2217	1425	380	399	13			

There are 30 discrepancies between the modelled and reference sequences:

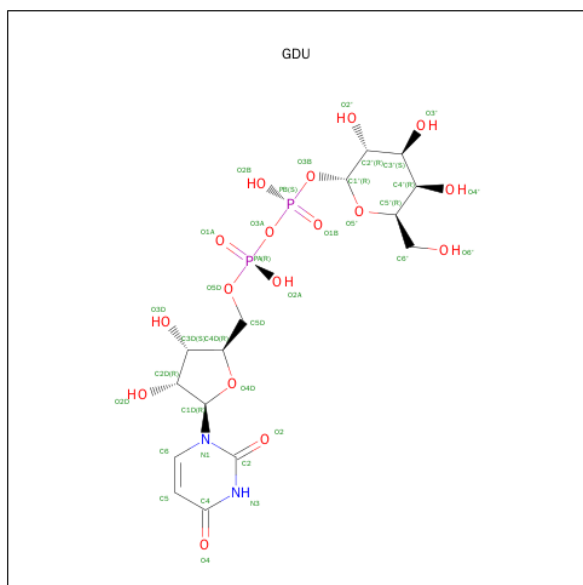
Chain	Residue	Modelled	Actual	Comment	Reference
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MET	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	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	228	LYS	ARG	ENGINEERED	UNP P08037
B	342	THR	CYS	ENGINEERED	UNP P08037
D	117	ALA	-	SEE REMARK 999	UNP P08037

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	118	SER	-	SEE REMARK 999	UNP P08037
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	228	LYS	ARG	ENGINEERED	UNP P08037
D	342	THR	CYS	ENGINEERED	UNP P08037

- Molecule 3 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

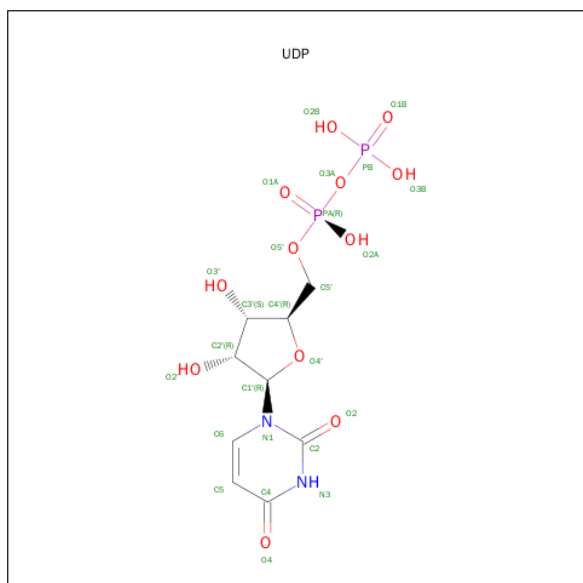
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



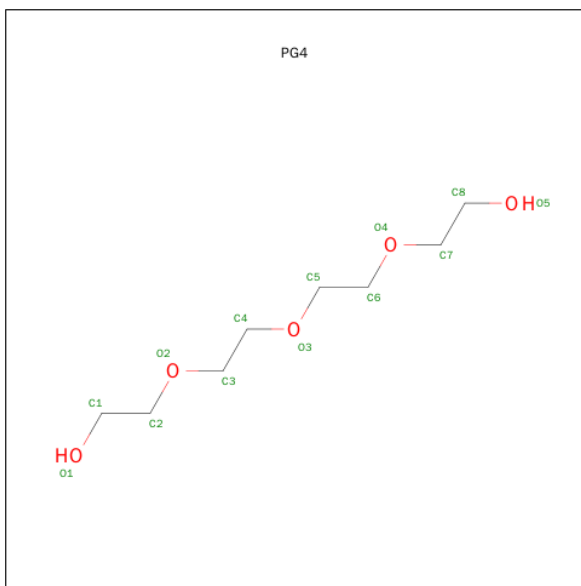
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O P 25 9 2 12 2	0	0
6	D	1	Total C N O P 25 9 2 12 2	0	0

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	8	5		
8	C	1	Total	C	O	0	0
			13	8	5		

