



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:03 am GMT

PDB ID : 2FYD  
Title : catalytic domain of bovine beta 1, 4-galactosyltransferase in complex with  
alpha-lactalbumin, glucose, Mn, and UDP-N-acetylgalactosamine  
Authors : Ramakrishnan, B.; Ramasamy, V.; Qasba, P.K.  
Deposited on : 2006-02-07  
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

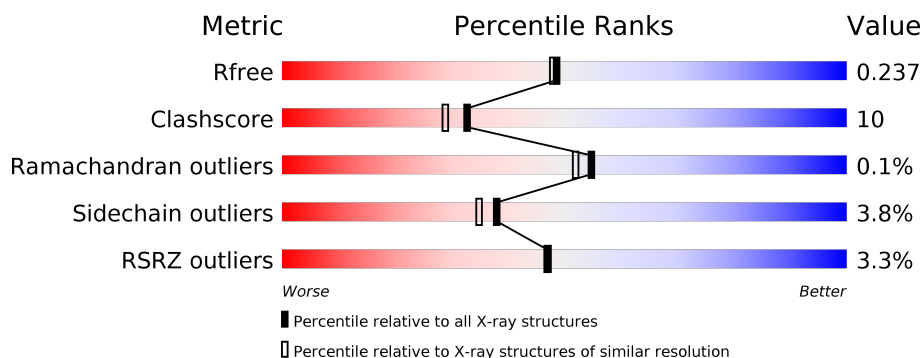
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>4%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>•</div> </div> </div>
1	C	123	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>24%</div> </div> </div>
2	B	286	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>•</div> <div>5%</div> </div> </div>
2	D	286	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>15%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NGA	B	404	-	-	X	X
4	NGA	D	529	-	-	X	X
8	PG4	A	850	-	-	-	X
8	PG4	C	851	-	-	-	X
9	MES	A	805	-	-	-	X
9	MES	C	806	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7045 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	2	0	0
			2210	1415	381	399	15			
2	D	272	Total	C	N	O	S	2	0	0
			2210	1415	381	399	15			

There are 32 discrepancies between the modelled and reference sequences:

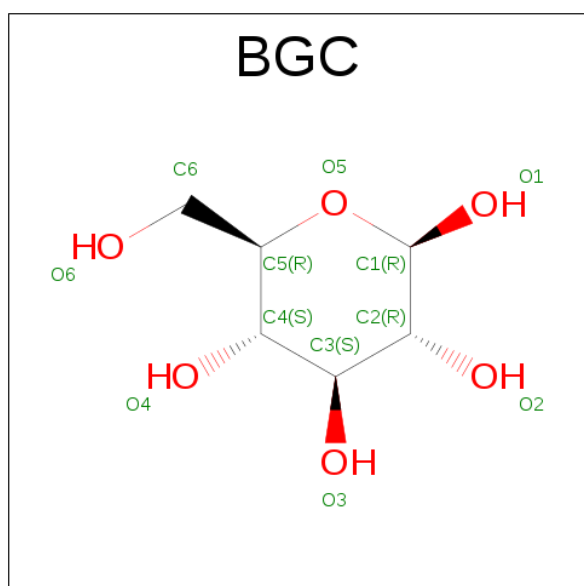
Chain	Residue	Modelled	Actual	Comment	Reference
B	117	ALA	-	CLONING ARTIFACT	GB 21450879
B	118	SER	-	CLONING ARTIFACT	GB 21450879
B	119	MET	-	CLONING ARTIFACT	GB 21450879
B	120	THR	-	CLONING ARTIFACT	GB 21450879
B	121	GLY	-	CLONING ARTIFACT	GB 21450879
B	122	GLY	-	CLONING ARTIFACT	GB 21450879
B	123	GLN	-	CLONING ARTIFACT	GB 21450879
B	124	GLN	-	CLONING ARTIFACT	GB 21450879
B	125	MET	-	CLONING ARTIFACT	GB 21450879
B	126	GLY	-	CLONING ARTIFACT	GB 21450879
B	127	ARG	-	CLONING ARTIFACT	GB 21450879
B	128	GLY	-	CLONING ARTIFACT	GB 21450879
B	129	SER	-	CLONING ARTIFACT	GB 21450879
B	312	CYS	TRP	ENGINEERED	GB 21450879
B	342	THR	CYS	ENGINEERED	GB 21450879
B	401	CYS	PRO	ENGINEERED	GB 21450879

