



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:52 AM GMT

PDB ID : 2BZD  
Title : GALACTOSE RECOGNITION BY THE CARBOHYDRATE-BINDING  
MODULE OF A BACTERIAL SIALIDASE.  
Authors : Newstead, S.L.; Taylor, G.  
Deposited on : 2005-08-16  
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 (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

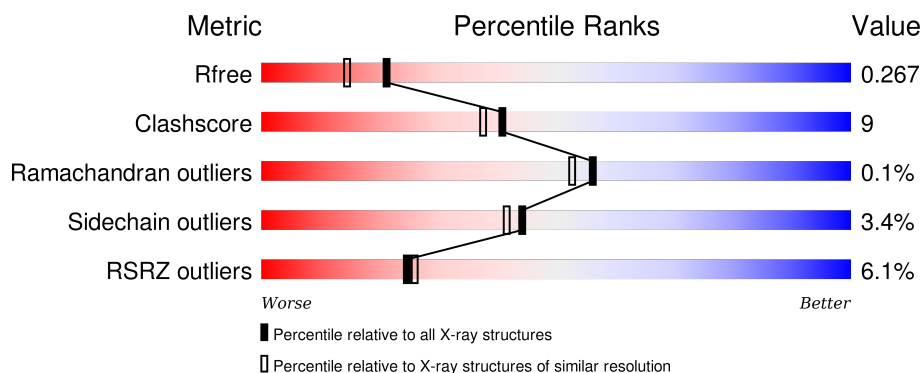
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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	601	<div> <div>14%</div> <div>72%</div> <div>27%</div> </div>
1	B	601	<div> <div>3%</div> <div>89%</div> <div>10%</div> </div>
1	C	601	<div> <div>%</div> <div>88%</div> <div>11%</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
3	GAL	A	1649	-	-	-	X
4	GOL	A	1650	-	-	X	-
4	GOL	C	1650	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15216 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 BACTERIAL SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	5	0
			4552	2820	823	901	8			
1	B	601	Total	C	N	O	S	0	12	0
			4573	2832	825	909	7			
1	C	600	Total	C	N	O	S	0	3	0
			4538	2814	818	897	9			

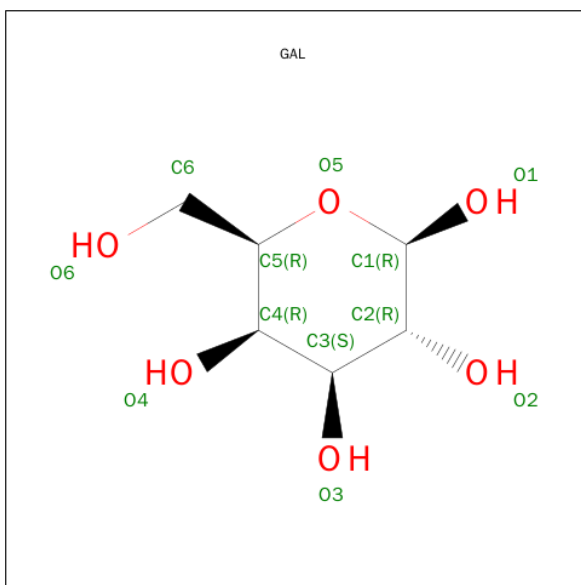
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	ALA	GLU	ENGINEERED MUTATION	UNP Q02834
B	260	ALA	GLU	ENGINEERED MUTATION	UNP Q02834
C	260	ALA	GLU	ENGINEERED MUTATION	UNP Q02834

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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

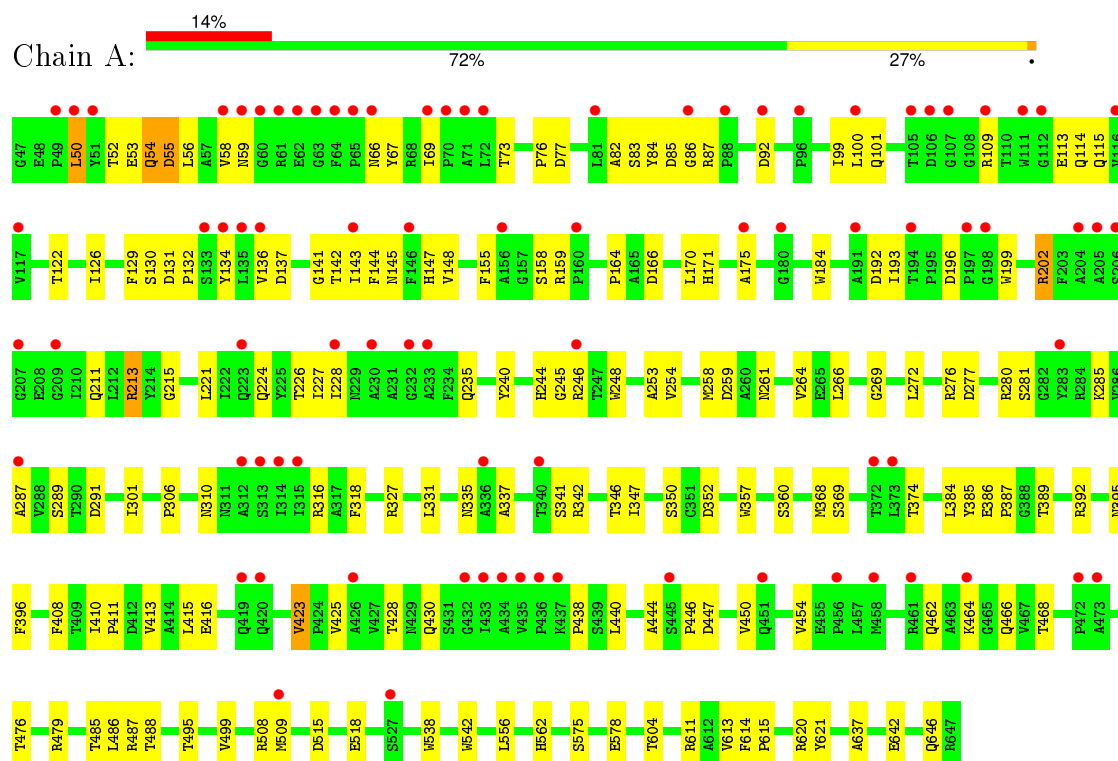
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	361	Total	O		0	0
			361	361			
5	B	488	Total	O		0	0
			488	488			
5	C	647	Total	O		0	0
			647	647			

