



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:12 PM UTC

PDB ID : 1EUU / pdb_00001euu
Title : SIALIDASE OR NEURAMINIDASE, LARGE 68KD FORM
Authors : Gaskell, A.; Crennell, S.J.; Taylor, G.L.
Deposited on : 1996-06-21
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

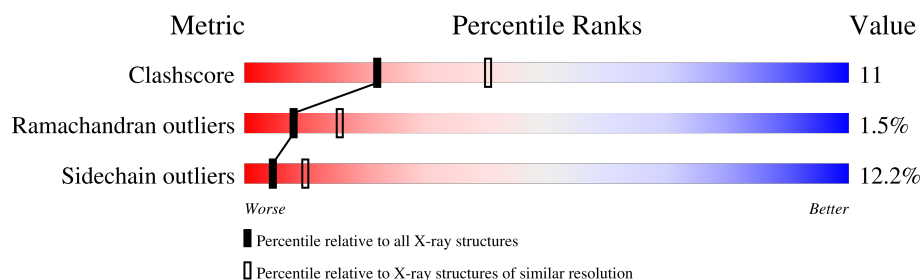
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	605	 70% 24% 5% ..

2 Entry composition [i](#)

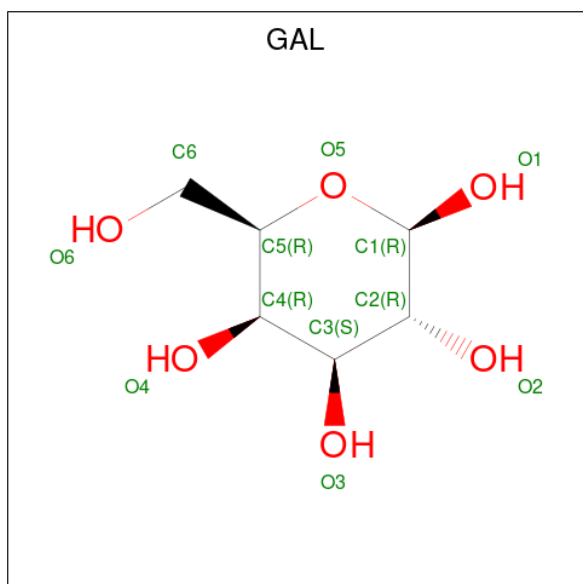
There are 3 unique types of molecules in this entry. The entry contains 4548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4535	2809	819	900	7			

