



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:59 PM UTC

PDB ID : 2BZD / pdb_00002bzd
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

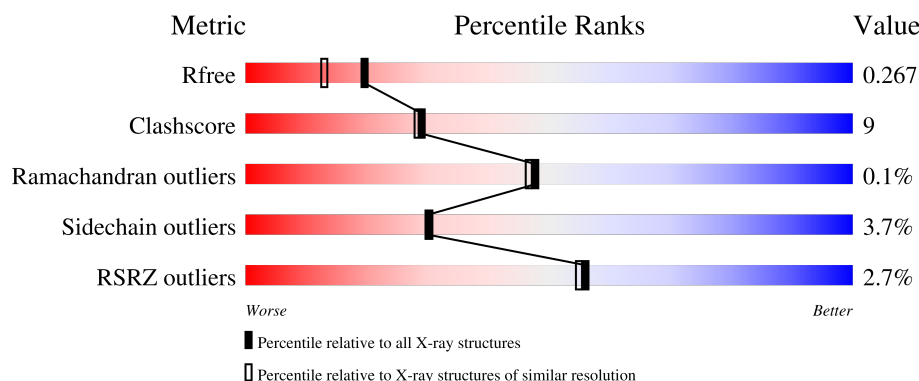
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	7% 72% 26% .
1	B	601	88% 11% .
1	C	601	87% 12% .

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
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			

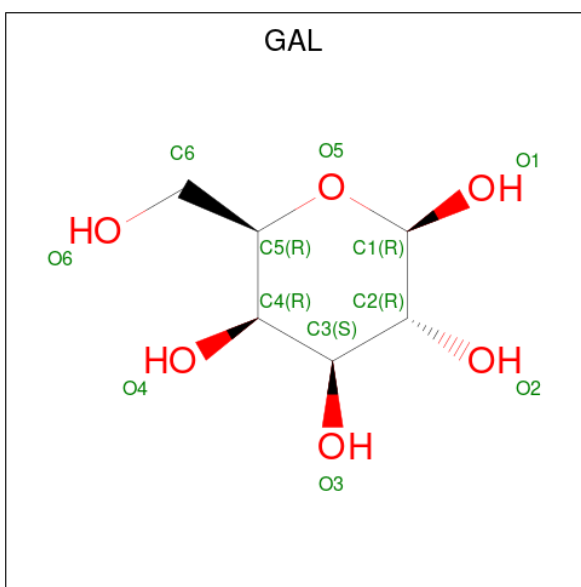
There are 3 discrepancies between the modelled and reference sequences:

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 (CCD ID: NA) (formula: Na).

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

- Molecule 3 is beta-D-galactopyranose (CCD ID: 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 (CCD ID: 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		

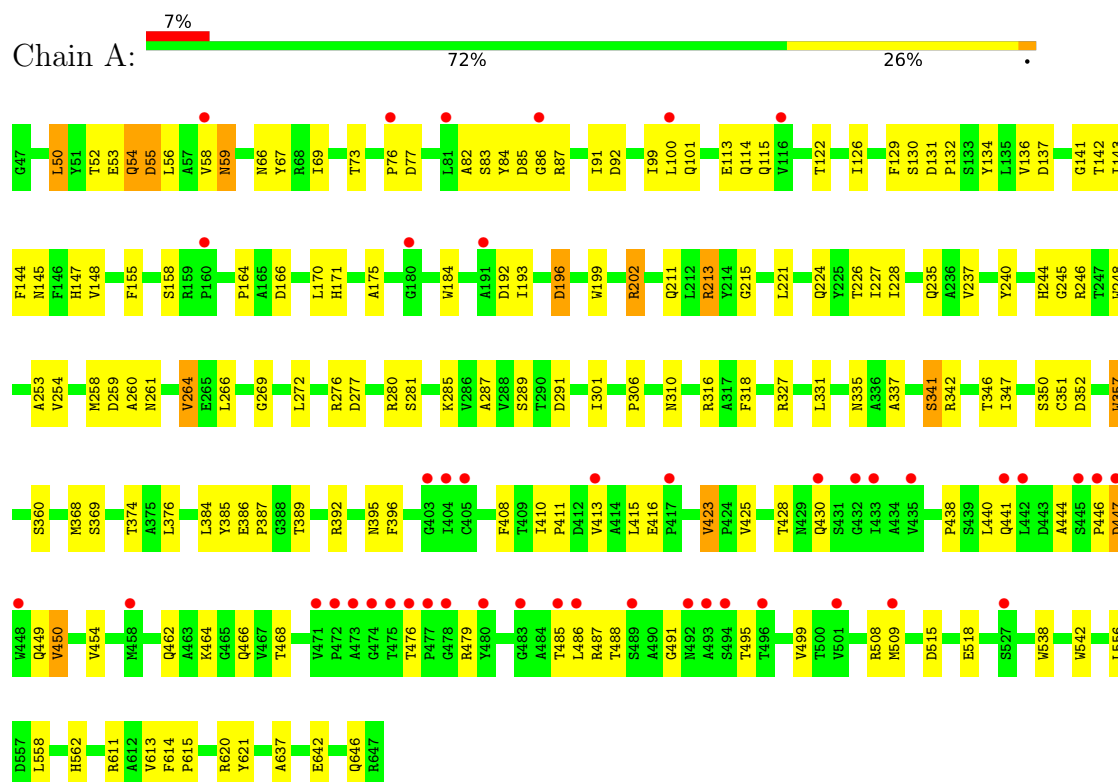
- Molecule 5 is water.