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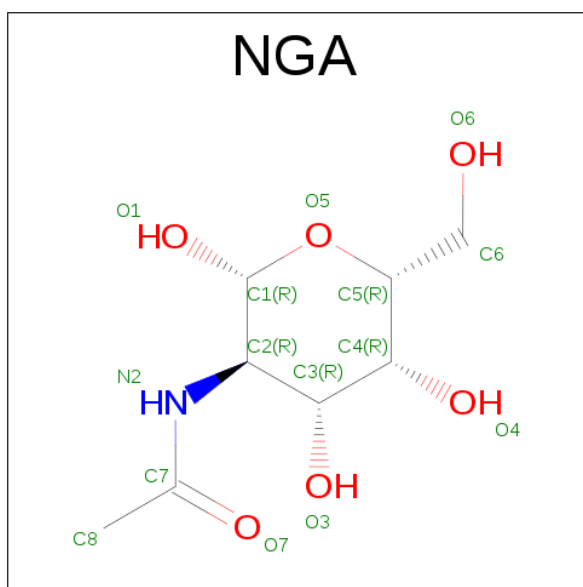
Chain	Residue	Modelled	Actual	Comment	Reference
D	117	ALA	-	CLONING ARTIFACT	GB 21450879
D	118	SER	-	CLONING ARTIFACT	GB 21450879
D	119	MET	-	CLONING ARTIFACT	GB 21450879
D	120	THR	-	CLONING ARTIFACT	GB 21450879
D	121	GLY	-	CLONING ARTIFACT	GB 21450879
D	122	GLY	-	CLONING ARTIFACT	GB 21450879
D	123	GLN	-	CLONING ARTIFACT	GB 21450879
D	124	GLN	-	CLONING ARTIFACT	GB 21450879
D	125	MET	-	CLONING ARTIFACT	GB 21450879
D	126	GLY	-	CLONING ARTIFACT	GB 21450879
D	127	ARG	-	CLONING ARTIFACT	GB 21450879
D	128	GLY	-	CLONING ARTIFACT	GB 21450879
D	129	SER	-	CLONING ARTIFACT	GB 21450879
D	312	CYS	TRP	ENGINEERED	GB 21450879
D	342	THR	CYS	ENGINEERED	GB 21450879
D	401	CYS	PRO	ENGINEERED	GB 21450879

- Molecule 3 is SUGAR (GLUCOSE) (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is SUGAR (N-ACETYL-D-GALACTOSAMINE) (three-letter code: NGA) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

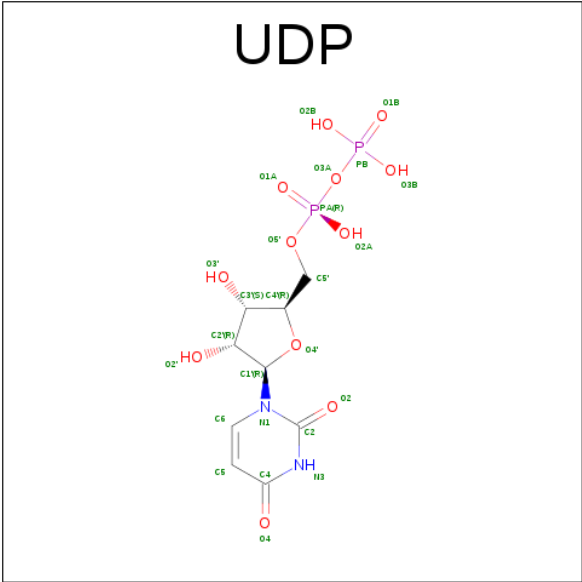
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

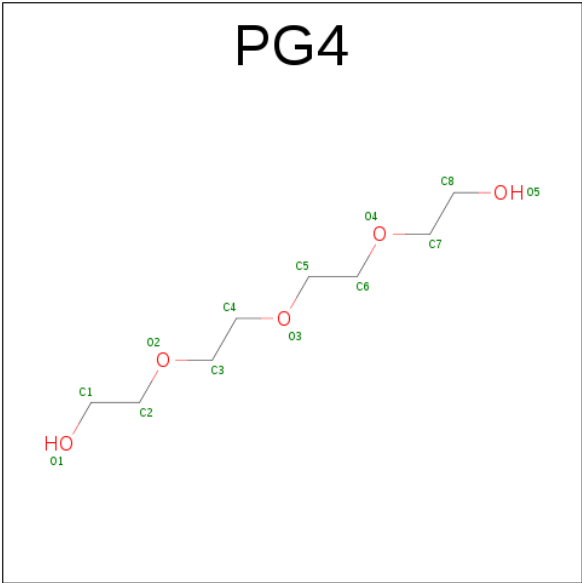
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mn	0	0
			1	1		
6	D	1	Total	Mn	0	0
			1	1		