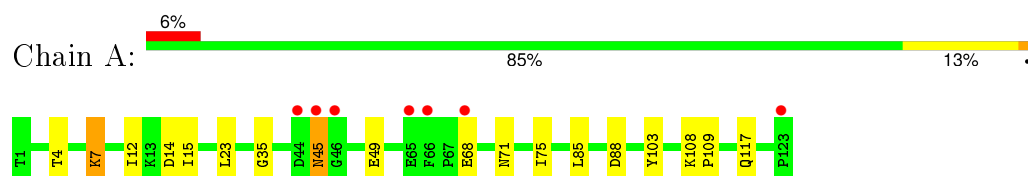
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	156	Total 156	O 156	0	0
9	B	253	Total 253	O 253	0	0
9	C	151	Total 151	O 151	0	0
9	D	270	Total 270	O 270	0	0

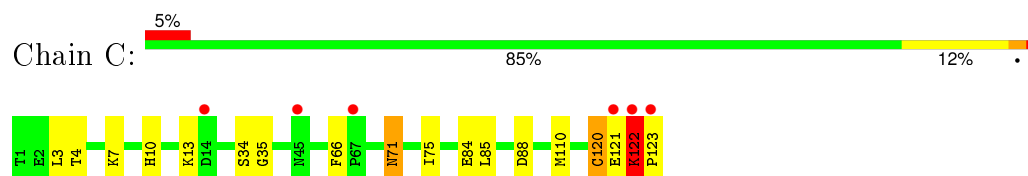
3 Residue-property plots [i](#)

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.

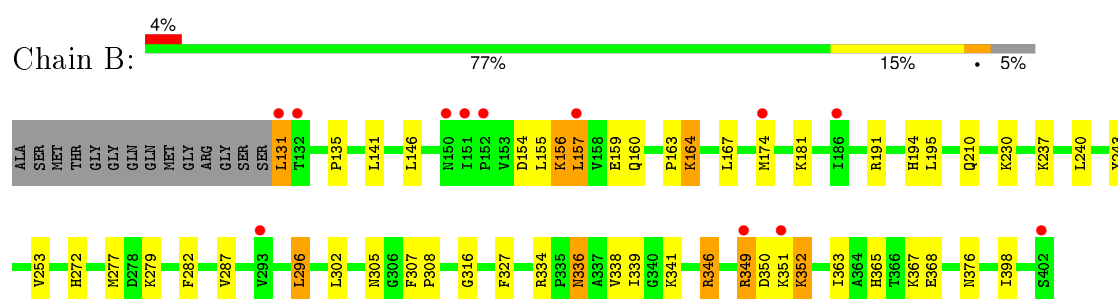
- Molecule 1: ALPHA-LACTALBUMIN



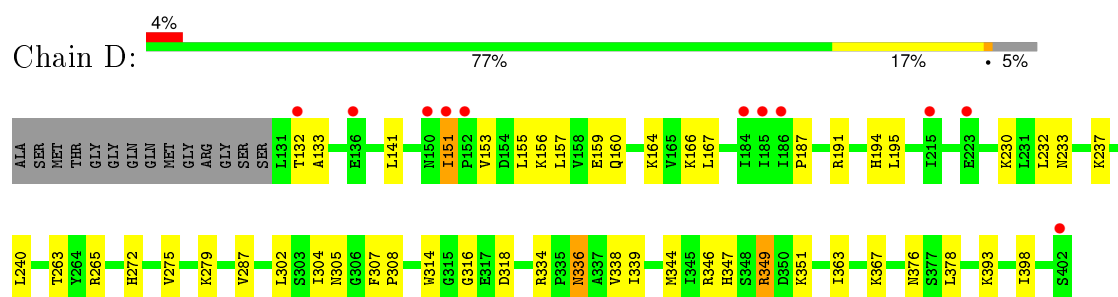
- Molecule 1: ALPHA-LACTALBUMIN



- 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, α , β , γ	57.33Å 94.09Å 99.70Å 90.00° 101.64° 90.00°	Depositor
Resolution (Å)	32.55 – 1.90 30.76 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.9 (32.55-1.90) 97.1 (30.76-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.88Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.225 0.185 , 0.221	Depositor DCC
R_{free} test set	8001 reflections (10.02%)	DCC
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 82354 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7388	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UDP, GDU, CA, MN, PG4, MES

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	0.58	0/1001	0.76	0/1350
1	C	0.62	0/1001	0.85	1/1350 (0.1%)
2	B	0.56	0/2277	0.76	1/3084 (0.0%)
2	D	0.57	0/2277	0.76	0/3084
All	All	0.58	0/6556	0.77	2/8868 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	LYS	N-CA-C	9.17	135.76	111.00
2	B	296	LEU	CA-CB-CG	5.55	128.07	115.30