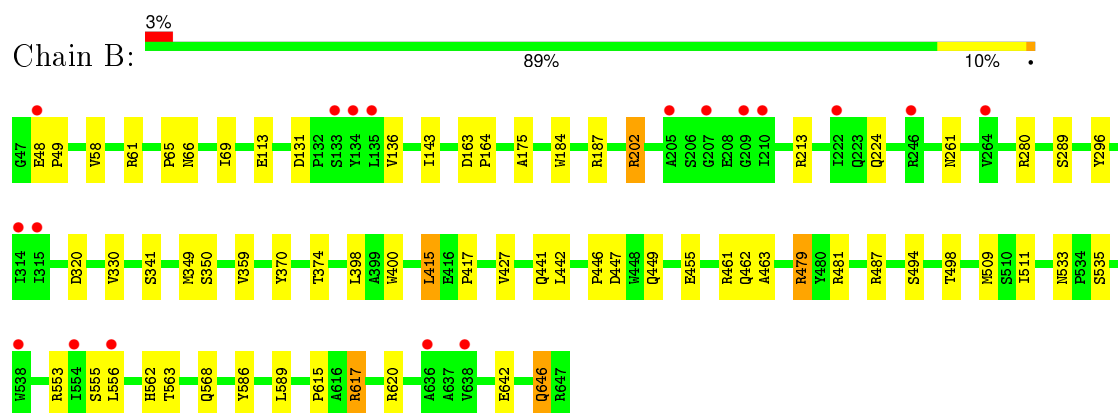
### 3 Residue-property plots [i](#)

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.

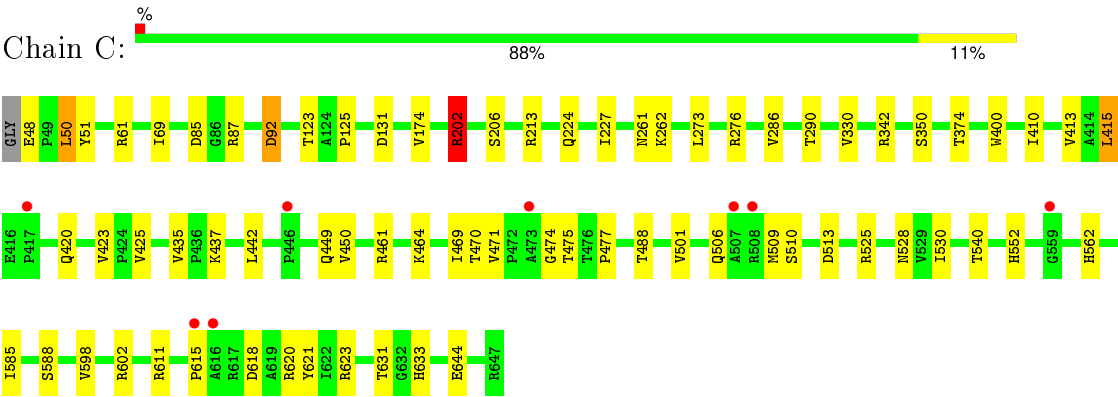
#### • Molecule 1: BACTERIAL SIALIDASE



#### • Molecule 1: BACTERIAL SIALIDASE



#### • Molecule 1: BACTERIAL SIALIDASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.46Å 141.46Å 158.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.17 – 2.00 30.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (122.17-2.00) 98.0 (30.15-2.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.193 , 0.267 0.195 , 0.267	Depositor DCC
$R_{free}$ test set	6102 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.7	EDS
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 121364 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, 0.375 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: GOL, GAL, NA

