



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:30 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 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/ValidationPDFNotes.html>

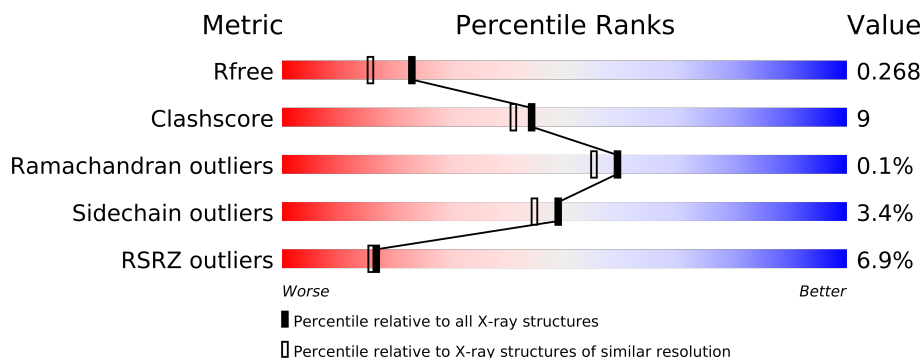
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	601	
1	B	601	
1	C	601	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GAL	A	1649	-	X
3	GAL	C	1649	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15216 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

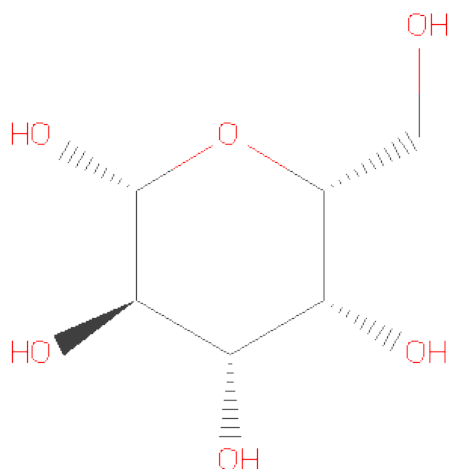
There are 3 discrepancies between the modelled and reference sequences:

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).

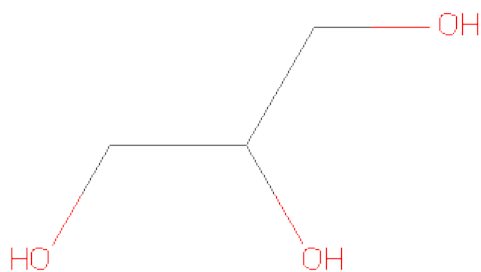
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: C₆H₁₂O₆).