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		

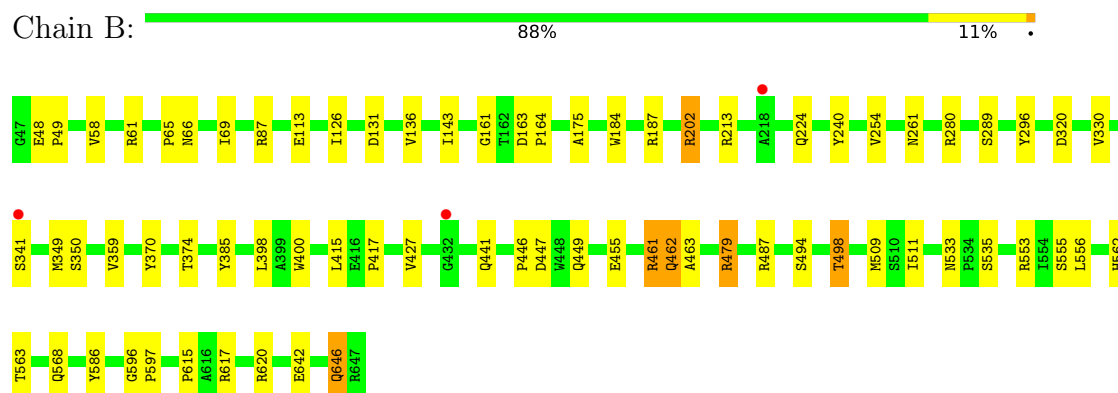
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: BACTERIAL SIALIDASE



• Molecule 1: BACTERIAL SIALIDASE



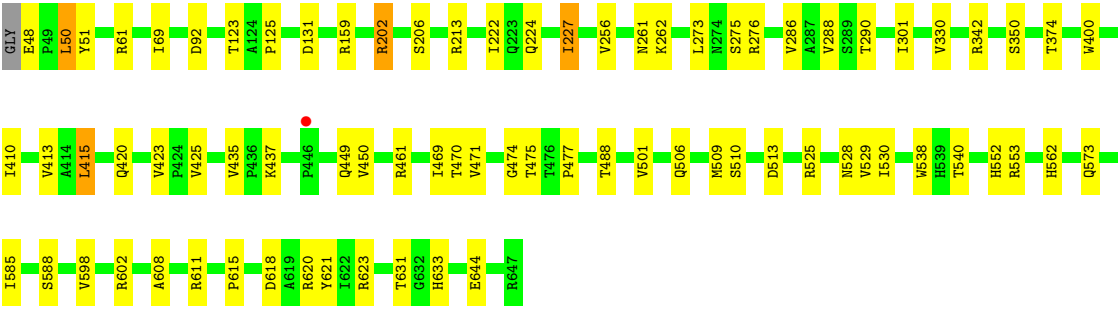
• Molecule 1: BACTERIAL SIALIDASE

Chain C:

87%

12%

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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 – 2.00 122.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (122.17-2.00) 97.9 (122.17-2.00)	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 0.195 , 0.267	Depositor DCC
R_{free} test set	6102 reflections (4.92%)	wwPDB-VP
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 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	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.