- Molecule 7 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



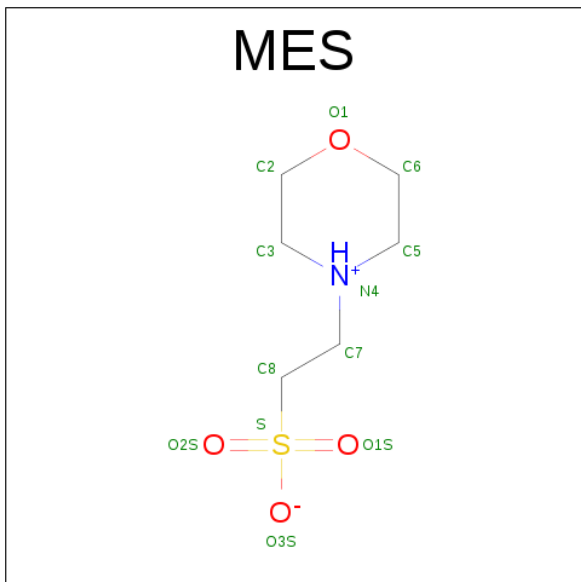
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
7	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 8 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
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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 10 is water.

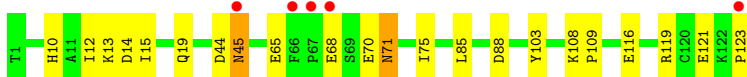
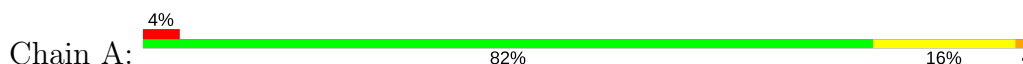
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	90	Total	O	0	0
			90	90		
10	B	153	Total	O	0	0
			153	153		
10	C	101	Total	O	0	0
			101	101		
10	D	165	Total	O	0	0
			165	165		



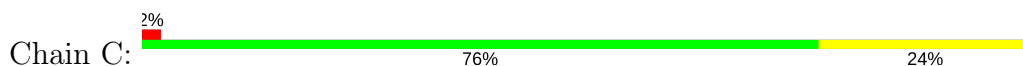
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

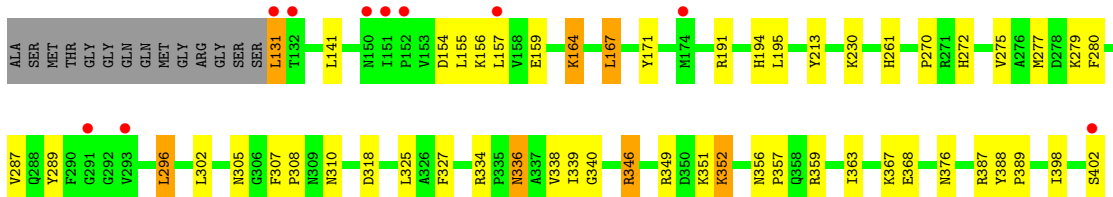
- Molecule 1: Alpha-lactalbumin



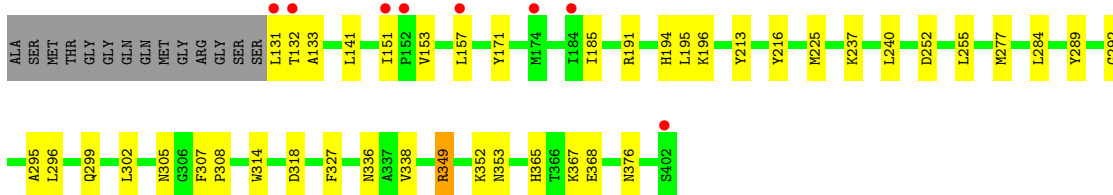
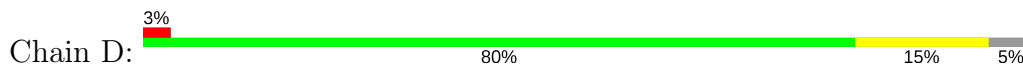
- Molecule 1: Alpha-lactalbumin



- 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, $\alpha$ , $\beta$ , $\gamma$	58.07Å 95.38Å 100.39Å 90.00° 101.33° 90.00°	Depositor
Resolution (Å)	32.08 – 2.00 32.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.9 (32.08-2.00) 94.8 (32.08-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.201 , 0.242 0.196 , 0.237	Depositor DCC
$R_{free}$ test set	6965 reflections (11.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7045	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, BGC, NGA, 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	0.62	0/1001	0.74	0/1350
1	C	0.61	0/1001	0.79	1/1350 (0.1%)
2	B	0.53	0/2267	0.74	1/3068 (0.0%)
2	D	0.58	0/2267	0.76	1/3068 (0.0%)
All	All	0.57	0/6536	0.75	3/8836 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	ASP	CB-CG-OD1	6.25	123.93	118.30
2	B	296	LEU	CA-CB-CG	5.48	127.91	115.30
2	D	284	LEU	CA-CB-CG	5.11	127.06	115.30