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	0.68	1/4682 (0.0%)	0.74	0/6392
1	B	0.70	0/4732	0.77	1/6460 (0.0%)
1	C	0.85	1/4657 (0.0%)	0.86	5/6360 (0.1%)
All	All	0.75	2/14071 (0.0%)	0.79	6/19212 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	THR	C-O	5.78	1.34	1.23
1	C	174	VAL	CB-CG2	5.57	1.64	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ASP	CB-CG-OD1	9.90	127.21	118.30
1	C	202	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	B	589	LEU	CA-CB-CG	-6.75	99.78	115.30
1	C	202	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	C	87	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	C	85	ASP	CB-CG-OD2	-5.13	113.69	118.30

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	4552	0	4368	134	0
1	B	4573	0	4382	49	0
1	C	4538	0	4365	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	12	0	12	0	0
4	A	6	0	8	6	0
4	B	6	0	8	1	0
4	C	6	0	8	4	0
5	A	361	0	0	51	0
5	B	488	0	0	10	1
5	C	647	0	0	16	3
All	All	15216	0	13175	232	3

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509[A]:MET:HE1	1:B:556[A]:LEU:HD13	1.15	1.12
1:C:413[A]:VAL:HG11	1:C:423:VAL:HG11	1.20	1.11
1:B:509[A]:MET:CE	1:B:556[A]:LEU:HD13	1.79	1.11
1:A:192:ASP:HB2	5:A:2149:HOH:O	1.52	1.07
1:B:509[A]:MET:HE1	1:B:556[A]:LEU:CD1	2.00	0.91
1:B:224:GLN:HE21	1:B:261:ASN:ND2	1.69	0.89
1:C:413[A]:VAL:HG11	1:C:423:VAL:CG1	2.04	0.88
1:A:259:ASP:HB3	1:A:276:ARG:HG2	1.59	0.85
1:A:509[B]:MET:CE	1:A:556:LEU:HD13	2.07	0.85
1:C:123:THR:HG22	5:C:2155:HOH:O	1.78	0.82
1:A:508:ARG:HG2	5:A:2130:HOH:O	1.79	0.81
1:B:224:GLN:HE21	1:B:261:ASN:HD21	1.29	0.79
1:B:509[A]:MET:CE	1:B:556[A]:LEU:CD1	2.57	0.78
1:A:509[B]:MET:HE1	1:A:556:LEU:HD13	1.67	0.77
1:A:253:ALA:HB1	5:A:2136:HOH:O	1.84	0.77
1:A:276:ARG:HH12	4:A:1650:GOL:H11	1.49	0.76
1:A:411:PRO:HD2	1:A:423:VAL:HG23	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ARG:NH1	4:C:1650:GOL:O3	2.13	0.75
1:A:213:ARG:HG3	5:A:2167:HOH:O	1.88	0.73
4:A:1650:GOL:H2	5:A:2361:HOH:O	1.89	0.72
1:B:479:ARG:CG	1:B:479:ARG:HH11	2.01	0.72
1:A:137:ASP:HB2	5:A:2052:HOH:O	1.89	0.71
1:A:446:PRO:HB3	5:C:2485:HOH:O	1.88	0.71
1:A:487:ARG:HB3	5:A:2274:HOH:O	1.91	0.70
1:A:136:VAL:HG22	5:A:2050:HOH:O	1.91	0.70
1:B:417:PRO:HG3	5:B:2336:HOH:O	1.90	0.70
1:B:441:GLN:OE1	1:B:487:ARG:NH1	2.26	0.68
1:B:113:GLU:HG3	5:B:2061:HOH:O	1.93	0.68
1:A:509[B]:MET:HE2	1:A:556:LEU:HD13	1.75	0.67
1:A:310:ASN:HB3	5:A:2188:HOH:O	1.93	0.67
1:A:285:LYS:HD2	5:A:2156:HOH:O	1.94	0.66
1:C:69:ILE:HG21	1:C:131:ASP:HA	1.77	0.66
1:A:352:ASP:HB3	1:A:430:GLN:HE22	1.60	0.66
1:A:221:LEU:HD22	5:A:2052:HOH:O	1.96	0.65
1:A:415:LEU:HD21	1:A:499:VAL:HG13	1.79	0.64
1:B:562:HIS:HE1	5:B:2399:HOH:O	1.79	0.64
1:C:413[A]:VAL:CG1	1:C:423:VAL:HG11	2.13	0.63
1:C:213:ARG:NH2	5:C:2283:HOH:O	2.32	0.63
1:C:415:LEU:HD11	1:C:471:VAL:HG21	1.81	0.63
1:C:224:GLN:HE21	1:C:261:ASN:HD21	1.47	0.63