²Theoretical 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: NA, GOL, GAL

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	0.90	2/4682 (0.0%)	0.99	10/6392 (0.2%)
1	B	0.92	2/4732 (0.0%)	1.00	6/6460 (0.1%)
1	C	1.07	0/4657	1.05	9/6360 (0.1%)
All	All	0.96	4/14071 (0.0%)	1.02	25/19212 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	THR	C-O	8.83	1.34	1.23
1	B	126	ILE	CA-CB	5.14	1.59	1.54
1	B	254	VAL	CA-CB	5.08	1.61	1.54
1	A	264	VAL	CA-CB	5.05	1.61	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ASP	CA-C-N	7.47	127.18	119.56
1	A	196	ASP	C-N-CA	7.47	127.18	119.56
1	B	161	GLY	N-CA-C	-7.04	104.39	111.85
1	C	573	GLN	N-CA-C	6.55	118.50	111.36
1	A	357	TRP	CA-C-N	6.45	126.38	119.28
1	A	357	TRP	C-N-CA	6.45	126.38	119.28
1	B	87	ARG	CA-C-N	6.19	126.08	119.28
1	B	87	ARG	C-N-CA	6.19	126.08	119.28
1	A	341	SER	N-CA-C	5.79	118.50	109.52
1	A	491	GLY	N-CA-C	5.73	119.90	112.68
1	A	237	VAL	N-CA-C	5.62	115.77	108.35
1	B	240	TYR	N-CA-C	5.58	117.67	109.24
1	A	447	ASP	N-CA-C	5.54	118.83	112.57
1	C	538	TRP	N-CA-C	-5.46	102.19	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	LEU	N-CA-C	5.46	116.95	110.07
1	A	59	ASN	N-CA-C	5.26	122.01	110.80
1	C	608	ALA	CA-C-N	5.11	125.40	119.93
1	C	608	ALA	C-N-CA	5.11	125.40	119.93
1	C	222	ILE	N-CA-C	5.09	115.31	107.77
1	B	461	ARG	N-CA-C	5.09	117.40	109.52
1	B	385	TYR	N-CA-C	5.06	116.68	109.14
1	C	159	ARG	CA-C-N	-5.05	114.52	119.92
1	C	159	ARG	C-N-CA	-5.05	114.52	119.92
1	C	275	SER	N-CA-C	5.05	117.80	109.72
1	C	256	VAL	N-CA-C	-5.05	101.33	108.65