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	980	0	936	15	0
1	C	980	0	936	26	0
2	B	2210	0	2178	49	0
2	D	2210	0	2178	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	12	1	0
3	D	12	0	12	2	0
4	B	14	0	12	8	0
4	D	14	0	12	10	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	25	0	11	1	0
7	D	25	0	11	2	0
8	A	13	0	18	0	0
8	C	13	0	18	1	0
9	A	12	0	13	1	0
9	C	12	0	13	1	0
10	A	90	0	0	1	0
10	B	153	0	0	2	0
10	C	101	0	0	3	0
10	D	165	0	0	2	0
All	All	7045	0	6360	128	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 10.

All (128) 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)
4:D:529:NGA:H82	7:D:528:UDP:O3B	1.58	1.02
2:B:310:ASN:ND2	2:B:402:SER:H	1.61	0.97
1:A:10:HIS:HA	1:A:13:LYS:HE2	1.48	0.95
1:C:62:LYS:HE3	1:C:63:SER:O	1.73	0.87
2:B:310:ASN:HD22	2:B:402:SER:H	1.27	0.82
2:D:225:MET:HE2	2:D:352:LYS:HE3	1.60	0.82
1:A:121:GLU:O	1:A:123:PRO:HD3	1.80	0.80
1:A:71:ASN:HD21	1:A:75:ILE:H	1.28	0.78
2:B:346:ARG:HA	2:B:346:ARG:HH11	1.49	0.76
2:B:191:ARG:HH11	2:B:194:HIS:HD2	1.34	0.75
2:D:305:ASN:HD21	2:D:376:ASN:H	1.35	0.74
1:C:4:THR:HG23	1:C:7:LYS:HE2	1.70	0.74
2:D:252:ASP:OD2	4:D:529:NGA:H83	1.89	0.72
2:B:336:ASN:HD22	2:B:338:VAL:H	1.38	0.70
2:D:349:ARG:HG2	2:D:349:ARG:HH11	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ASN:HD21	1:C:75:ILE:H	1.38	0.68
2:B:349:ARG:HD3	10:B:1034:HOH:O	1.94	0.67
1:A:44:ASP:O	1:A:45:ASN:HB2	1.94	0.67
2:D:151:ILE:O	2:D:151:ILE:HG13	1.95	0.66
2:B:336:ASN:ND2	2:B:339:ILE:HG22	2.11	0.65
1:C:4:THR:H	1:C:7:LYS:HE3	1.62	0.64
2:B:327:PHE:CZ	2:B:367:LYS:HB2	2.33	0.63
1:C:4:THR:H	1:C:7:LYS:CE	2.11	0.62
2:B:351:LYS:O	2:B:352:LYS:HB2	1.98	0.62
2:D:314:TRP:CD1	4:D:529:NGA:H61	2.35	0.61
2:D:327:PHE:CZ	2:D:367:LYS:HB2	2.34	0.61
2:B:336:ASN:ND2	2:B:338:VAL:H	1.99	0.61
2:B:305:ASN:HD21	2:B:376:ASN:H	1.48	0.61
2:D:349:ARG:CG	2:D:349:ARG:HH11	2.14	0.60
1:C:6:CYS:SG	1:C:122:LYS:HB2	2.41	0.60
2:D:225:MET:CE	2:D:352:LYS:HE3	2.30	0.59
2:B:131:LEU:HD12	2:B:131:LEU:N	2.18	0.59
2:B:164:LYS:HG3	10:B:1395:HOH:O	2.03	0.58
1:A:10:HIS:O	1:A:13:LYS:HG2	2.03	0.57
2:B:191:ARG:NH1	2:B:194:HIS:HD2	2.02	0.57
2:B:272:HIS:HB3	2:B:334:ARG:HG2	1.87	0.57