- Molecule 2 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

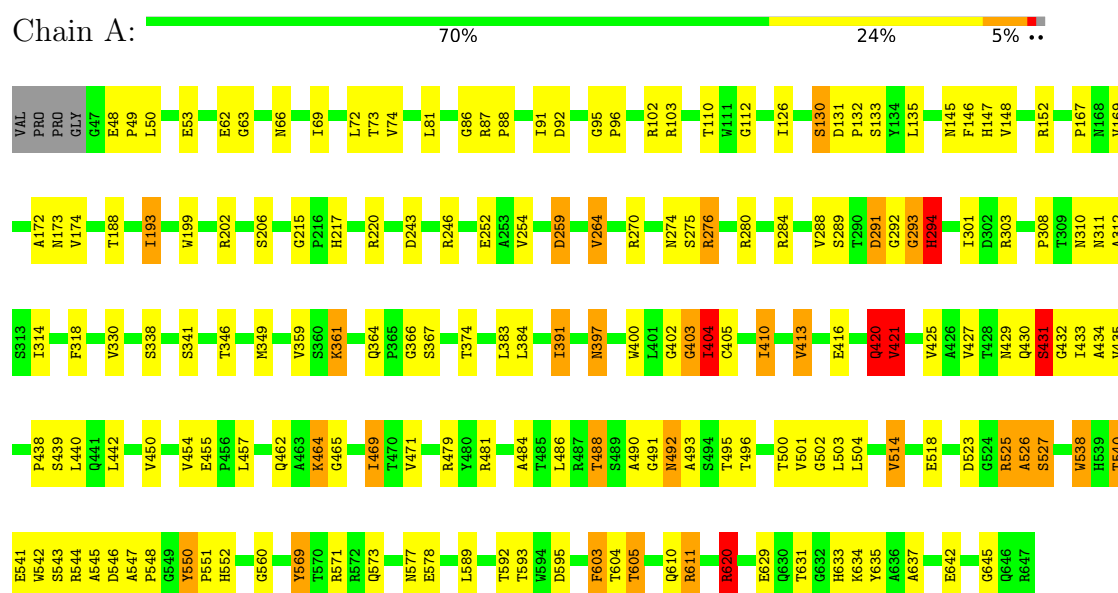
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: SIALIDASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.87Å 116.99Å 60.00Å 90.00° 95.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.228 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4548	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.82	2/4642 (0.0%)	1.27	45/6339 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	410	ILE	CA-CB	-6.25	1.49	1.54
1	A	391	ILE	CA-CB	5.39	1.61	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	TYR	CA-C-N	-12.63	104.05	119.84
1	A	550	TYR	C-N-CA	-12.63	104.05	119.84
1	A	550	TYR	N-CA-C	11.63	135.51	109.81
1	A	573	GLN	N-CA-C	10.89	122.91	111.14
1	A	275	SER	N-CA-C	9.51	125.06	109.95
1	A	403	GLY	N-CA-C	8.90	121.77	110.38
1	A	634	LYS	N-CA-C	8.50	123.88	113.17
1	A	95	GLY	CA-C-N	8.37	130.30	119.84
1	A	95	GLY	C-N-CA	8.37	130.30	119.84
1	A	276	ARG	N-CA-C	-8.09	99.09	110.50
1	A	63	GLY	N-CA-C	7.75	125.00	114.92
1	A	544	ARG	N-CA-C	-7.73	100.50	111.56
1	A	294	HIS	N-CA-C	7.56	126.91	110.80
1	A	420	GLN	N-CA-C	7.55	123.40	114.04
1	A	404	ILE	N-CA-C	7.17	124.25	109.34
1	A	421	VAL	N-CA-C	7.11	124.13	109.34
1	A	188	THR	N-CA-C	-6.90	97.28	108.52
1	A	291	ASP	N-CA-C	6.85	125.38	110.80
1	A	577	ASN	N-CA-C	6.78	121.26	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	SER	N-CA-C	6.59	119.18	109.24
1	A	193	ILE	N-CA-C	6.50	118.34	112.17
1	A	526	ALA	N-CA-C	-6.41	97.21	108.23
1	A	604	THR	N-CA-C	6.37	118.09	110.19
1	A	402	GLY	N-CA-C	-6.26	98.34	113.18
1	A	293	GLY	CA-C-N	6.20	133.38	121.54
1	A	293	GLY	C-N-CA	6.20	133.38	121.54
1	A	86	GLY	N-CA-C	-6.08	98.76	113.18
1	A	429	ASN	N-CA-C	6.06	119.95	110.32
1	A	413	VAL	N-CA-C	6.05	117.30	108.53
1	A	330	VAL	N-CA-C	5.92	116.97	107.73
1	A	215	GLY	CA-C-N	5.75	126.26	120.04
1	A	215	GLY	C-N-CA	5.75	126.26	120.04
1	A	280	ARG	N-CA-C	5.74	123.02	110.80
1	A	431	SER	N-CA-C	5.61	122.74	110.80
1	A	551	PRO	N-CA-C	-5.60	100.94	112.47
1	A	502	GLY	N-CA-C	5.59	123.52	114.90
1	A	293	GLY	N-CA-C	-5.59	99.93	113.18
1	A	434	ALA	N-CA-C	-5.44	96.91	107.62
1	A	538	TRP	N-CA-C	-5.37	100.94	109.96
1	A	514	VAL	CB-CA-C	-5.34	101.57	111.18
1	A	620	ARG	N-CA-C	-5.23	107.27	113.97
1	A	318	PHE	CA-C-N	5.10	124.71	119.05
1	A	318	PHE	C-N-CA	5.10	124.71	119.05
1	A	413	VAL	CB-CA-C	-5.08	103.08	110.81
1	A	605	THR	N-CA-CB	-5.04	103.17	110.47

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	4535	0	4353	95	0
2	A	12	0	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4548	0	4365	95	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 11.