1:A:59:ASN:HB2	5:A:2013:HOH:O	1.99	0.63
1:C:509[A]:MET:HE3	1:C:530:ILE:HG21	1.80	0.63
1:A:69:ILE:HG21	1:A:131:ASP:HA	1.81	0.62
1:A:306:PRO:HB2	5:A:2210:HOH:O	1.99	0.62
1:A:53:GLU:HG2	1:A:392:ARG:HD3	1.81	0.61
1:A:52:THR:HG22	1:A:395:ASN:HB3	1.83	0.61
1:A:113:GLU:HG3	1:A:115:GLN:HG3	1.83	0.60
1:C:224:GLN:HE21	1:C:261:ASN:ND2	1.99	0.60
1:A:509[B]:MET:HE1	1:A:556:LEU:CD1	2.32	0.59
1:A:410:ILE:HG12	1:A:425:VAL:HG22	1.85	0.59
1:A:416:GLU:HG3	1:A:646[B]:GLN:HE22	1.68	0.59
1:A:428:THR:HG23	1:A:462:GLN:HE21	1.67	0.59
1:A:277:ASP:HA	5:A:2156:HOH:O	2.01	0.59
1:A:276:ARG:HH22	4:A:1650:GOL:C1	2.16	0.59
1:A:92[B]:ASP:HB2	5:A:2048:HOH:O	2.02	0.59
1:A:342:ARG:HH22	4:A:1650:GOL:H12	1.68	0.59
1:A:196:ASP:HB2	5:A:2109:HOH:O	2.02	0.59
1:A:411:PRO:HD2	1:A:423:VAL:CG2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG23	5:A:2194:HOH:O	2.03	0.58
1:A:387:PRO:HG3	1:A:392:ARG:HB2	1.86	0.57
1:C:435:VAL:HG11	1:C:488:THR:HB	1.86	0.57
1:B:646:GLN:HB3	5:B:2480:HOH:O	2.04	0.57
1:B:479:ARG:HG3	1:B:479:ARG:HH11	1.68	0.56
1:A:276:ARG:HH12	4:A:1650:GOL:C1	2.15	0.56
1:A:137:ASP:O	1:A:141:GLY:N	2.38	0.56
1:C:631:THR:OG1	1:C:633:HIS:CE1	2.58	0.56
1:A:316:ARG:HD3	5:A:2166:HOH:O	2.05	0.56
1:A:82:ALA:O	1:A:101:GLN:HA	2.06	0.56
1:A:76:PRO:HA	5:A:2054:HOH:O	2.06	0.56
1:A:136:VAL:CG2	5:A:2050:HOH:O	2.49	0.55
1:B:479:ARG:CG	1:B:479:ARG:NH1	2.67	0.55
1:C:342:ARG:HH22	4:C:1650:GOL:C3	2.19	0.55
1:A:277:ASP:OD2	1:A:281:SER:HB3	2.06	0.55
1:C:123:THR:CG2	5:C:2158:HOH:O	2.55	0.54
1:B:479:ARG:NH1	1:B:479:ARG:HG3	2.21	0.54
1:B:49:PRO:HB3	1:B:400:TRP:HA	1.89	0.54
1:C:125:PRO:HB2	5:C:2161:HOH:O	2.06	0.54
1:A:272:LEU:HD12	1:A:287:ALA:O	2.08	0.54
1:A:253:ALA:CB	5:A:2136:HOH:O	2.50	0.54
1:A:144:PHE:CZ	1:A:245:GLY:HA3	2.43	0.54
1:C:509[A]:MET:CE	1:C:530:ILE:CG2	2.86	0.54
1:A:509[B]:MET:CE	1:A:556:LEU:CD1	2.82	0.54
1:A:202:ARG:HD3	5:A:2105:HOH:O	2.07	0.54
1:B:69:ILE:HG21	1:B:131:ASP:HA	1.90	0.53
1:B:479:ARG:HD3	1:B:498:THR:HG21	1.91	0.53
1:B:187:ARG:HG2	5:B:2114:HOH:O	2.10	0.52
1:A:142:THR:HB	5:A:2060:HOH:O	2.10	0.52
1:A:143:ILE:HG12	5:A:2089:HOH:O	2.10	0.52
1:A:538:TRP:O	1:A:637:ALA:HA	2.10	0.52
1:A:562:HIS:HE1	5:A:2311:HOH:O	1.92	0.51
1:A:84:TYR:HA	1:A:132:PRO:HG3	1.93	0.51
1:B:58:VAL:HB	1:B:61:ARG:HD2	1.93	0.51
1:A:416:GLU:HG3	1:A:646[B]:GLN:NE2	2.25	0.51
1:C:342:ARG:HH22	4:C:1650:GOL:H32	1.75	0.50
1:A:211:GLN:HG3	1:A:221:LEU:HD23	1.92	0.50
1:A:83:SER:HB2	1:A:134:TYR:CZ	2.47	0.50
1:A:73:THR:HG21	5:A:2050:HOH:O	2.12	0.50
1:A:155:PHE:HA	5:A:2113:HOH:O	2.11	0.50
1:B:646:GLN:HG2	5:B:2482:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:VAL:O	1:B:462:GLN:HG3	2.12	0.50
1:A:244:HIS:CE1	5:A:2144:HOH:O	2.63	0.50
1:A:199:TRP:CZ2	1:A:253:ALA:HB2	2.47	0.49
1:A:347:ILE:O	1:A:360:SER:HA	2.11	0.49
1:B:615:PRO:O	1:B:617[B]:ARG:HD2	2.12	0.49
1:A:142:THR:CB	5:A:2060:HOH:O	2.59	0.49