1:C:13:LYS:HD3	1:C:23:LEU:CD1	2.35	0.57
2:B:336:ASN:HD22	2:B:336:ASN:C	2.08	0.56
2:B:191:ARG:HD2	2:B:194:HIS:CD2	2.42	0.54
1:C:84:GLU:HG3	10:C:1121:HOH:O	2.08	0.54
1:C:120:CYS:SG	1:C:122:LYS:HB2	2.47	0.54
1:C:58:ARG:HD2	1:C:59:PHE:CE2	2.42	0.54
2:B:279:LYS:HE2	4:B:404:NGA:H81	1.90	0.54
2:D:336:ASN:HD22	2:D:338:VAL:H	1.56	0.54
2:D:295:ALA:O	2:D:296:LEU:HD12	2.07	0.53
2:B:277:MET:CE	2:B:279:LYS:HD3	2.38	0.53
2:D:185:ILE:HD13	2:D:216:TYR:HB2	1.90	0.53
2:D:255:LEU:HD11	4:D:529:NGA:H81	1.90	0.52
1:A:68:GLU:HG2	1:A:68:GLU:O	2.10	0.52
2:B:336:ASN:ND2	2:B:339:ILE:H	2.07	0.52
1:A:108:LYS:HB3	1:A:109:PRO:HD3	1.90	0.52
2:B:277:MET:HE1	4:B:404:NGA:O7	2.10	0.52
2:B:277:MET:SD	4:B:404:NGA:O7	2.69	0.51
2:B:307:PHE:HB3	2:B:308:PRO:HD2	1.91	0.51
2:B:336:ASN:HD22	2:B:338:VAL:N	2.06	0.51
2:D:349:ARG:HD2	2:D:353:ASN:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:327:PHE:CE2	2:D:367:LYS:HD2	2.47	0.50
1:A:14:ASP:CG	1:A:14:ASP:O	2.48	0.50
1:A:116:GLU:OE1	1:A:119:ARG:NH2	2.45	0.50
1:C:9:SER:O	1:C:13:LYS:HG2	2.12	0.49
2:D:365:HIS:HD2	2:D:368:GLU:OE1	1.95	0.49
2:D:132:THR:CG2	2:D:133:ALA:N	2.74	0.49
2:B:289:TYR:OH	4:B:404:NGA:N2	2.46	0.49
2:B:310:ASN:HD22	2:B:402:SER:N	2.04	0.49
2:D:153:VAL:HG22	2:D:196:LYS:HB3	1.94	0.49
2:D:277:MET:HE1	4:D:529:NGA:O7	2.13	0.49
2:B:261:HIS:O	2:B:339:ILE:HD11	2.14	0.48
2:B:289:TYR:OH	4:B:404:NGA:C7	2.61	0.48
8:C:851:PG4:H11	3:D:530:BGC:O6	2.14	0.48
2:D:307:PHE:HB3	2:D:308:PRO:HD2	1.95	0.48
1:C:13:LYS:HD3	1:C:23:LEU:HD13	1.96	0.47
1:A:108:LYS:HB3	1:A:109:PRO:CD	2.44	0.47
1:C:66:PHE:HB2	10:C:1017:HOH:O	2.13	0.47
2:D:132:THR:HG22	2:D:133:ALA:N	2.28	0.47
2:B:191:ARG:HH11	2:B:194:HIS:CD2	2.23	0.47
3:D:530:BGC:O4	4:D:529:NGA:C1	2.62	0.47
2:B:191:ARG:NH1	2:B:194:HIS:CD2	2.83	0.46
2:D:237:LYS:HD2	10:D:1403:HOH:O	2.14	0.46
1:C:13:LYS:HD3	1:C:23:LEU:HD11	1.97	0.46
2:D:191:ARG:HH11	2:D:194:HIS:HD2	1.63	0.46
2:D:252:ASP:OD2	4:D:529:NGA:C8	2.62	0.46
2:B:336:ASN:ND2	2:B:336:ASN:C	2.69	0.46
2:B:230:LYS:HD3	2:B:398:ILE:HB	1.98	0.45
1:A:70:GLU:HG3	10:A:1402:HOH:O	2.16	0.45
2:B:279:LYS:HE3	2:B:280:PHE:CZ	2.51	0.45
