



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:55 AM UTC

PDB ID : 6TL8 / pdb_00006tl8
Title : Structural basis of SALM3 dimerization and adhesion complex formation with the presynaptic receptor protein tyrosine phosphatases
Authors : Karki, S.; Shkumatov, A.V.; Bae, S.; Ko, J.; Kajander, T.
Deposited on : 2019-12-02
Resolution : 2.80 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

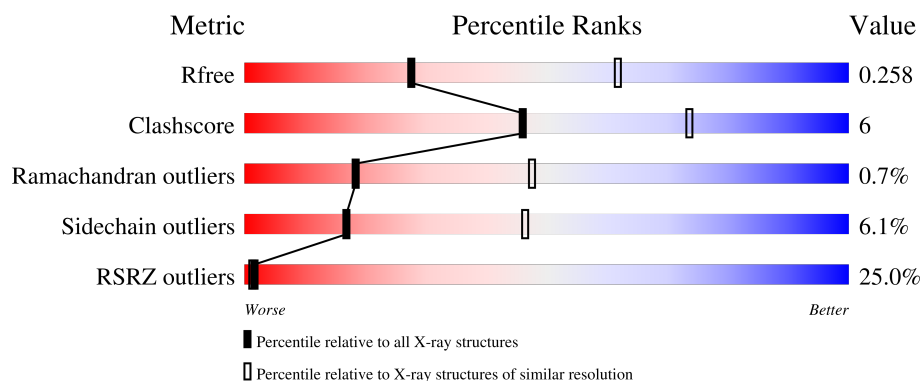
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	299	24% 67% 16% • 16%
1	B	299	21% 69% 14% • 15%
1	C	299	20% 71% 13% • 15%
1	D	299	19% 71% 12% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7304 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 Myeloid cell surface antigen CD33,Leucine-rich repeat and fibronectin type-III domain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1809	1147	319	333	10			
1	B	253	Total	C	N	O	S	0	0	0
			1811	1138	321	342	10			
1	C	253	Total	C	N	O	S	0	0	0
			1821	1148	310	353	10			
1	D	253	Total	C	N	O	S	0	0	0
			1817	1149	318	340	10			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	linker	UNP P20138
A	14	ASP	-	linker	UNP P20138
A	15	LYS	-	linker	UNP P20138
A	16	LEU	-	linker	UNP P20138
A	285	GLY	-	cloning artifact	UNP Q80XU8
A	286	THR	-	cloning artifact	UNP Q80XU8
A	287	ARG	-	cloning artifact	UNP Q80XU8
A	288	GLY	-	cloning artifact	UNP Q80XU8
A	289	SER	-	cloning artifact	UNP Q80XU8
A	290	LEU	-	cloning artifact	UNP Q80XU8
A	291	GLU	-	cloning artifact	UNP Q80XU8
A	292	VAL	-	cloning artifact	UNP Q80XU8
A	293	LEU	-	cloning artifact	UNP Q80XU8
A	294	PHE	-	cloning artifact	UNP Q80XU8
A	295	GLN	-	cloning artifact	UNP Q80XU8
B	13	MET	-	linker	UNP P20138
B	14	ASP	-	linker	UNP P20138
B	15	LYS	-	linker	UNP P20138
B	16	LEU	-	linker	UNP P20138
B	285	GLY	-	cloning artifact	UNP Q80XU8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	286	THR	-	cloning artifact	UNP Q80XU8
B	287	ARG	-	cloning artifact	UNP Q80XU8
B	288	GLY	-	cloning artifact	UNP Q80XU8
B	289	SER	-	cloning artifact	UNP Q80XU8
B	290	LEU	-	cloning artifact	UNP Q80XU8
B	291	GLU	-	cloning artifact	UNP Q80XU8
B	292	VAL	-	cloning artifact	UNP Q80XU8
B	293	LEU	-	cloning artifact	UNP Q80XU8
B	294	PHE	-	cloning artifact	UNP Q80XU8
B	295	GLN	-	cloning artifact	UNP Q80XU8
C	13	MET	-	linker	UNP P20138
C	14	ASP	-	linker	UNP P20138
C	15	LYS	-	linker	UNP P20138
C	16	LEU	-	linker	UNP P20138
C	285	GLY	-	cloning artifact	UNP Q80XU8
C	286	THR	-	cloning artifact	UNP Q80XU8
C	287	ARG	-	cloning artifact	UNP Q80XU8
C	288	GLY	-	cloning artifact	UNP Q80XU8
C	289	SER	-	cloning artifact	UNP Q80XU8
C	290	LEU	-	cloning artifact	UNP Q80XU8
C	291	GLU	-	cloning artifact	UNP Q80XU8
C	292	VAL	-	cloning artifact	UNP Q80XU8
C	293	LEU	-	cloning artifact	UNP Q80XU8
C	294	PHE	-	cloning artifact	UNP Q80XU8
C	295	GLN	-	cloning artifact	UNP Q80XU8
D	13	MET	-	linker	UNP P20138
D	14	ASP	-	linker	UNP P20138
D	15	LYS	-	linker	UNP P20138
D	16	LEU	-	linker	UNP P20138
D	285	GLY	-	cloning artifact	UNP Q80XU8
D	286	THR	-	cloning artifact	UNP Q80XU8
D	287	ARG	-	cloning artifact	UNP Q80XU8
D	288	GLY	-	cloning artifact	UNP Q80XU8
D	289	SER	-	cloning artifact	UNP Q80XU8
D	290	LEU	-	cloning artifact	UNP Q80XU8
D	291	GLU	-	cloning artifact	UNP Q80XU8
D	292	VAL	-	cloning artifact	UNP Q80XU8
D	293	LEU	-	cloning artifact	UNP Q80XU8
D	294	PHE	-	cloning artifact	UNP Q80XU8
D	295	GLN	-	cloning artifact	UNP Q80XU8