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	4552	0	4368	135	0
1	B	4573	0	4382	51	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	235	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 (235) 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	1.19	1.16
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	1.91	1.00
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: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
1:C:276:ARG:NH1	4:C:1650:GOL:O3	2.13	0.75
1:A:509[B]:MET:HE2	1:A:556:LEU:HD13	1.68	0.73
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:509[A]:MET:CE	1:B:556[A]:LEU:CD1	2.57	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:A:509[B]:MET:HE1	1:A:556:LEU:HD13	1.74	0.69
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLN:HE21	1:C:261:ASN:HD21	1.47	0.63
1:C:415:LEU:HD11	1:C:471:VAL:HG21	1.81	0.63
1:A:59:ASN:HB2	5:A:2013:HOH:O	1.99	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:C:509[A]:MET:HE3	1:C:530:ILE:HG21	1.82	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: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:92[B]:ASP:HB2	5:A:2048:HOH:O	2.02	0.59
1:A:276:ARG:HH22	4:A:1650:GOL:C1	2.16	0.59
1:A:196:ASP:HB2	5:A:2109:HOH:O	2.02	0.59
1:A:342:ARG:HH22	4:A:1650:GOL:H12	1.68	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
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:HH11	1:B:479:ARG:HG3	1.68	0.56
1:A:137:ASP:O	1:A:141:GLY:N	2.38	0.56
1:A:276:ARG:HH12	4:A:1650:GOL:C1	2.15	0.56
1:A:316:ARG:HD3	5:A:2166:HOH:O	2.05	0.56
1:C:631:THR:OG1	1:C:633:HIS:CE1	2.58	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:A:277:ASP:OD2	1:A:281:SER:HB3	2.06	0.55
1:C:342:ARG:HH22	4:C:1650:GOL:C3	2.19	0.55
1:A:509[B]:MET:HE1	1:A:556:LEU:CD1	2.37	0.55
1:B:479:ARG:HG3	1:B:479:ARG:NH1	2.21	0.54
1:C:123:THR:CG2	5:C:2158:HOH:O	2.55	0.54
1:B:49:PRO:HB3	1:B:400:TRP:HA	1.89	0.54
1:A:272:LEU:HD12	1:A:287:ALA:O	2.08	0.54
1:C:125:PRO:HB2	5:C:2161:HOH:O	2.06	0.54
1:A:144:PHE:CZ	1:A:245:GLY:HA3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ALA:CB	5:A:2136:HOH:O	2.50	0.54
1:C:509[A]:MET:CE	1:C:530:ILE:CG2	2.86	0.54
1:A:202:ARG:HD3	5:A:2105:HOH:O	2.07	0.54
1:A:509[B]:MET:CE	1:A:556:LEU:CD1	2.82	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:A:142:THR:HB	5:A:2060:HOH:O	2.10	0.52
1:B:187:ARG:HG2	5:B:2114: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:A:337:ALA:C	5:A:2210:HOH:O	2.54	0.50
1:B:415:LEU:HD12	1:B:415:LEU:C	2.36	0.50
1:C:342:ARG:HH22	4:C:1650:GOL:H32	1.75	0.50
1:A:83:SER:HB2	1:A:134:TYR:CZ	2.47	0.50
1:A:211:GLN:HG3	1:A:221:LEU:HD23	1.92	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:A:244:HIS:CE1	5:A:2144:HOH:O	2.63	0.50
1:B:427:VAL:O	1:B:462:GLN:HG3	2.12	0.50
1:B:646:GLN:HG2	5:B:2482:HOH:O	2.11	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:OD1	1:B:447:ASP:N	2.41	0.49
1:A:341:SER:HB3	5:A:2214:HOH:O	2.13	0.49
1:B:553:ARG:HB2	5:B:2395:HOH:O	2.11	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:C:509[A]:MET:HE1	1:C:530:ILE:HG22	1.95	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:A:227:ILE:HD12	1:A:228:ILE:C	2.38	0.48
1:C:420:GLN:HG3	1:C:470:THR:OG1	2.13	0.48
1:C:513:ASP:OD2	1:C:623:ARG:NH2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:HIS:HE1	5:C:2577:HOH:O	1.96	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:B:136:VAL:HG22	1:B:143:ILE:HG12	1.97	0.47
1:B:461:ARG:NE	5:B:2329:HOH:O	2.48	0.47
1:C:123:THR:HG21	5:C:2158:HOH:O	2.14	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:A:408:PHE:CE2	1:A:486:LEU:HB2	2.49	0.47
1:B:463:ALA:HB2	5:B:2328:HOH:O	2.14	0.47
1:A:350:SER:HB2	1:A:357:TRP:CE3	2.50	0.46
1:A:518:GLU:HG2	1:A:542:TRP:NE1	2.30	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:C:506:GLN:HA	1:C:509[A]:MET:HE2	1.98	0.46
1:A:476:THR:HG23	1:A:611:ARG:NH1	2.31	0.46
1:A:368:MET:HG2	1:A:385:TYR:CD1	2.51	0.46
1:C:450:VAL:HG22	1:C:469:ILE:HG23	1.98	0.45
1:C:588:SER:HB3	1:C:621:TYR:HB2	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:A:614:PHE:O	1:A:615:PRO:C	2.59	0.45
1:C:474:GLY:O	1:C:475:THR:C	2.59	0.45
1:B:511:ILE:HD13	1:B:556[B]:LEU:HD12	1.98	0.45
1:A:145:ASN:C	1:A:145:ASN:OD1	2.59	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:100:LEU:HD12	5:A:2026:HOH:O	2.16	0.44
1:A:479:ARG:HD2	1:A:642:GLU:OE2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:620:ARG:O	1:B:620:ARG:HG2	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:509[A]:MET:CE	1:C:530:ILE:HG21	2.46	0.43
1:C:92:ASP:HB3	5:C:2088:HOH:O	2.17	0.43
1:C:540:THR:HG21	1:C:552:HIS:CG	2.53	0.43
1:A:259:ASP:O	1:A:260:ALA:C	2.62	0.43
1:B:596:GLY:CA	1:B:597:PRO:C	2.91	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:50:LEU:O	1:A:396:PHE:HA	2.18	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:199:TRP:CD1	1:A:227:ILE:HD13	2.53	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:A:306:PRO:HG2	5:A:2210:HOH:O	2.19	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:B:509[A]:MET:HE2	1:B:556[A]:LEU:HD13	1.89	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: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:HD23	1:B:398:LEU:HA	1.85	0.42
1:B:415:LEU:C	1:B:415:LEU:CD1	2.93	0.42
1:C:477:PRO:HA	1:C:501:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:87:ARG:HH12	1:A:92[A]:ASP:CG	2.28	0.41
1:A:509[B]:MET:HE3	1:A:558:LEU:HD23	2.02	0.41
1:B:568:GLN:HB2	1:B:642:GLU:HB2	2.02	0.41
1:C:202:ARG:HB3	1:C:227:ILE:HG22	2.02	0.41
1:C:585:ILE:HG22	1:C:598:VAL:HG22	2.02	0.41
1:A:54:GLN:HE21	1:A:54:GLN:HB3	1.75	0.41
1:A:254:VAL:HG23	5:A:2179:HOH:O	2.19	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:A:58:VAL:HA	1:A:389:THR:O	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:56:LEU:HD12	1:A:384:LEU:HD11	2.02	0.41
1:B:415:LEU:HD12	1:B:415:LEU:O	2.21	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:A:369:SER:HB2	1:A:386:GLU:HB2	2.02	0.41
1:B:213:ARG:NH1	1:B:320:ASP:OD1	2.52	0.41
1:A:99:ILE:HG13	1:A:147:HIS:CG	2.56	0.41
1:A:248:TRP:HB2	5:A:2149:HOH:O	2.21	0.41
1:A:83:SER:HB2	1:A:134:TYR:CE1	2.56	0.40
1:A:166:ASP:CB	5:A:2081:HOH:O	2.69	0.40
1:A:258:MET:O	1:A:259:ASP:HB2	2.21	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: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:C:410:ILE:HG12	1:C:425:VAL:HG22	2.04	0.40
1:A:164:PRO:HA	1:A:171:HIS:CE1	2.56	0.40
1:B:479:ARG:HH11	1:B:479:ARG:HG2	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%)	43	42
1	C	601/601 (100%)	582 (97%)	19 (3%)	0	100	100
All	All	1816/1803 (101%)	1743 (96%)	72 (4%)	1 (0%)	48	46