1:C:49:GLU:OE1	9:C:806:MES:H52	2.16	0.45
2:D:314:TRP:NE1	4:D:529:NGA:H61	2.32	0.45
1:C:19:GLN:HG3	1:C:19:GLN:O	2.17	0.45
2:D:132:THR:HG22	2:D:133:ALA:O	2.17	0.45
2:B:155:LEU:O	2:B:159:GLU:HG3	2.16	0.45
2:B:336:ASN:HD21	2:B:339:ILE:H	1.63	0.45
1:C:10:HIS:HA	1:C:13:LYS:HE2	1.99	0.45
4:B:404:NGA:H83	7:B:406:UDP:PB	2.57	0.44
1:A:116:GLU:OE2	1:A:119:ARG:HD2	2.17	0.44
2:B:388:TYR:HB3	2:B:389:PRO:HD2	1.99	0.44
2:D:194:HIS:HE1	10:D:982:HOH:O	2.00	0.44
2:B:327:PHE:CE1	2:B:367:LYS:HB2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:403:BGC:O4	4:B:404:NGA:C1	2.65	0.44
2:B:261:HIS:C	2:B:339:ILE:HD11	2.38	0.44
1:C:121:GLU:O	1:C:122:LYS:C	2.56	0.44
2:D:171:TYR:HB3	2:D:213:TYR:CE2	2.52	0.44
2:B:277:MET:CE	4:B:404:NGA:O7	2.65	0.44
1:C:3:LEU:HA	1:C:7:LYS:HE3	2.00	0.44
2:D:318:ASP:OD1	2:D:318:ASP:N	2.50	0.43
1:A:12:ILE:O	1:A:15:ILE:HG22	2.18	0.43
2:D:292:GLY:HA2	4:D:529:NGA:H83	2.01	0.43
1:C:58:ARG:HB3	10:C:1261:HOH:O	2.18	0.43
2:B:167:LEU:HD13	2:B:387:ARG:HB3	2.00	0.42
2:D:289:TYR:OH	4:D:529:NGA:N2	2.52	0.42
1:A:103:TYR:CE2	9:A:805:MES:H51	2.54	0.42
2:B:359:ARG:O	2:B:363:ILE:HG23	2.20	0.42
1:A:65:GLU:CD	1:A:65:GLU:H	2.23	0.42
2:B:275:VAL:HG22	2:B:340:GLY:HA3	2.00	0.42
1:C:4:THR:H	1:C:7:LYS:HE2	1.83	0.41
1:C:18:TYR:O	1:C:19:GLN:HB3	2.20	0.41
2:B:368:GLU:HG2	2:B:368:GLU:H	1.66	0.41
2:B:318:ASP:OD1	2:B:318:ASP:N	2.50	0.41
2:D:252:ASP:HB3	7:D:528:UDP:O3'	2.21	0.41
2:B:356:ASN:HA	2:B:357:PRO:HD3	1.88	0.41
1:C:43:ASN:HD21	1:C:45:ASN:HA	1.86	0.41
1:C:4:THR:N	1:C:7:LYS:CE	2.81	0.41
2:B:351:LYS:O	2:B:352:LYS:CB	2.67	0.41
1:C:65:GLU:O	1:C:67:PRO:HD3	2.21	0.41
2:D:349:ARG:CG	2:D:349:ARG:NH1	2.82	0.40
2:B:171:TYR:HB3	2:B:213:TYR:CE2	2.56	0.40
2:B:270:PRO:HG2	2:B:325:LEU:HD22	2.03	0.40
2:B:154:ASP:OD1	2:B:156:LYS:HB2	2.22	0.40
1:C:10:HIS:HA	1:C:13:LYS:HG2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	118 (98%)	2 (2%)	1 (1%)	22	15
1	C	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	B	270/286 (94%)	265 (98%)	5 (2%)	0	100	100
2	D	270/286 (94%)	265 (98%)	5 (2%)	0	100	100
All	All	782/818 (96%)	763 (98%)	18 (2%)	1 (0%)	55	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN