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

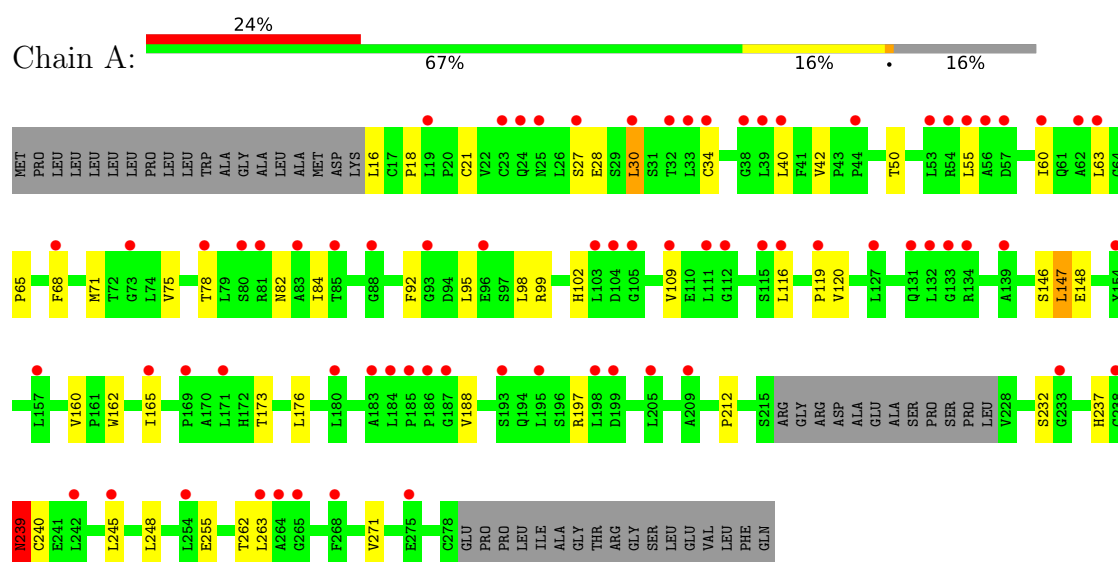
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	1	Total	O	0	0
			1	1		
3	C	5	Total	O	0	0
			5	5		
3	D	7	Total	O	0	0
			7	7		