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	19	0
2	B	2217	0	2187	46	0
2	D	2217	0	2187	43	0
3	B	36	0	22	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	36	0	22	4	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	25	0	11	0	0
6	D	25	0	11	0	0
7	A	12	0	13	2	0
8	A	13	0	18	1	0
8	C	13	0	18	2	0
9	A	156	0	0	3	0
9	B	253	0	0	7	0
9	C	151	0	0	4	0
9	D	270	0	0	7	0
All	All	7388	0	6361	121	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 9.

All (121) 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)
2:B:346:ARG:HB3	2:B:346:ARG:HH11	1.30	0.96
2:D:349:ARG:HG2	2:D:349:ARG:HH11	1.39	0.85
2:D:346:ARG:HD3	9:D:1182:HOH:O	1.78	0.82
1:A:71:ASN:HD21	1:A:75:ILE:H	1.28	0.81
2:B:327:PHE:CZ	2:B:367:LYS:HB2	2.16	0.80
2:B:305:ASN:HD21	2:B:376:ASN:H	1.30	0.77
2:D:151:ILE:HD13	2:D:151:ILE:H	1.53	0.74
2:B:237:LYS:HD2	9:B:1398:HOH:O	1.89	0.73
1:C:4:THR:H	1:C:7:LYS:HE3	1.54	0.72
2:B:277:MET:CE	2:B:279:LYS:HE2	2.21	0.70
2:B:336:ASN:HD22	2:B:338:VAL:H	1.40	0.69
2:B:277:MET:HE1	2:B:279:LYS:HE2	1.72	0.69
2:B:191:ARG:HH11	2:B:194:HIS:HD2	1.39	0.69
2:B:346:ARG:CB	2:B:346:ARG:HH11	2.06	0.68
2:D:336:ASN:HD22	2:D:338:VAL:H	1.41	0.67
2:D:191:ARG:HH11	2:D:194:HIS:HD2	1.43	0.65
1:C:71:ASN:HD21	1:C:75:ILE:H	1.43	0.64
2:B:349:ARG:HD3	2:B:350:ASP:H	1.62	0.64
2:B:131:LEU:HD23	2:B:131:LEU:N	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:SER:HA	8:C:807:PG4:H51	1.81	0.63
2:D:155:LEU:O	2:D:159:GLU:HG3	1.97	0.63
2:D:279:LYS:HD2	2:D:346:ARG:HH12	1.64	0.62
2:B:352:LYS:HE3	9:B:1361:HOH:O	1.99	0.62
2:D:305:ASN:HD21	2:D:376:ASN:H	1.48	0.62
2:D:349:ARG:CG	2:D:349:ARG:HH11	2.11	0.62
2:B:351:LYS:O	2:B:352:LYS:HB2	1.99	0.61
1:C:7:LYS:HD3	9:C:1216:HOH:O	2.00	0.61
2:B:174:MET:HG2	9:B:1468:HOH:O	2.01	0.60
2:D:316:GLY:HA2	2:D:363:ILE:HD11	1.83	0.60
2:D:151:ILE:CD1	2:D:151:ILE:H	2.15	0.60
1:C:66:PHE:HB2	9:C:996:HOH:O	2.02	0.59
2:B:191:ARG:NH1	2:B:194:HIS:HD2	2.00	0.59
2:B:272:HIS:HB3	2:B:334:ARG:HG2	1.85	0.58
1:A:7:LYS:HE3	9:A:1510:HOH:O	2.03	0.58
2:D:151:ILE:N	2:D:151:ILE:HD13	2.18	0.58
1:C:35:GLY:N	8:C:807:PG4:H32	2.18	0.57
2:B:160:GLN:O	2:B:163:PRO:HD3	2.06	0.56
1:C:122:LYS:HG3	9:C:1270:HOH:O	2.04	0.56
1:A:12:ILE:O	1:A:15:ILE:HG22	2.06	0.56
1:A:49:GLU:OE1	7:A:805:MES:H52	2.07	0.55
2:D:164:LYS:HD2	9:D:1443:HOH:O	2.05	0.55
1:C:4:THR:HG23	1:C:7:LYS:HE2	1.87	0.55
2:B:365:HIS:O	2:B:368:GLU:HG2	2.08	0.54
2:B:191:ARG:HD2	2:B:194:HIS:CD2	2.43	0.54
2:D:132:THR:HG22	2:D:133:ALA:N	2.22	0.53
2:D:314:TRP:NE1	3:D:528:GDU:H6'1	2.24	0.52
1:A:108:LYS:HB3	1:A:109:PRO:CD	2.39	0.52
2:D:279:LYS:HB2	2:D:346:ARG:NH1	2.23	0.52
2:D:344:MET:HE3	2:D:347:HIS:CD2	2.43	0.52
1:C:110:MET:HE3	9:D:1407:HOH:O	2.08	0.52
2:D:367:LYS:HE3	9:D:1726:HOH:O	2.09	0.52
1:C:10:HIS:CD2	1:C:13:LYS:NZ	2.78	0.52
1:A:45:ASN:OD1	1:A:45:ASN:O	2.29	0.51
2:B:327:PHE:CE2	2:B:367:LYS:HD2	2.46	0.51
1:C:10:HIS:O	1:C:13:LYS:HG3	2.11	0.51
2:B:327:PHE:CE1	2:B:367:LYS:HB2	2.45	0.51
2:B:336:ASN:ND2	2:B:339:ILE:H	2.08	0.51
1:A:117:GLN:NE2	2:B:287:VAL:HG12	2.25	0.51
2:D:318:ASP:OD2	3:D:528:GDU:O4'	2.22	0.51