### 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%)	39	36
1	C	109/109 (100%)	106 (97%)	3 (3%)	49	49
2	B	245/254 (96%)	233 (95%)	12 (5%)	29	24
2	D	245/254 (96%)	237 (97%)	8 (3%)	43	41
All	All	708/726 (98%)	681 (96%)	27 (4%)	38	35

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	71	ASN
1	A	85	LEU
1	A	88	ASP
2	B	131	LEU
2	B	141	LEU
2	B	157	LEU

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Mol	Chain	Res	Type
2	B	164	LYS
2	B	167	LEU
2	B	195	LEU
2	B	287	VAL
2	B	296	LEU
2	B	302	LEU
2	B	336	ASN
2	B	346	ARG
2	B	352	LYS
1	C	44	ASP
1	C	85	LEU
1	C	88	ASP
2	D	131	LEU
2	D	141	LEU
2	D	157	LEU
2	D	195	LEU
2	D	240	LEU
2	D	299	GLN
2	D	302	LEU
2	D	349	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
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
1	C	43	ASN
1	C	71	ASN
2	D	161	GLN
2	D	194	HIS
2	D	207	GLN
2	D	299	GLN
2	D	305	ASN
2	D	310	ASN
2	D	336	ASN
2	D	365	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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$
9	MES	A	805	-	12,12,12	1.48	3 (25%)	14,16,16	1.41	2 (14%)
8	PG4	A	850	-	12,12,12	0.40	0	11,11,11	0.46	0
3	BGC	B	403	-	12,12,12	0.37	0	17,17,17	0.48	0
4	NGA	B	404	-	14,14,15	2.45	5 (35%)	15,19,21	4.06	10 (66%)
7	UDP	B	406	6	21,26,26	2.09	7 (33%)	22,40,40	3.64	7 (31%)
9	MES	C	806	-	12,12,12	1.11	0	14,16,16	1.24	1 (7%)
8	PG4	C	851	-	12,12,12	0.48	0	11,11,11	0.37	0
7	UDP	D	528	6	21,26,26	2.21	8 (38%)	22,40,40	3.63	9 (40%)
4	NGA	D	529	-	14,14,15	2.47	5 (35%)	15,19,21	3.95	11 (73%)
3	BGC	D	530	-	12,12,12	0.44	0	17,17,17	0.37	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
9	MES	A	805	-	-	0/6/14/14	0/1/1/1
8	PG4	A	850	-	-	0/10/10/10	0/0/0/0
3	BGC	B	403	-	-	0/2/22/22	0/1/1/1
4	NGA	B	404	-	-	0/6/23/26	0/1/1/1
7	UDP	B	406	6	-	0/12/32/32	0/2/2/2
9	MES	C	806	-	-	0/6/14/14	0/1/1/1
8	PG4	C	851	-	-	0/10/10/10	0/0/0/0
7	UDP	D	528	6	-	0/12/32/32	0/2/2/2
4	NGA	D	529	-	-	0/6/23/26	0/1/1/1
3	BGC	D	530	-	-	0/2/22/22	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	529	NGA	O5-C1	-6.73	1.32	1.43
4	B	404	NGA	O5-C1	-5.05	1.35	1.43
7	D	528	UDP	C2'-C1'	-3.70	1.47	1.53
7	B	406	UDP	PB-O3A	-2.98	1.55	1.60
7	B	406	UDP	C2'-C1'	-2.85	1.49	1.53
7	D	528	UDP	PB-O3B	-2.83	1.43	1.54
4	D	529	NGA	O4-C4	-2.63	1.36	1.43
7	D	528	UDP	PB-O3A	-2.28	1.56	1.60
4	B	404	NGA	O4-C4	-2.26	1.37	1.43
7	B	406	UDP	C6-C5	-2.26	1.33	1.38
7	D	528	UDP	O5'-C5'	-2.11	1.36	1.44
7	D	528	UDP	PB-O1B	2.07	1.57	1.50
4	D	529	NGA	C4-C3	2.14	1.57	1.52
7	B	406	UDP	PB-O1B	2.16	1.58	1.50
9	A	805	MES	C3-N4	2.29	1.53	1.47
4	B	404	NGA	C8-C7	2.38	1.55	1.50
9	A	805	MES	C5-N4	2.47	1.53	1.47
4	D	529	NGA	C3-C2	2.54	1.58	1.52
9	A	805	MES	C7-N4	2.67	1.53	1.47
7	D	528	UDP	O4'-C1'	2.68	1.45	1.41
7	B	406	UDP	O4'-C1'	2.69	1.45	1.41
4	B	404	NGA	C2-N2	2.80	1.51	1.46
4	D	529	NGA	O5-C5	3.12	1.50	1.43
7	D	528	UDP	C6-N1	3.75	1.40	1.35
7	B	406	UDP	C4-N3	4.12	1.40	1.33
7	B	406	UDP	C6-N1	4.44	1.41	1.35
7	D	528	UDP	C4-N3	4.79	1.41	1.33
4	B	404	NGA	O5-C5	5.11	1.54	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	406	UDP	O4'-C4'-C3'	-4.43	96.37	105.17
7	D	528	UDP	O4'-C4'-C3'	-4.07	97.08	105.17
7	D	528	UDP	C5-C4-N3	-3.48	114.80	123.12
7	B	406	UDP	C5-C4-N3	-3.41	114.97	123.12
9	C	806	MES	O2S-S-C8	-3.33	103.93	106.79
4	B	404	NGA	O4-C4-C5	-3.14	101.37	109.28