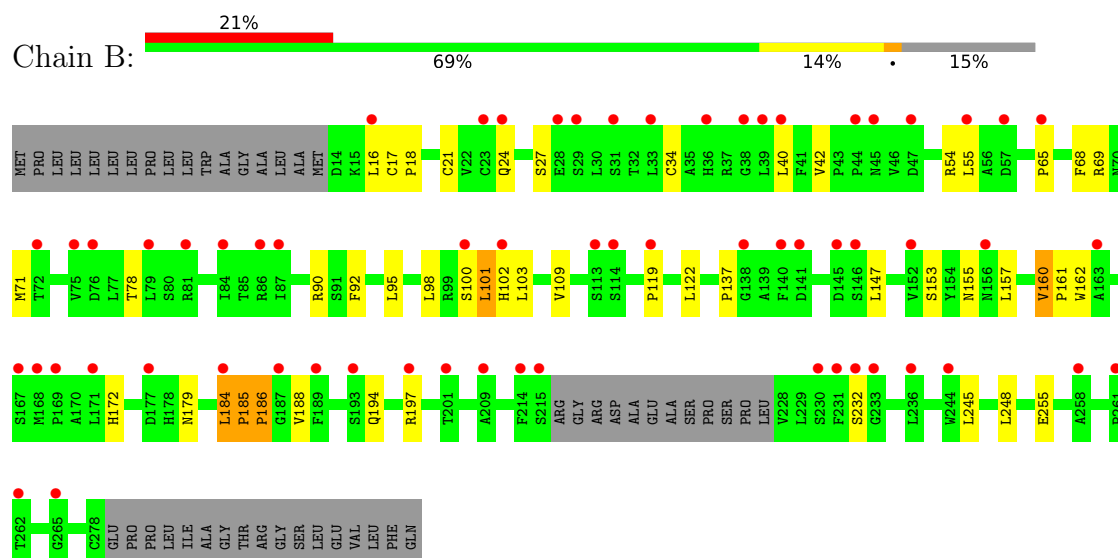
3 Residue-property plots

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.

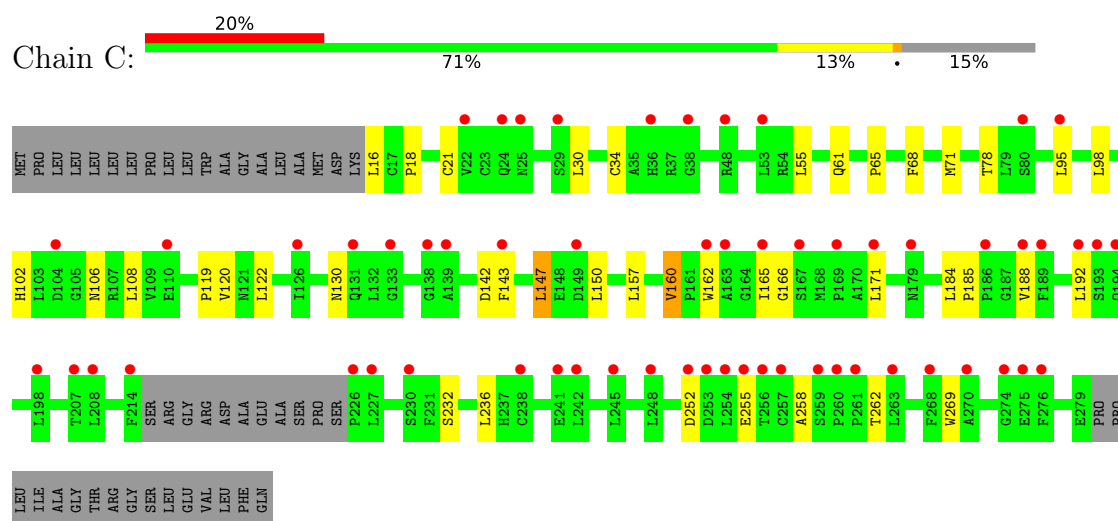
- Molecule 1: Myeloid cell surface antigen CD33, Leucine-rich repeat and fibronectin type-III domain-containing protein 4