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		

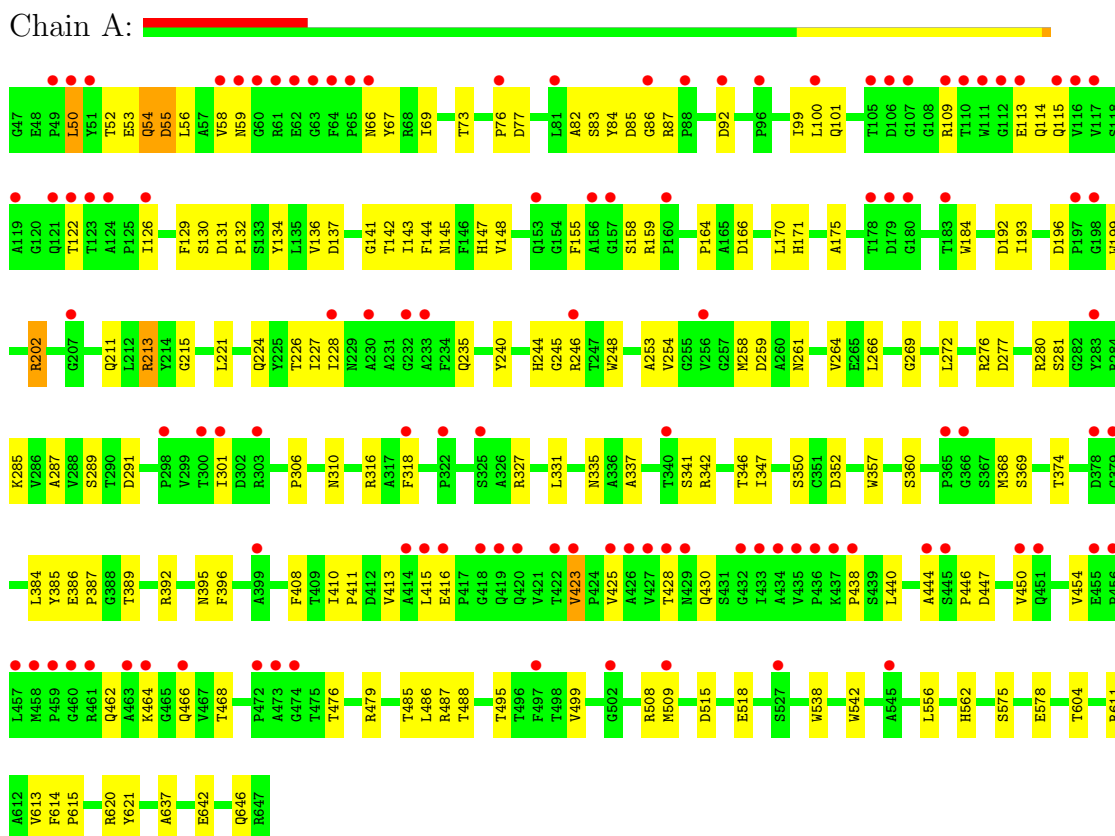
- Molecule 5 is water.

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		

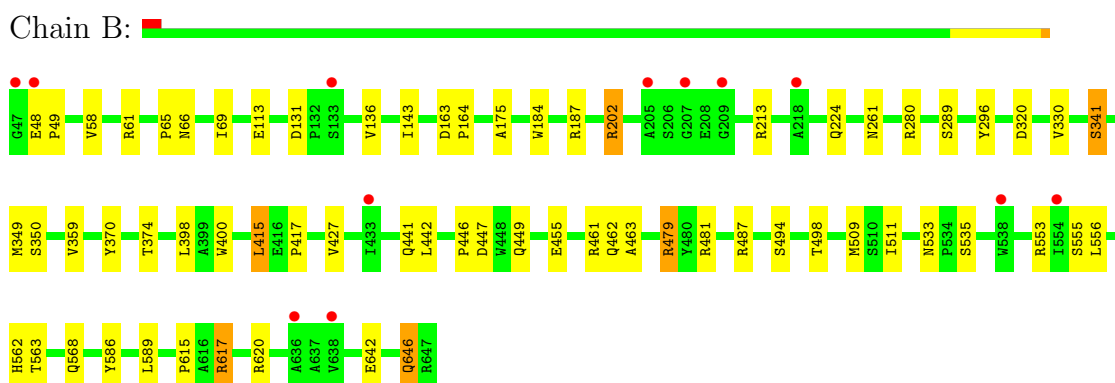
3 Residue-property plots

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.