1:A:266:LEU:HA	5:A:2166:HOH:O	2.13	0.49
1:B:447:ASP:N	1:B:447:ASP:OD1	2.41	0.49
1:B:553:ARG:HB2	5:B:2395:HOH:O	2.11	0.49
1:A:341:SER:HB3	5:A:2214:HOH:O	2.13	0.49
1:C:213:ARG:HD2	5:C:2401:HOH:O	2.13	0.49
1:A:92[A]:ASP:HB3	5:A:2048:HOH:O	2.11	0.49
1:B:370:TYR:OH	4:B:1650:GOL:H12	2.13	0.49
1:A:224:GLN:HE21	1:A:261:ASN:ND2	2.11	0.48
1:A:87:ARG:NH1	1:A:92[A]:ASP:OD1	2.44	0.48
1:C:420:GLN:HG3	1:C:470:THR:OG1	2.13	0.48
1:C:562:HIS:HE1	5:C:2577:HOH:O	1.96	0.48
1:C:513:ASP:OD2	1:C:623:ARG:NH2	2.43	0.48
1:A:269:GLY:O	5:A:2170:HOH:O	2.20	0.48
1:B:449[A]:GLN:HE22	1:C:602:ARG:HD3	1.78	0.48
1:A:613:VAL:HG23	1:C:290:THR:HB	1.94	0.48
1:B:330:VAL:HA	1:B:350:SER:O	2.14	0.48
1:A:170:LEU:HD23	1:A:202:ARG:O	2.13	0.48
1:A:620:ARG:HG2	1:A:621:TYR:CE2	2.49	0.47
1:C:123:THR:HG21	5:C:2158:HOH:O	2.14	0.47
1:B:461:ARG:NE	5:B:2329:HOH:O	2.48	0.47
1:B:136:VAL:HG22	1:B:143:ILE:HG12	1.97	0.47
1:C:330:VAL:HA	1:C:350:SER:O	2.15	0.47
1:A:337:ALA:HB2	1:A:346:THR:HB	1.97	0.47
1:C:202:ARG:HD3	5:C:2260:HOH:O	2.14	0.47
1:A:440:LEU:HD12	1:A:485:THR:O	2.15	0.47
1:B:463:ALA:HB2	5:B:2328:HOH:O	2.14	0.47
1:A:408:PHE:CE2	1:A:486:LEU:HB2	2.49	0.47
1:A:518:GLU:HG2	1:A:542:TRP:NE1	2.30	0.46
1:A:350:SER:HB2	1:A:357:TRP:CE3	2.50	0.46
1:A:192:ASP:CB	5:A:2149:HOH:O	2.34	0.46
1:A:144:PHE:HZ	1:A:245:GLY:HA3	1.78	0.46
1:A:69:ILE:HG22	1:A:132:PRO:HD2	1.97	0.46
1:A:184:TRP:HD1	5:A:2093:HOH:O	1.99	0.46
1:A:276:ARG:HH22	4:A:1650:GOL:H12	1.81	0.46
1:A:384:LEU:HD12	1:A:392:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:THR:HG23	1:A:611:ARG:NH1	2.31	0.46
1:C:509[A]:MET:HE1	1:C:530:ILE:HG22	1.97	0.46
1:A:368:MET:HG2	1:A:385:TYR:CD1	2.51	0.46
1:B:415:LEU:C	1:B:415:LEU:HD12	2.36	0.46
1:C:588:SER:HB3	1:C:621:TYR:HB2	1.98	0.45
1:C:450:VAL:HG22	1:C:469:ILE:HG23	1.98	0.45
1:A:444:ALA:HB3	1:A:450:VAL:HG21	1.98	0.45
1:A:310:ASN:ND2	1:A:369:SER:O	2.48	0.45
1:B:511:ILE:HD13	1:B:556[B]:LEU:HD12	1.98	0.45
1:A:337:ALA:C	5:A:2210:HOH:O	2.54	0.45
1:C:509[A]:MET:CE	1:C:530:ILE:HG22	2.47	0.45
1:A:55:ASP:HA	1:A:392:ARG:HA	1.99	0.44
1:A:479:ARG:HD2	1:A:642:GLU:OE2	2.17	0.44
1:A:100:LEU:HD12	5:A:2026:HOH:O	2.16	0.44
1:A:143:ILE:HG23	5:A:2050:HOH:O	2.16	0.44
1:A:276:ARG:NH1	5:A:2231:HOH:O	2.48	0.44
1:A:175:ALA:HB1	1:A:184:TRP:CE3	2.53	0.44
1:A:86:GLY:CA	5:A:2026:HOH:O	2.65	0.44
1:C:50:LEU:HD22	5:C:2244:HOH:O	2.17	0.44
1:A:227:ILE:HD12	1:A:228:ILE:C	2.38	0.44
1:B:620:ARG:HG2	1:B:620:ARG:O	2.18	0.44
1:A:277:ASP:OD2	1:A:281:SER:CB	2.65	0.44
1:B:533:ASN:OD1	1:B:535[B]:SER:OG	2.33	0.44
1:A:193:ILE:HG23	5:A:2149:HOH:O	2.18	0.44
1:C:540:THR:HG21	1:C:552:HIS:CG	2.53	0.43
1:C:92:ASP:HB3	5:C:2088:HOH:O	2.17	0.43
1:C:50:LEU:HB2	5:C:2006:HOH:O	2.18	0.43
1:C:206:SER:O	1:C:262:LYS:HE2	2.18	0.43
1:C:611:ARG:NE	1:C:644:GLU:OE2	2.40	0.43
1:A:408:PHE:CE1	1:A:495:THR:HG22	2.52	0.43
1:B:65:PRO:HG2	1:B:66[B]:ASN:HD22	1.83	0.43