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%)	457 (95%)	24 (5%)	22	20
1	B	488/476 (102%)	475 (97%)	13 (3%)	39	42
1	C	479/476 (101%)	462 (96%)	17 (4%)	32	32
All	All	1448/1428 (101%)	1394 (96%)	54 (4%)	30	30

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	54	GLN

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Mol	Chain	Res	Type
1	A	55	ASP
1	A	77	ASP
1	A	91	ILE
1	A	122	THR
1	A	126	ILE
1	A	202	ARG
1	A	213	ARG
1	A	280	ARG
1	A	301	ILE
1	A	335	ASN
1	A	351	CYS
1	A	374	THR
1	A	413	VAL
1	A	423	VAL
1	A	441	GLN
1	A	447	ASP
1	A	449	GLN
1	A	450	VAL
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	455	GLU
1	B	462	GLN
1	B	479	ARG
1	B	494	SER
1	B	498	THR
1	B	555	SER
1	B	646	GLN
1	C	48	GLU
1	C	50	LEU
1	C	61	ARG
1	C	202	ARG
1	C	227	ILE
1	C	288	VAL
1	C	301	ILE

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Mol	Chain	Res	Type
1	C	374	THR
1	C	415	LEU
1	C	437	LYS
1	C	449	GLN
1	C	461	ARG
1	C	510	SER
1	C	529	VAL
1	C	553	ARG
1	C	618	ASP
1	C	620	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	211	GLN
1	A	224	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	114	GLN
1	B	173	ASN
1	B	261	ASN
1	B	355	GLN
1	B	395	ASN
1	B	462	GLN
1	B	562	HIS
1	B	573	GLN
1	B	630	GLN
1	C	66	ASN
1	C	151	GLN
1	C	217	HIS
1	C	223	GLN
1	C	224	GLN
1	C	261	ASN
1	C	344	GLN
1	C	355	GLN
1	C	395	ASN
1	C	441	GLN

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Mol	Chain	Res	Type
1	C	449	GLN
1	C	562	HIS
1	C	573	GLN

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 oligosaccharides 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	$\# Z > 2$
4	GOL	C	1650	-	5,5,5	0.73	0	5,5,5	0.85	0
3	GAL	C	1649	-	12,12,12	0.46	0	17,17,17	1.18	1 (5%)
3	GAL	A	1649	-	12,12,12	0.65	0	17,17,17	0.72	0
4	GOL	A	1650	-	5,5,5	0.89	0	5,5,5	0.86	0
4	GOL	B	1650	-	5,5,5	0.93	0	5,5,5	0.85	0
3	GAL	B	1649	-	12,12,12	0.68	0	17,17,17	0.85	1 (5%)