2:B:316:GLY:HA2	2:B:363:ILE:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HG3	9:A:1545:HOH:O	2.11	0.51
1:C:84:GLU:HG3	9:C:1148:HOH:O	2.10	0.50
2:B:164:LYS:HD3	9:B:1026:HOH:O	2.12	0.50
1:A:68:GLU:O	1:A:68:GLU:HG2	2.11	0.50
2:B:164:LYS:HE2	9:B:1341:HOH:O	2.12	0.50
1:C:4:THR:H	1:C:7:LYS:CE	2.23	0.49
2:D:314:TRP:CD1	3:D:528:GDU:H6'1	2.47	0.49
1:C:120:CYS:O	1:C:122:LYS:N	2.45	0.49
2:B:155:LEU:O	2:B:159:GLU:HG3	2.13	0.49
2:D:156:LYS:O	2:D:160:GLN:HG3	2.13	0.49
2:B:336:ASN:HD22	2:B:338:VAL:N	2.08	0.48
2:B:336:ASN:ND2	2:B:338:VAL:H	2.08	0.48
2:B:277:MET:HE1	9:B:964:HOH:O	2.14	0.48
2:D:191:ARG:NH1	2:D:194:HIS:HD2	2.09	0.47
2:D:230:LYS:HD3	2:D:398:ILE:HB	1.96	0.47
1:C:4:THR:N	1:C:7:LYS:HE3	2.27	0.47
2:D:336:ASN:ND2	2:D:339:ILE:H	2.12	0.47
1:A:4:THR:OG1	1:A:7:LYS:HB2	2.15	0.46
2:D:272:HIS:HB3	2:D:334:ARG:HG2	1.97	0.46
2:D:275:VAL:HG11	9:D:1362:HOH:O	2.15	0.46
2:B:194:HIS:HE1	9:B:1132:HOH:O	1.99	0.46
2:D:237:LYS:HD3	2:D:378:LEU:HD23	1.98	0.45
2:D:132:THR:CG2	2:D:133:ALA:N	2.79	0.45
2:D:307:PHE:HB3	2:D:308:PRO:HD2	1.99	0.45
2:B:230:LYS:HD3	2:B:398:ILE:HB	1.98	0.45
2:B:277:MET:HE2	2:B:279:LYS:HE2	1.95	0.45
2:D:314:TRP:CE2	3:D:528:GDU:H6'1	2.51	0.45
2:B:135:PRO:HD2	2:B:210:GLN:HE22	1.81	0.45
1:C:10:HIS:HA	1:C:13:LYS:HE3	1.99	0.45
2:D:187:PRO:HD3	2:D:232:LEU:HD21	1.99	0.45
2:B:277:MET:HE2	2:B:279:LYS:HG2	2.00	0.44
2:D:191:ARG:HD2	2:D:194:HIS:CD2	2.53	0.44
2:D:166:LYS:HE3	9:D:1447:HOH:O	2.16	0.44
1:A:103:TYR:CE2	7:A:805:MES:H51	2.53	0.44
2:D:263:THR:HG22	2:D:265:ARG:HG3	2.00	0.44
1:A:108:LYS:HB3	1:A:109:PRO:HD3	1.99	0.43
1:C:10:HIS:CD2	1:C:13:LYS:HE3	2.54	0.43
2:B:346:ARG:HB3	2:B:346:ARG:NH1	2.14	0.43
2:D:155:LEU:HD23	2:D:155:LEU:HA	1.83	0.43
2:B:282:PHE:CD2	2:B:341:LYS:HD2	2.54	0.43
2:D:151:ILE:O	2:D:151:ILE:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:ARG:NH1	2:B:194:HIS:CD2	2.85	0.43
2:D:304:ILE:O	2:D:305:ASN:HB3	2.19	0.43
1:C:3:LEU:HA	1:C:7:LYS:HE3	1.99	0.43
2:B:156:LYS:HE3	2:B:156:LYS:HA	2.01	0.43
2:B:349:ARG:HA	2:B:349:ARG:NE	2.33	0.42
1:A:35:GLY:N	8:A:806:PG4:H52	2.34	0.42
2:B:253:VAL:HG12	3:B:403:GDU:H2D	2.01	0.42
2:D:346:ARG:HA	2:D:346:ARG:HD2	1.63	0.42
2:D:351:LYS:HE2	2:D:351:LYS:HB2	1.74	0.42
2:D:233:ASN:HB3	2:D:378:LEU:HD22	2.01	0.42
2:D:393:LYS:HD2	9:D:1163:HOH:O	2.20	0.42
2:B:131:LEU:CD2	2:B:131:LEU:N	2.83	0.42
2:B:368:GLU:HG2	2:B:368:GLU:H	1.61	0.42
2:B:181:LYS:HD3	2:B:243:TYR:CE2	2.55	0.41
2:B:307:PHE:HB3	2:B:308:PRO:HD2	2.01	0.41
2:D:336:ASN:ND2	2:D:338:VAL:HB	2.35	0.41
1:C:122:LYS:HA	1:C:123:PRO:HD3	1.56	0.41
2:D:164:LYS:HD3	2:D:164:LYS:N	2.37	0.40
2:B:154:ASP:HB3	2:B:157:LEU:HB2	2.03	0.40
1:A:14:ASP:HA	9:A:1083:HOH:O	2.22	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%)	119 (98%)	1 (1%)	1 (1%)	24	11
1	C	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	24	11
2	B	270/286 (94%)	264 (98%)	6 (2%)	0	100	100
2	D	270/286 (94%)	265 (98%)	5 (2%)	0	100	100
All	All	782/818 (96%)	764 (98%)	16 (2%)	2 (0%)	46	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	C	122	LYS