1:B:349:MET:HB3	1:B:359:VAL:HB	2.00	0.43
1:A:235:GLN:HB2	5:A:2136:HOH:O	2.18	0.43
1:B:289:SER:HB2	1:B:296:TYR:CD1	2.53	0.43
1:A:50:LEU:O	1:A:396:PHE:HA	2.18	0.43
1:A:199:TRP:CD1	1:A:227:ILE:HD13	2.53	0.43
1:A:306:PRO:HG2	5:A:2210:HOH:O	2.19	0.43
1:A:85:ASP:OD2	1:A:130:SER:HB2	2.19	0.43
1:A:215:GLY:HA3	5:A:2046:HOH:O	2.18	0.43
1:C:51:TYR:HB2	1:C:400:TRP:CD1	2.53	0.43
1:A:331:LEU:HD21	5:A:2166:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:HG21	1:A:259:ASP:HA	2.01	0.42
4:C:1650:GOL:H2	5:C:2646:HOH:O	2.18	0.42
1:A:246:ARG:HG3	5:A:2145:HOH:O	2.19	0.42
1:A:615:PRO:HG3	5:C:2372:HOH:O	2.19	0.42
1:A:59:ASN:OD1	1:A:67:TYR:N	2.47	0.42
1:A:100:LEU:HD13	1:A:114:GLN:HG2	2.02	0.42
1:A:129:PHE:HA	1:A:148:VAL:O	2.19	0.42
1:C:525:ARG:O	1:C:528:ASN:HB2	2.19	0.42
1:C:506:GLN:HA	1:C:509[A]:MET:HE2	2.01	0.42
1:B:202:ARG:HD3	5:B:2135:HOH:O	2.19	0.42
1:A:221:LEU:O	1:A:240:TYR:HA	2.20	0.42
1:B:398:LEU:HA	1:B:398:LEU:HD23	1.85	0.42
1:C:477:PRO:HA	1:C:501:VAL:O	2.20	0.42
1:A:438:PRO:HG2	1:A:454:VAL:HG13	2.02	0.42
1:C:615:PRO:HD3	5:C:2340:HOH:O	2.19	0.42
1:B:163:ASP:HA	1:B:164:PRO:HD3	1.93	0.41
1:C:202:ARG:HB3	1:C:227:ILE:HG22	2.02	0.41
1:B:568:GLN:HB2	1:B:642:GLU:HB2	2.02	0.41
1:C:585:ILE:HG22	1:C:598:VAL:HG22	2.02	0.41
1:A:54:GLN:HB3	1:A:54:GLN:HE21	1.75	0.41
1:A:254:VAL:HG23	5:A:2179:HOH:O	2.19	0.41
1:A:575:SER:HG	1:A:578:GLU:CD	2.24	0.41
1:A:202:ARG:NH2	5:A:2076:HOH:O	2.50	0.41
1:C:273:LEU:O	1:C:286:VAL:HA	2.20	0.41
1:B:563:THR:HB	1:B:646:GLN:HG3	2.03	0.41
1:C:562:HIS:CE1	5:C:2577:HOH:O	2.71	0.41
1:A:58:VAL:HA	1:A:389:THR:O	2.20	0.41
1:C:506:GLN:HG2	1:C:509[A]:MET:HE1	2.03	0.41
1:A:56:LEU:HD12	1:A:384:LEU:HD11	2.02	0.41
1:B:415:LEU:O	1:B:415:LEU:HD12	2.21	0.41
1:B:509[A]:MET:HE3	1:B:556[A]:LEU:CD1	2.47	0.41
1:A:369:SER:HB2	1:A:386:GLU:HB2	2.02	0.41
1:A:66:ASN:OD1	1:A:87:ARG:HD2	2.20	0.41
1:A:158:SER:HB2	5:A:2113:HOH:O	2.21	0.41
1:B:213:ARG:NH1	1:B:320:ASP:OD1	2.52	0.41
1:A:248:TRP:HB2	5:A:2149:HOH:O	2.21	0.41
1:A:99:ILE:HG13	1:A:147:HIS:CG	2.56	0.41
1:A:258:MET:O	1:A:259:ASP:HB2	2.21	0.40
1:A:83:SER:HB2	1:A:134:TYR:CE1	2.56	0.40
1:B:175:ALA:HB1	1:B:184:TRP:HB3	2.03	0.40
1:B:586:TYR:CD2	1:B:586:TYR:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:CB	5:A:2081:HOH:O	2.69	0.40
1:A:289:SER:OG	1:A:291:ASP:OD1	2.40	0.40
1:A:318:PHE:CE1	1:A:327:ARG:NH2	2.89	0.40
1:A:614:PHE:O	1:A:615:PRO:C	2.59	0.40
1:C:474:GLY:O	1:C:475:THR:C	2.59	0.40
1:C:410:ILE:HG12	1:C:425:VAL:HG22	2.04	0.40
1:A:145:ASN:OD1	1:A:145:ASN:C	2.59	0.40
1:A:604:THR:HG1	1:A:604:THR:H	1.55	0.40
1:A:164:PRO:HA	1:A:171:HIS:CE1	2.56	0.40
1:B:479:ARG:HG2	1:B:479:ARG:HH11	1.80	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2155:HOH:O	5:C:2155:HOH:O[4_555]	1.90	0.30
5:C:2247:HOH:O	5:C:2247:HOH:O[6_555]	2.05	0.15
5:B:2427:HOH:O	5:C:2025:HOH:O[5_555]	2.09	0.11