7	D	528	UDP	O5'-PA-O1A	-3.13	96.61	109.25
7	B	406	UDP	O5'-PA-O1A	-2.89	97.60	109.25
9	A	805	MES	O2S-S-C8	-2.88	104.32	106.79
4	D	529	NGA	O3-C3-C4	-2.81	104.25	110.36
4	D	529	NGA	O4-C4-C5	-2.66	102.58	109.28
4	B	404	NGA	O3-C3-C4	-2.65	104.58	110.36
7	D	528	UDP	O3A-PB-O1B	-2.64	95.18	111.44
7	B	406	UDP	O3A-PB-O1B	-2.41	96.61	111.44
4	D	529	NGA	O7-C7-C8	-2.35	117.78	122.06
4	B	404	NGA	C4-C3-C2	2.09	114.08	111.02
7	D	528	UDP	O2B-PB-O1B	2.12	118.80	110.50
7	B	406	UDP	O2A-PA-O5'	2.20	118.52	108.14
7	D	528	UDP	C4'-O4'-C1'	2.29	112.21	109.77
4	D	529	NGA	O6-C6-C5	2.36	119.29	111.34
4	D	529	NGA	C8-C7-N2	2.42	120.48	116.11
4	B	404	NGA	C8-C7-N2	2.44	120.52	116.11
7	D	528	UDP	O3B-PB-O1B	2.56	120.52	110.50
4	D	529	NGA	C1-C2-N2	2.59	114.91	110.49
7	D	528	UDP	O2A-PA-O5'	2.73	121.04	108.14
7	B	406	UDP	O3B-PB-O1B	2.83	121.59	110.50
9	A	805	MES	O1S-S-C8	3.71	109.98	106.79
4	B	404	NGA	O3-C3-C2	3.86	117.66	109.39
4	D	529	NGA	O3-C3-C2	3.97	117.90	109.39
4	B	404	NGA	C1-O5-C5	5.24	119.39	112.17
4	B	404	NGA	C6-C5-C4	5.58	126.06	113.00
4	B	404	NGA	C2-N2-C7	5.99	131.69	122.94
4	D	529	NGA	C2-N2-C7	6.36	132.22	122.94
4	D	529	NGA	O5-C1-C2	6.62	120.69	111.47
4	D	529	NGA	C1-O5-C5	6.70	121.40	112.17
4	B	404	NGA	O5-C1-C2	6.73	120.84	111.47
4	D	529	NGA	C6-C5-C4	6.81	128.93	113.00
4	B	404	NGA	C1-C2-N2	7.77	123.76	110.49
7	D	528	UDP	C4-N3-C2	14.36	126.47	114.13
7	B	406	UDP	C4-N3-C2	14.54	126.62	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	805	MES	1	0
3	B	403	BGC	1	0
4	B	404	NGA	8	0
7	B	406	UDP	1	0
9	C	806	MES	1	0
8	C	851	PG4	1	0
7	D	528	UDP	2	0
4	D	529	NGA	10	0
3	D	530	BGC	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<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%)	-0.32	5 (4%) 38 38	20, 28, 51, 65	0
1	C	123/123 (100%)	-0.24	3 (2%) 59 59	18, 28, 49, 82	0
2	B	272/286 (95%)	-0.09	10 (3%) 42 43	21, 31, 50, 63	2 (0%)
2	D	272/286 (95%)	-0.11	8 (2%) 52 52	20, 29, 47, 62	2 (0%)
All	All	790/818 (96%)	-0.16	26 (3%) 47 47	18, 29, 50, 82	4 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	PRO	11.7
1	C	122	LYS	6.5
1	A	123	PRO	6.3
2	D	131	LEU	3.9
2	B	151	ILE	3.7
2	D	402	SER	3.7
2	B	131	LEU	3.5
2	D	132	THR	3.5
2	B	152	PRO	3.4
1	A	66	PHE	3.4
2	D	151	ILE	3.3
2	B	157	LEU	3.2
1	A	68	GLU	3.2
1	C	45	ASN	3.1
1	A	45	ASN	2.8
2	B	402	SER	2.7
2	B	174	MET	2.7
2	D	152	PRO	2.7
1	A	67	PRO	2.4
2	D	174	MET	2.3
2	B	150	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	157	LEU	2.1
2	B	293	VAL	2.1
2	B	291	GLY	2.1
2	D	184	ILE	2.0
2	B	132	THR	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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NGA	B	404	14/15	0.58	0.43	8.58	40,54,72,72	0
4	NGA	D	529	14/15	0.75	0.35	5.33	31,53,72,72	0
8	PG4	C	851	13/13	0.78	0.21	5.13	44,49,57,59	0
9	MES	A	805	12/12	0.89	0.19	2.98	52,55,61,61	0
8	PG4	A	850	13/13	0.86	0.20	2.80	45,46,53,55	0
9	MES	C	806	12/12	0.77	0.23	2.72	54,56,65,65	0
3	BGC	B	403	12/12	0.93	0.15	0.21	42,45,48,48	0
7	UDP	B	406	25/25	0.96	0.13	0.05	25,28,37,61	0
7	UDP	D	528	25/25	0.96	0.10	-0.49	21,24,30,32	0
5	CA	A	124	1/1	0.99	0.07	-1.04	23,23,23,23	0
3	BGC	D	530	12/12	0.95	0.08	-1.23	27,32,33,35	0
5	CA	C	526	1/1	0.98	0.06	-1.41	27,27,27,27	0
6	MN	B	405	1/1	0.99	0.09	-	28,28,28,28	0
6	MN	D	527	1/1	0.99	0.09	-	27,27,27,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.