5.3.2 Protein sidechains ⓘ

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%)	41	29
1	C	109/109 (100%)	103 (94%)	6 (6%)	27	14
2	B	245/254 (96%)	230 (94%)	15 (6%)	23	11
2	D	245/254 (96%)	234 (96%)	11 (4%)	34	21
All	All	708/726 (98%)	672 (95%)	36 (5%)	29	17

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	23	LEU
1	A	85	LEU
1	A	88	ASP
2	B	131	LEU
2	B	141	LEU
2	B	146	LEU
2	B	156	LYS
2	B	157	LEU
2	B	164	LYS
2	B	167	LEU
2	B	195	LEU
2	B	240	LEU
2	B	296	LEU
2	B	302	LEU
2	B	336	ASN
2	B	346	ARG
2	B	349	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	352	LYS
1	C	71	ASN
1	C	85	LEU
1	C	88	ASP
1	C	120	CYS
1	C	121	GLU
1	C	122	LYS
2	D	141	LEU
2	D	151	ILE
2	D	153	VAL
2	D	157	LEU
2	D	167	LEU
2	D	195	LEU
2	D	240	LEU
2	D	287	VAL
2	D	302	LEU
2	D	336	ASN
2	D	349	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	45	ASN
1	A	71	ASN
2	B	160	GLN
2	B	161	GLN
2	B	194	HIS
2	B	210	GLN
2	B	305	ASN
2	B	310	ASN
2	B	336	ASN
2	B	365	HIS
1	C	10	HIS
1	C	32	HIS
1	C	71	ASN
2	D	160	GLN
2	D	161	GLN
2	D	194	HIS
2	D	207	GLN
2	D	305	ASN
2	D	310	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	336	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z > 2$
7	MES	A	805	-	11,12,12	1.21	2 (18%)	14,16,16	1.49	3 (21%)
8	PG4	A	806	-	12,12,12	0.50	0	11,11,11	0.40	0
3	GDU	B	403	5	29,38,38	1.77	6 (20%)	43,58,58	2.69	9 (20%)
6	UDP	B	405	-	18,26,26	1.88	4 (22%)	26,40,40	3.03	7 (26%)
8	PG4	C	807	-	12,12,12	0.50	0	11,11,11	0.34	0
3	GDU	D	528	5	29,38,38	1.97	7 (24%)	43,58,58	2.76	9 (20%)
6	UDP	D	530	-	18,26,26	1.86	4 (22%)	26,40,40	3.04	6 (23%)