## 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	604/601 (100%)	565 (94%)	39 (6%)	0	100	100
1	B	611/601 (102%)	596 (98%)	14 (2%)	1 (0%)	52	48
1	C	601/601 (100%)	582 (97%)	19 (3%)	0	100	100
All	All	1816/1803 (101%)	1743 (96%)	72 (4%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	446	PRO

### 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	481/476 (101%)	460 (96%)	21 (4%)	35	30
1	B	488/476 (102%)	472 (97%)	16 (3%)	45	43
1	C	479/476 (101%)	465 (97%)	14 (3%)	50	49
All	All	1448/1428 (101%)	1397 (96%)	51 (4%)	44	40

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

Mol	Chain	Res	Type
1	A	50	LEU
1	A	54	GLN
1	A	55	ASP
1	A	77	ASP
1	A	109	ARG
1	A	122	THR
1	A	126	ILE
1	A	159	ARG
1	A	202	ARG
1	A	213	ARG
1	A	280	ARG
1	A	301	ILE
1	A	335	ASN
1	A	374	THR
1	A	413	VAL
1	A	423	VAL
1	A	447	ASP
1	A	464	LYS
1	A	466	GLN
1	A	488	THR
1	A	515	ASP
1	B	48	GLU

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Mol	Chain	Res	Type
1	B	202	ARG
1	B	280	ARG
1	B	341[A]	SER
1	B	341[B]	SER
1	B	374	THR
1	B	415	LEU
1	B	442	LEU
1	B	455	GLU
1	B	479	ARG
1	B	481	ARG
1	B	494	SER
1	B	555	SER
1	B	617[A]	ARG
1	B	617[B]	ARG
1	B	646	GLN
1	C	48	GLU
1	C	50	LEU
1	C	61	ARG
1	C	202	ARG
1	C	374	THR
1	C	415	LEU
1	C	437	LYS
1	C	442	LEU
1	C	449	GLN
1	C	461	ARG
1	C	464	LYS
1	C	510	SER
1	C	618	ASP
1	C	620	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	261	ASN
1	A	395	ASN
1	A	430	GLN
1	A	462	GLN
1	A	466	GLN
1	A	562	HIS
1	B	261	ASN
1	B	451	GLN