All (95) 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:A:547:ALA:HB1	1:A:548:PRO:HD2	1.45	0.98
1:A:488:THR:HG22	1:A:490:ALA:H	1.31	0.93
1:A:481:ARG:H	1:A:481:ARG:HD3	1.41	0.86
1:A:433:ILE:HG23	1:A:435:VAL:HG23	1.56	0.85
1:A:50:LEU:H	1:A:397:ASN:HD21	1.31	0.76
1:A:217:HIS:CE1	1:A:292:GLY:HA3	2.22	0.74
1:A:603:PHE:H	1:A:603:PHE:HD1	1.38	0.70
1:A:145:ASN:HD22	1:A:147:HIS:HD2	1.40	0.70
1:A:264:VAL:HG22	1:A:314:ILE:HG23	1.75	0.67
1:A:611:ARG:NE	1:A:611:ARG:H	1.92	0.67
1:A:274:ASN:ND2	1:A:284:ARG:HE	1.94	0.66
1:A:410:ILE:HG12	1:A:425:VAL:HG22	1.78	0.65
1:A:631:THR:HG23	1:A:633:HIS:ND1	2.11	0.65
1:A:547:ALA:HB1	1:A:548:PRO:CD	2.23	0.65
1:A:420:GLN:H	1:A:420:GLN:CD	2.05	0.64
1:A:438:PRO:HG2	1:A:454:VAL:HG13	1.79	0.63
1:A:433:ILE:HG23	1:A:435:VAL:CG2	2.27	0.62
1:A:349:MET:HB3	1:A:359:VAL:HB	1.82	0.62
1:A:603:PHE:N	1:A:603:PHE:CD1	2.68	0.61
1:A:479:ARG:HD3	1:A:500:THR:HG22	1.83	0.60
1:A:603:PHE:HD1	1:A:603:PHE:N	1.98	0.60
1:A:361:LYS:HE3	1:A:400:TRP:O	2.03	0.59
1:A:69:ILE:HG21	1:A:131:ASP:HA	1.85	0.59
1:A:50:LEU:H	1:A:397:ASN:ND2	1.98	0.58
1:A:538:TRP:O	1:A:637:ALA:HA	2.02	0.58
1:A:364:GLN:HE21	1:A:366:GLY:H	1.51	0.57
1:A:243:ASP:OD2	1:A:246:ARG:HB2	2.05	0.57
1:A:397:ASN:HD22	1:A:397:ASN:H	1.53	0.57
1:A:102:ARG:HD2	1:A:112:GLY:O	2.05	0.56
1:A:403:GLY:O	1:A:492:ASN:O	2.23	0.56
1:A:405:CYS:HB2	1:A:430:GLN:HB3	1.88	0.55
1:A:592:THR:HG23	1:A:593:THR:HG23	1.87	0.55
1:A:484:ALA:HB3	1:A:495:THR:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:ND2	1:A:147:HIS:HD2	2.04	0.54
1:A:569:TYR:N	1:A:569:TYR:CD1	2.72	0.54
1:A:259:ASP:HB3	1:A:276:ARG:HD2	1.90	0.54
1:A:523:ASP:OD1	1:A:525:ARG:HD3	2.08	0.54
1:A:433:ILE:HG22	1:A:433:ILE:O	2.07	0.53
1:A:259:ASP:HB3	1:A:276:ARG:HB3	1.90	0.53
1:A:420:GLN:CD	1:A:420:GLN:N	2.66	0.53
1:A:421:VAL:HG13	1:A:469:ILE:HD12	1.90	0.52
1:A:220:ARG:HH12	1:A:292:GLY:HA2	1.75	0.52
1:A:420:GLN:O	1:A:469:ILE:O	2.29	0.51
1:A:518:GLU:HG2	1:A:542:TRP:CD1	2.46	0.50
1:A:220:ARG:HH11	1:A:294:HIS:HD2	1.59	0.50
1:A:66:ASN:HB3	1:A:87:ARG:HB2	1.94	0.50
1:A:550:TYR:CE2	1:A:629:GLU:HB2	2.47	0.49
1:A:431:SER:O	1:A:433:ILE:N	2.45	0.49
1:A:560:GLY:C	1:A:620:ARG:HG2	2.38	0.49
1:A:571:ARG:NH1	1:A:603:PHE:CE2	2.81	0.48
1:A:310:ASN:ND2	1:A:311:ASN:H	2.11	0.48
1:A:526:ALA:O	1:A:527:SER:HB3	2.14	0.48
1:A:503:LEU:HD13	1:A:642:GLU:CG	2.43	0.48
1:A:550:TYR:O	1:A:552:HIS:N	2.46	0.47
1:A:435:VAL:HB	1:A:457:LEU:HB2	1.94	0.47
1:A:311:ASN:HD22	1:A:312:ALA:H	1.62	0.47
1:A:464:LYS:HG2	1:A:465:GLY:N	2.30	0.47
1:A:427:VAL:O	1:A:462:GLN:HG3	2.15	0.47
1:A:102:ARG:NH1	1:A:112:GLY:O	2.48	0.46
1:A:133:SER:HB2	1:A:206:SER:HA	1.97	0.46
1:A:364:GLN:HE21	1:A:366:GLY:N	2.13	0.46
1:A:569:TYR:H	1:A:569:TYR:HD1	1.63	0.46
1:A:88:PRO:HG2	1:A:96:PRO:HG2	1.97	0.46
1:A:518:GLU:HG2	1:A:542:TRP:NE1	2.30	0.45
1:A:220:ARG:NH1	1:A:292:GLY:HA2	2.32	0.45
1:A:504:LEU:HD11	1:A:645:GLY:HA3	1.98	0.45
1:A:542:TRP:HA	1:A:635:TYR:CE1	2.52	0.45
1:A:569:TYR:CE2	1:A:603:PHE:CZ	3.04	0.45
1:A:291:ASP:OD1	1:A:294:HIS:HA	2.17	0.45
1:A:454:VAL:HG22	1:A:455:GLU:O	2.18	0.44
1:A:504:LEU:HD12	1:A:504:LEU:N	2.32	0.44
1:A:486:LEU:HB3	1:A:493:ALA:HB3	2.00	0.44
1:A:338:SER:HB3	1:A:341:SER:O	2.18	0.44
1:A:503:LEU:HD13	1:A:642:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASN:ND2	1:A:312:ALA:H	2.16	0.43
1:A:432:GLY:O	1:A:433:ILE:HD13	2.19	0.43
1:A:132:PRO:HA	1:A:146:PHE:O	2.18	0.43
1:A:308:PRO:HD3	1:A:338:SER:O	2.19	0.43
1:A:397:ASN:HD22	1:A:397:ASN:N	2.15	0.43
1:A:403:GLY:HA3	1:A:491:GLY:HA3	2.01	0.42
1:A:259:ASP:CB	1:A:276:ARG:HD2	2.47	0.42
1:A:404:ILE:HD11	1:A:433:ILE:HG21	2.02	0.42
1:A:50:LEU:N	1:A:397:ASN:HD21	2.07	0.42
1:A:314:ILE:HG23	1:A:314:ILE:O	2.19	0.42
1:A:288:VAL:HG22	1:A:289:SER:N	2.35	0.41
1:A:152:ARG:HG3	1:A:167:PRO:HB2	2.02	0.41
1:A:540:THR:HG21	1:A:552:HIS:CE1	2.54	0.41
1:A:603:PHE:HB2	1:A:610:GLN:NE2	2.36	0.41
1:A:48:GLU:HA	1:A:49:PRO:HD3	1.87	0.41
1:A:172:ALA:CB	1:A:193:ILE:HD11	2.50	0.41
1:A:270:ARG:HH11	1:A:288:VAL:HG21	1.84	0.41
1:A:73:THR:HG22	1:A:81:LEU:HB2	2.02	0.40
1:A:571:ARG:HG2	1:A:571:ARG:HH11	1.85	0.40
1:A:404:ILE:HD12	1:A:488:THR:HG21	2.02	0.40
1:A:433:ILE:HD13	1:A:433:ILE:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/605 (99%)	555 (93%)	35 (6%)	9 (2%)	8	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	HIS
1	A	404	ILE
1	A	421	VAL
1	A	431	SER
1	A	527	SER
1	A	543	SER
1	A	545	ALA
1	A	259	ASP
1	A	293	GLY