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
4	GOL	C	1650	-	-	4/4/4/4	-
3	GAL	C	1649	-	-	2/2/22/22	0/1/1/1
3	GAL	A	1649	-	-	2/2/22/22	0/1/1/1
4	GOL	A	1650	-	-	2/4/4/4	-
4	GOL	B	1650	-	-	3/4/4/4	-
3	GAL	B	1649	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1649	GAL	C4-C3-C2	2.33	114.91	110.83
3	B	1649	GAL	O5-C5-C6	2.24	111.99	106.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1650	GOL	C1-C2-C3-O3
4	B	1650	GOL	C1-C2-C3-O3
4	B	1650	GOL	O2-C2-C3-O3
4	C	1650	GOL	O1-C1-C2-O2
4	C	1650	GOL	O1-C1-C2-C3
4	C	1650	GOL	C1-C2-C3-O3
4	C	1650	GOL	O2-C2-C3-O3
3	A	1649	GAL	C4-C5-C6-O6
3	C	1649	GAL	C4-C5-C6-O6
3	A	1649	GAL	O5-C5-C6-O6
3	C	1649	GAL	O5-C5-C6-O6
4	A	1650	GOL	O2-C2-C3-O3
3	B	1649	GAL	O5-C5-C6-O6
4	B	1650	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1650	GOL	4	0
4	A	1650	GOL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1650	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	601/601 (100%)	0.52	45 (7%)	20 19	6, 18, 25, 28	10 (1%)
1	B	601/601 (100%)	0.03	3 (0%)	87 87	8, 17, 21, 28	22 (3%)
1	C	600/601 (99%)	-0.57	1 (0%)	91 90	2, 13, 31, 39	7 (1%)
All	All	1802/1803 (99%)	-0.00	49 (2%)	56 55	2, 17, 26, 39	39 (2%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	GLY	5.2
1	A	509[A]	MET	4.6
1	A	476	THR	4.0
1	A	527	SER	3.9
1	A	448	TRP	3.9
1	A	417	PRO	3.8
1	A	472	PRO	3.7
1	A	458[A]	MET	3.6
1	A	485	THR	3.6
1	A	86	GLY	3.4
1	A	496	THR	3.4
1	A	180	GLY	3.3
1	A	447	ASP	3.3
1	A	405	CYS	3.2
1	A	483	GLY	3.1
1	A	116	VAL	3.1
1	A	191	ALA	3.1
1	A	435	VAL	2.8
1	B	432	GLY	2.8
1	A	474	GLY	2.7
1	A	471	VAL	2.7
1	A	446	PRO	2.7
1	A	404	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	100	LEU	2.6
1	A	501	VAL	2.5
1	A	433	ILE	2.5
1	A	494	SER	2.5
1	A	432	GLY	2.5
1	A	478	GLY	2.5
1	A	441	GLN	2.4
1	A	489	SER	2.4
1	A	81	LEU	2.3
1	A	442	LEU	2.3
1	A	58	VAL	2.3
1	A	430	GLN	2.3
1	B	218	ALA	2.2
1	A	475	THR	2.2
1	A	413	VAL	2.2
1	A	493	ALA	2.2
1	A	477	PRO	2.2
1	A	480	TYR	2.2
1	A	445	SER	2.1
1	A	486	LEU	2.1
1	A	160	PRO	2.1
1	B	341[A]	SER	2.1
1	A	76	PRO	2.1
1	A	473	ALA	2.1
1	A	492	ASN	2.0
1	C	446	PRO	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	1650	6/6	0.77	0.11	30,32,36,37	0
3	GAL	A	1649	12/12	0.83	0.11	58,60,61,61	0
4	GOL	C	1650	6/6	0.86	0.11	27,34,35,36	0
4	GOL	B	1650	6/6	0.88	0.09	16,23,24,26	0
3	GAL	C	1649	12/12	0.89	0.09	35,40,43,44	0
2	NA	C	1648	1/1	0.90	0.06	16,16,16,16	0
3	GAL	B	1649	12/12	0.90	0.08	21,26,30,31	0
2	NA	B	1648	1/1	0.95	0.05	8,8,8,8	0
2	NA	A	1648	1/1	0.99	0.05	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.