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
7	MES	A	805	-	-	0/6/14/14	0/1/1/1
8	PG4	A	806	-	-	0/10/10/10	0/0/0/0
3	GDU	B	403	5	-	0/19/59/59	0/3/3/3
6	UDP	B	405	-	-	0/12/32/32	0/2/2/2
8	PG4	C	807	-	-	0/10/10/10	0/0/0/0
3	GDU	D	528	5	-	0/19/59/59	0/3/3/3
6	UDP	D	530	-	-	0/12/32/32	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	528	GDU	PB-O3B	-5.29	1.46	1.60
3	B	403	GDU	PB-O3B	-3.71	1.50	1.60
6	D	530	UDP	C6-C5	-2.54	1.32	1.38
6	B	405	UDP	C6-C5	-2.47	1.32	1.38
3	D	528	GDU	C6-C5	-2.16	1.33	1.38
3	D	528	GDU	PA-O2A	-2.13	1.45	1.54
3	B	403	GDU	C6-C5	-2.02	1.33	1.38
7	A	805	MES	C3-N4	2.02	1.52	1.46
7	A	805	MES	C5-N4	2.26	1.53	1.46
3	B	403	GDU	O5'-C5'	2.63	1.50	1.44
3	B	403	GDU	O5'-C1'	2.68	1.48	1.41
6	D	530	UDP	PB-O1B	2.95	1.60	1.51
6	B	405	UDP	PB-O1B	3.23	1.61	1.51
3	D	528	GDU	O5'-C1'	3.42	1.50	1.41
3	B	403	GDU	C4-N3	3.73	1.40	1.33
3	D	528	GDU	C6-N1	3.77	1.41	1.35
6	B	405	UDP	C6-N1	3.97	1.41	1.35
3	D	528	GDU	O5'-C5'	4.12	1.54	1.44
6	D	530	UDP	C6-N1	4.20	1.41	1.35
6	D	530	UDP	C4-N3	4.29	1.41	1.33
6	B	405	UDP	C4-N3	4.34	1.41	1.33
3	D	528	GDU	C4-N3	4.41	1.41	1.33
3	B	403	GDU	C6-N1	4.58	1.42	1.35