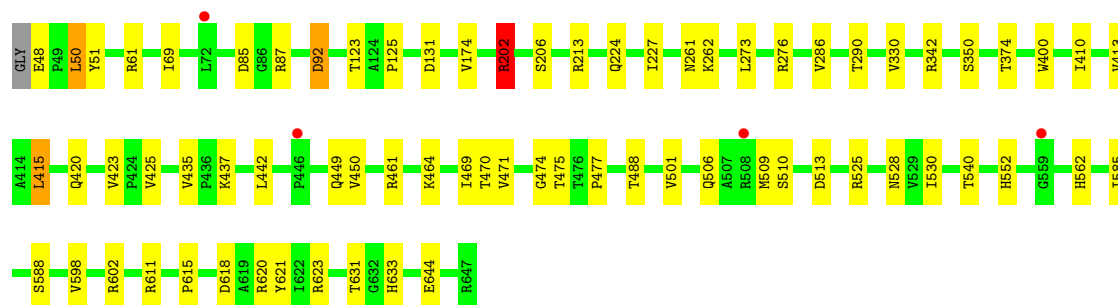
• Molecule 1: BACTERIAL SIALIDASE



• Molecule 1: BACTERIAL SIALIDASE



● Molecule 1: BACTERIAL SIALIDASE

Chain C: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 97.9 (30.15-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.193 , 0.267 0.197 , 0.268	Depositor DCC
R_{free} test set	6102 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.4	EDS
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 121364 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15216	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4552	0	4368	134	0
1	B	4573	0	4382	49	1
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	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (232) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:A:264:VAL:HG23	5:A:2194:HOH:O	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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 (4) 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	Distance(Å)	Clash(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
1:B:341[B]:SER:CB	1:B:449[B]:GLN:NE2[5_555]	2.08	0.12
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%)	56	51
1	C	601/601 (100%)	582 (97%)	19 (3%)	0	100	100
All	All	1816/1803 (101%)	1743 (96%)	72 (4%)	1 (0%)	59	55

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%)	39	32
1	B	488/476 (102%)	472 (97%)	16 (3%)	50	46
1	C	479/476 (101%)	465 (97%)	14 (3%)	55	52
All	All	1448/1428 (101%)	1397 (96%)	51 (4%)	49	43

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
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

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Mol	Chain	Res	Type
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
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 ⓘ