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Mol	Chain	Res	Type
1	B	462	GLN
1	B	562	HIS
1	B	573	GLN
1	C	261	ASN
1	C	344	GLN
1	C	395	ASN
1	C	441	GLN
1	C	562	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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GAL	A	1649	-	12,12,12	0.63	0	17,17,17	0.69	0
4	GOL	A	1650	-	5,5,5	0.82	0	5,5,5	0.80	0
3	GAL	B	1649	-	12,12,12	0.66	0	17,17,17	0.86	1 (5%)
4	GOL	B	1650	-	5,5,5	0.85	0	5,5,5	0.83	0
3	GAL	C	1649	-	12,12,12	0.45	0	17,17,17	1.32	2 (11%)
4	GOL	C	1650	-	5,5,5	0.66	0	5,5,5	0.79	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
3	GAL	A	1649	-	-	0/2/22/22	0/1/1/1
4	GOL	A	1650	-	-	0/4/4/4	0/0/0/0
3	GAL	B	1649	-	-	0/2/22/22	0/1/1/1
4	GOL	B	1650	-	-	0/4/4/4	0/0/0/0
3	GAL	C	1649	-	-	0/2/22/22	0/1/1/1
4	GOL	C	1650	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1649	GAL	C4-C3-C2	2.21	114.91	110.79
3	B	1649	GAL	O5-C5-C6	2.23	111.99	106.36
3	C	1649	GAL	C1-C2-C3	2.66	114.38	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1650	GOL	6	0
4	B	1650	GOL	1	0
4	C	1650	GOL	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, 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	601/601 (100%)	0.89	84 (13%) 4 4	8, 18, 25, 28	7 (1%)
1	B	601/601 (100%)	0.09	18 (2%) 54 55	11, 17, 21, 28	11 (1%)
1	C	600/601 (99%)	-0.39	8 (1%) 79 80	2, 13, 31, 39	4 (0%)
All	All	1802/1803 (99%)	0.20	110 (6%) 25 26	2, 17, 26, 39	22 (1%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458[A]	MET	6.3
1	A	116	VAL	5.0
1	A	509[A]	MET	5.0
1	A	461	ARG	4.8
1	A	61	ARG	4.5
1	A	62	GLU	4.4
1	A	230	ALA	4.0
1	A	527	SER	3.9
1	A	65	PRO	3.9
1	A	58	VAL	3.8
1	A	435	VAL	3.8
1	A	51	TYR	3.7
1	C	559	GLY	3.7
1	A	86	GLY	3.6
1	A	473	ALA	3.6
1	A	107	GLY	3.6
1	A	50	LEU	3.5
1	A	207	GLY	3.5
1	A	436	PRO	3.4
1	A	205	ALA	3.4
1	A	88	PRO	3.4
1	A	133	SER	3.4
1	A	60	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	210	ILE	3.3
1	A	372	THR	3.3
1	C	446	PRO	3.3
1	A	134	TYR	3.2
1	A	228	ILE	3.2
1	A	373	LEU	3.2
1	A	464	LYS	3.2
1	A	456	PRO	3.1
1	A	433	ILE	3.1
1	A	106	ASP	3.1
1	A	246	ARG	3.1
1	A	81	LEU	3.1
1	B	207	GLY	3.0
1	B	209	GLY	3.0
1	A	432	GLY	3.0
1	A	156	ALA	2.9
1	A	314	ILE	2.9
1	A	49	PRO	2.9
1	A	340	THR	2.9
1	B	135	LEU	2.9
1	A	109	ARG	2.9
1	C	508	ARG	2.8
1	B	205	ALA	2.8
1	A	64	PHE	2.8
1	A	232	GLY	2.8
1	A	135	LEU	2.7
1	A	312	ALA	2.7
1	A	72	LEU	2.7
1	A	160	PRO	2.7
1	A	420	GLN	2.7
1	A	136	VAL	2.7
1	A	71	ALA	2.7
1	A	180	GLY	2.7
1	C	616	ALA	2.6
1	A	233	ALA	2.6
1	B	554	ILE	2.6
1	A	426	ALA	2.6
1	A	63	GLY	2.6
1	C	473	ALA	2.6
1	A	283	TYR	2.5
1	A	191	ALA	2.5
1	C	507	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	70	PRO	2.5
1	B	48	GLU	2.5
1	B	538	TRP	2.5
1	A	66	ASN	2.4
1	A	315	ILE	2.4
1	A	96	PRO	2.4
1	B	133	SER	2.4
1	A	204	ALA	2.4
1	A	206	SER	2.4
1	A	445	SER	2.4
1	A	194	THR	2.3
1	A	59	ASN	2.3
1	A	287	ALA	2.3
1	A	472	PRO	2.3
1	A	105	THR	2.3
1	A	100	LEU	2.3
1	A	198	GLY	2.3
1	A	69	ILE	2.3
1	B	314	ILE	2.3
1	A	434	ALA	2.3
1	B	264	VAL	2.2
1	A	313	SER	2.2
1	B	636	ALA	2.2
1	C	615	PRO	2.2
1	A	143	ILE	2.2
1	A	111	TRP	2.2
1	A	419	GLN	2.2
1	B	134	TYR	2.2
1	A	209	GLY	2.2
1	B	556[A]	LEU	2.2
1	A	451	GLN	2.2
1	B	246	ARG	2.2
1	A	146	PHE	2.2
1	A	175	ALA	2.1
1	B	222	ILE	2.1
1	B	315	ILE	2.1
1	A	197	PRO	2.1
1	A	336	ALA	2.1
1	A	117	VAL	2.1
1	A	437	LYS	2.1
1	A	92[A]	ASP	2.0
1	B	638	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	417	PRO	2.0
1	A	223	GLN	2.0
1	A	112	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, 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
3	GAL	A	1649	12/12	0.85	0.18	5.08	58,60,61,61	0
3	GAL	C	1649	12/12	0.89	0.15	1.69	35,40,43,44	0
4	GOL	C	1650	6/6	0.88	0.15	1.53	27,34,35,36	0
3	GAL	B	1649	12/12	0.88	0.15	1.34	21,26,30,31	0
2	NA	A	1648	1/1	0.99	0.06	-2.20	20,20,20,20	0
2	NA	B	1648	1/1	0.98	0.05	-2.87	8,8,8,8	0
2	NA	C	1648	1/1	0.97	0.06	-3.11	16,16,16,16	0
4	GOL	A	1650	6/6	0.83	0.15	-	30,32,36,37	0
4	GOL	B	1650	6/6	0.92	0.12	-	16,23,24,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.