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	GDU	O5'-C5'-C6'	-3.91	96.48	106.36
3	B	403	GDU	O4D-C4D-C3D	-3.59	97.92	105.15
7	A	805	MES	O2S-S-C8	-3.52	103.90	106.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	528	GDU	C5-C4-N3	-3.50	114.14	123.12
6	D	530	UDP	C5-C4-N3	-3.40	114.41	123.12
3	D	528	GDU	O5'-C5'-C6'	-3.36	97.85	106.36
3	D	528	GDU	O4D-C4D-C3D	-3.35	98.39	105.15
6	B	405	UDP	C5-C4-N3	-3.32	114.59	123.12
3	B	403	GDU	C5-C4-N3	-3.29	114.68	123.12
3	B	403	GDU	O3A-PA-O5D	-3.12	94.66	102.94
3	D	528	GDU	O3'-C3'-C4'	-2.97	103.65	110.34
3	B	403	GDU	O3'-C3'-C4'	-2.65	104.37	110.34
6	B	405	UDP	O3A-PA-O5'	-2.56	96.14	102.94
3	D	528	GDU	O3A-PA-O5D	-2.47	96.38	102.94
6	B	405	UDP	O4'-C4'-C3'	-2.42	100.28	105.15
7	A	805	MES	C2-C3-N4	-2.18	106.83	110.12
6	D	530	UDP	C6-C5-C4	2.04	121.09	117.28
3	B	403	GDU	O2A-PA-O3A	2.05	114.41	105.09
3	D	528	GDU	C6-C5-C4	2.18	121.36	117.28
6	B	405	UDP	O4'-C4'-C5'	2.21	117.23	109.32
6	D	530	UDP	C4'-O4'-C1'	2.67	112.65	109.72
7	A	805	MES	O1S-S-C8	3.07	109.52	106.91
6	D	530	UDP	O5'-C5'-C4'	3.69	122.73	109.12
6	B	405	UDP	O5'-C5'-C4'	4.17	124.49	109.12
3	B	403	GDU	O5'-C1'-O3B	4.43	117.20	111.36
6	B	405	UDP	O3B-PB-O1B	4.70	125.69	110.58
6	D	530	UDP	O3B-PB-O1B	4.95	126.50	110.58
3	D	528	GDU	O3B-PB-O1B	5.02	129.19	109.46
3	B	403	GDU	O3B-PB-O1B	5.87	132.55	109.46
3	D	528	GDU	O5'-C1'-O3B	6.87	120.43	111.36
3	B	403	GDU	C4-N3-C2	12.59	126.61	114.14
6	B	405	UDP	C4-N3-C2	12.59	126.61	114.14
6	D	530	UDP	C4-N3-C2	12.63	126.65	114.14
3	D	528	GDU	C4-N3-C2	12.78	126.80	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	805	MES	2	0
8	A	806	PG4	1	0
3	B	403	GDU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	807	PG4	2	0
3	D	528	GDU	4	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, 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	123/123 (100%)	-0.06	7 (5%)	27	30	19, 25, 51, 62	0
1	C	123/123 (100%)	0.03	6 (4%)	33	36	17, 25, 48, 82	0
2	B	272/286 (95%)	0.04	12 (4%)	38	41	18, 28, 49, 60	0
2	D	272/286 (95%)	-0.06	11 (4%)	42	46	18, 27, 44, 58	0
All	All	790/818 (96%)	-0.01	36 (4%)	36	39	17, 27, 48, 82	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	PRO	13.7
1	C	122	LYS	9.8
2	D	402	SER	8.3
1	A	45	ASN	7.3
1	C	67	PRO	5.6
1	A	123	PRO	5.6
2	B	402	SER	5.2
1	A	66	PHE	4.1
1	A	68	GLU	3.7
2	D	151	ILE	3.6
1	C	45	ASN	3.5
2	B	152	PRO	3.4
2	B	151	ILE	3.3
2	D	152	PRO	3.3
2	B	351	LYS	3.3
2	D	136	GLU	3.3
2	B	174	MET	3.1
1	A	65	GLU	3.0
2	D	186	ILE	2.6
2	D	132	THR	2.6
2	D	185	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	186	ILE	2.5
2	B	131	LEU	2.5
2	D	215	ILE	2.5
2	D	184	ILE	2.3
2	B	150	ASN	2.2
2	B	293	VAL	2.2
2	D	223	GLU	2.2
2	B	157	LEU	2.2
1	A	44	ASP	2.2
1	C	14	ASP	2.1
2	B	349	ARG	2.1
1	C	121	GLU	2.1
2	D	150	ASN	2.0
2	B	132	THR	2.0
1	A	46	GLY	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, 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	LLDF	B-factors(Å ²)	Q<0.9
8	PG4	C	807	13/13	0.73	0.24	6.42	46,50,58,61	0
8	PG4	A	806	13/13	0.69	0.30	4.17	51,53,58,61	0
6	UDP	D	530	25/25	0.58	0.25	2.73	62,80,98,98	0
6	UDP	B	405	25/25	0.63	0.23	2.29	70,79,98,99	0
7	MES	A	805	12/12	0.87	0.16	1.02	42,46,50,52	0
3	GDU	D	528	36/36	0.96	0.10	-0.22	19,24,33,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	A	124	1/1	1.00	0.08	-0.32	21,21,21,21	0
3	GDU	B	403	36/36	0.96	0.10	-0.44	20,25,29,31	0
4	CA	C	124	1/1	0.99	0.07	-0.75	26,26,26,26	0
5	MN	B	404	1/1	1.00	0.04	-2.07	25,25,25,25	0
5	MN	D	529	1/1	1.00	0.07	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.