There are no RNA chains 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 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	0.62	0	17,17,17	0.67	0
4	GOL	A	1650	-	5,5,5	0.77	0	5,5,5	0.82	0
3	GAL	B	1649	-	12,12,12	0.65	0	17,17,17	0.86	1 (5%)
4	GOL	B	1650	-	5,5,5	0.78	0	5,5,5	0.72	0
3	GAL	C	1649	-	12,12,12	0.45	0	17,17,17	1.31	2 (11%)
4	GOL	C	1650	-	5,5,5	0.61	0	5,5,5	0.80	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	C1-C2-C3	2.43	114.38	110.53
3	B	1649	GAL	O5-C5-C6	2.30	111.99	106.34
3	C	1649	GAL	C4-C3-C2	2.22	114.91	110.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	601/601 (100%)	1.01	109 (18%) 2 2	8, 18, 25, 28	7 (1%)
1	B	601/601 (100%)	0.07	12 (1%) 62 62	11, 17, 21, 28	11 (1%)
1	C	600/601 (99%)	-0.02	4 (0%) 84 85	2, 13, 31, 39	4 (0%)
All	All	1802/1803 (99%)	0.35	125 (6%) 17 16	2, 17, 26, 39	22 (1%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458[A]	MET	6.8
1	A	116	VAL	5.4
1	A	473	ALA	5.2
1	A	230	ALA	4.7
1	A	61	ARG	4.6
1	A	434	ALA	4.6
1	A	461	ARG	4.4
1	A	86	GLY	4.4
1	A	60	GLY	4.3
1	A	340	THR	4.2
1	A	456	PRO	4.1
1	A	232	GLY	4.1
1	A	105	THR	4.0
1	A	62	GLU	4.0
1	A	433	ILE	3.9
1	A	418	GLY	3.9
1	A	457	LEU	3.8
1	A	436	PRO	3.7
1	A	423	VAL	3.7
1	A	464	LYS	3.6
1	A	58	VAL	3.6
1	A	460	GLY	3.6
1	A	435	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	432	GLY	3.5
1	A	88	PRO	3.5
1	A	228	ILE	3.4
1	A	420	GLN	3.4
1	A	198	GLY	3.3
1	A	49	PRO	3.3
1	A	119	ALA	3.3
1	A	65	PRO	3.3
1	A	122	THR	3.3
1	A	180	GLY	3.3
1	A	81	LEU	3.3
1	A	474	GLY	3.2
1	A	451	GLN	3.2
1	A	450	VAL	3.2
1	A	123	THR	3.2
1	A	109	ARG	3.2
1	A	51	TYR	3.1
1	A	106	ASP	3.1
1	A	426	ALA	3.1
1	A	126	ILE	3.1
1	A	64	PHE	3.0
1	A	156	ALA	3.0
1	A	63	GLY	3.0
1	A	509[A]	MET	3.0
1	A	301	ILE	2.9
1	A	197	PRO	2.9
1	A	463	ALA	2.9
1	A	545	ALA	2.9
1	A	76	PRO	2.9
1	A	66	ASN	2.9
1	A	425	VAL	2.8
1	A	59	ASN	2.8
1	A	107	GLY	2.8
1	A	283	TYR	2.8
1	A	50	LEU	2.8
1	A	419	GLN	2.8
1	A	428	THR	2.8
1	A	415	LEU	2.8
1	C	559	GLY	2.8
1	A	399	ALA	2.7
1	C	446	PRO	2.7
1	A	183	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	325	SER	2.7
1	A	445	SER	2.6
1	A	111	TRP	2.6
1	A	246	ARG	2.6
1	A	497	PHE	2.6
1	A	437	LYS	2.5
1	A	466	GLN	2.5
1	A	121	GLN	2.5
1	A	160	PRO	2.4
1	A	366	GLY	2.4
1	B	133	SER	2.4
1	B	205	ALA	2.4
1	A	178	THR	2.4
1	A	300	THR	2.4
1	A	455	GLU	2.4
1	B	638	VAL	2.4
1	B	433	ILE	2.4
1	A	427	VAL	2.4
1	A	112	GLY	2.3
1	A	115	GLN	2.3
1	A	378	ASP	2.3
1	A	207	GLY	2.3
1	A	256	VAL	2.3
1	B	48	GLU	2.3
1	A	110	THR	2.3
1	A	303	ARG	2.3
1	A	157	GLY	2.3
1	A	422	THR	2.3
1	B	636	ALA	2.3
1	A	298	PRO	2.3
1	A	429	ASN	2.3
1	A	472	PRO	2.3
1	A	379	GLY	2.3
1	A	233	ALA	2.2
1	A	322	PRO	2.2
1	A	502	GLY	2.2
1	B	47	GLY	2.2
1	A	527	SER	2.2
1	A	459	PRO	2.2
1	A	444	ALA	2.2
1	A	92[A]	ASP	2.2
1	B	538	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	100	LEU	2.2
1	A	414	ALA	2.1
1	C	508	ARG	2.1
1	B	207	GLY	2.1
1	B	209	GLY	2.1
1	C	72	LEU	2.1
1	A	318	PHE	2.1
1	A	124	ALA	2.0
1	A	117	VAL	2.0
1	A	113	GLU	2.0
1	B	218	ALA	2.0
1	A	96	PRO	2.0
1	A	416	GLU	2.0
1	A	179	ASP	2.0
1	A	365	PRO	2.0
1	A	438	PRO	2.0
1	A	153	GLN	2.0
1	B	554	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GAL	A	1649	12/12	0.21	9.97	58,60,61,61	0
3	GAL	C	1649	12/12	0.19	4.46	35,40,43,44	0
3	GAL	B	1649	12/12	0.16	1.76	21,26,30,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	B	1650	6/6	0.15	1.71	16,23,24,26	0
4	GOL	C	1650	6/6	0.17	1.20	27,34,35,36	0
4	GOL	A	1650	6/6	0.19	0.51	30,32,36,37	0
2	NA	A	1648	1/1	0.13	0.17	20,20,20,20	0
2	NA	B	1648	1/1	0.08	-1.74	8,8,8,8	0
2	NA	C	1648	1/1	0.06	-2.94	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.