5.3.2 Protein sidechains [i](#)

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	477/480 (99%)	419 (88%)	58 (12%)	5 10

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	62	GLU
1	A	72	LEU
1	A	74	VAL
1	A	91	ILE
1	A	92	ASP
1	A	103	ARG
1	A	110	THR
1	A	126	ILE
1	A	130	SER
1	A	135	LEU
1	A	148	VAL
1	A	169	VAL
1	A	173	ASN
1	A	174	VAL
1	A	199	TRP
1	A	202	ARG
1	A	252	GLU

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Mol	Chain	Res	Type
1	A	254	VAL
1	A	264	VAL
1	A	301	ILE
1	A	303	ARG
1	A	346	THR
1	A	361	LYS
1	A	367	SER
1	A	374	THR
1	A	383	LEU
1	A	384	LEU
1	A	391	ILE
1	A	397	ASN
1	A	404	ILE
1	A	413	VAL
1	A	416	GLU
1	A	420	GLN
1	A	439	SER
1	A	440	LEU
1	A	442	LEU
1	A	450	VAL
1	A	464	LYS
1	A	469	ILE
1	A	471	VAL
1	A	488	THR
1	A	492	ASN
1	A	496	THR
1	A	501	VAL
1	A	514	VAL
1	A	525	ARG
1	A	540	THR
1	A	541	GLU
1	A	546	ASP
1	A	569	TYR
1	A	578	GLU
1	A	589	LEU
1	A	595	ASP
1	A	603	PHE
1	A	605	THR
1	A	611	ARG
1	A	620	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	66	ASN
1	A	101	GLN
1	A	115	GLN
1	A	145	ASN
1	A	147	HIS
1	A	168	ASN
1	A	186	HIS
1	A	224	GLN
1	A	274	ASN
1	A	294	HIS
1	A	310	ASN
1	A	311	ASN
1	A	355	GLN
1	A	364	GLN
1	A	397	ASN
1	A	430	GLN
1	A	492	ASN
1	A	573	GLN
1	A	610	GLN
1	A	630	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
2	GAL	A	2	-	12,12,12	0.40	0	17,17,17	0.54	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
2	GAL	A	2	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	GAL	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.