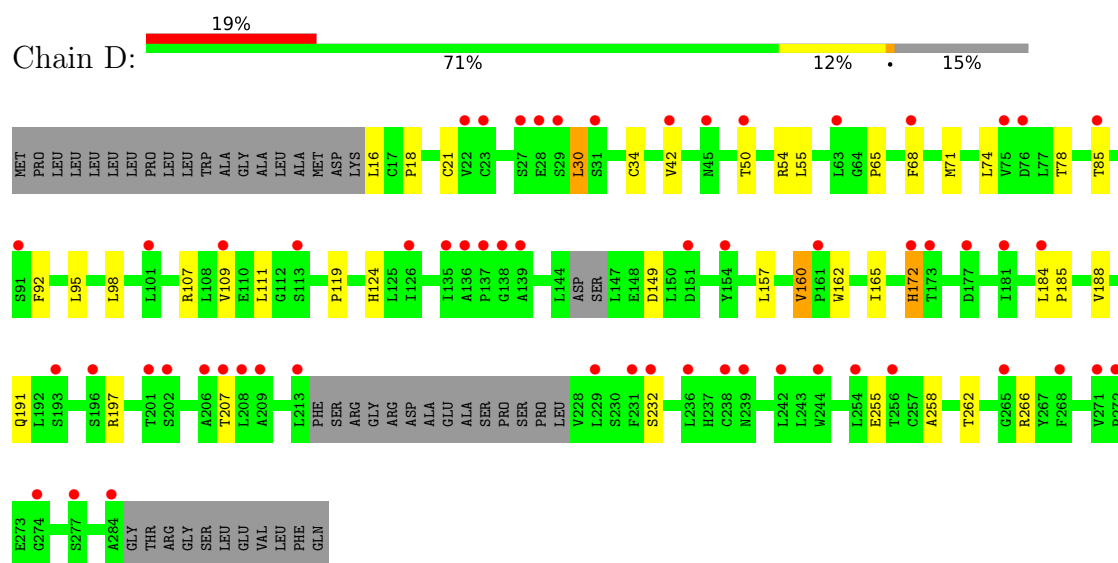
- Molecule 1: Myeloid cell surface antigen CD33, Leucine-rich repeat and fibronectin type-III domain-containing protein 4



- Molecule 1: Myeloid cell surface antigen CD33, Leucine-rich repeat and fibronectin type-III domain-containing protein 4



- Molecule 1: Myeloid cell surface antigen CD33, Leucine-rich repeat and fibronectin type-III domain-containing protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	31.45Å 132.16Å 134.18Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.80) 99.3 (30.00-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.80Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.262 , 0.285 0.254 , 0.258	Depositor DCC
R_{free} test set	1347 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 96.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.349 for h,-k,-l	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	7304	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: NAG

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	0.63	0/1850	1.00	2/2537 (0.1%)
1	B	0.64	0/1849	0.98	3/2536 (0.1%)
1	C	0.63	0/1862	0.93	1/2554 (0.0%)
1	D	0.63	0/1859	0.96	1/2551 (0.0%)
All	All	0.63	0/7420	0.97	7/10178 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	GLN	CA-C-N	6.54	131.86	121.66
1	B	24	GLN	C-N-CA	6.54	131.86	121.66
1	B	65	PRO	N-CA-C	5.57	117.50	110.70
1	D	65	PRO	N-CA-C	5.50	117.41	110.70
1	A	65	PRO	N-CA-C	5.45	117.35	110.70
1	C	65	PRO	N-CA-C	5.27	117.13	110.70
1	A	239	ASN	CA-CB-CG	5.12	117.72	112.60

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	1809	0	1687	23	0
1	B	1811	0	1680	23	0
1	C	1821	0	1669	20	0
1	D	1817	0	1686	18	0
2	C	14	0	13	1	0
2	D	14	0	13	0	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
3	C	5	0	0	0	0
3	D	7	0	0	0	0
All	All	7304	0	6748	82	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 6.

All (82) 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:30:LEU:HB3	1:A:50:THR:HA	1.68	0.75
1:B:162:TRP:HB3	1:B:188:VAL:HG21	1.73	0.71
1:D:157:LEU:HD13	1:D:160:VAL:HG23	1.79	0.64
1:D:162:TRP:HA	1:D:165:ILE:CG1	2.29	0.63
1:A:162:TRP:HA	1:A:165:ILE:CG1	2.29	0.62
1:A:232:SER:HA	1:A:255:GLU:HG3	1.85	0.58
1:C:232:SER:HA	1:C:255:GLU:HG3	1.86	0.58
1:D:30:LEU:HB3	1:D:50:THR:HA	1.86	0.57
1:A:160:VAL:HG21	1:A:176:LEU:HD22	1.87	0.57
1:B:232:SER:HA	1:B:255:GLU:HG3	1.87	0.57
1:B:98:LEU:HB3	1:B:119:PRO:HB3	1.87	0.57
1:C:252:ASP:OD1	1:C:269:TRP:HD1	1.87	0.57
1:C:162:TRP:HA	1:C:165:ILE:CG1	2.34	0.57
1:C:252:ASP:HA	1:C:269:TRP:CD1	2.40	0.57
1:B:157:LEU:HD13	1:B:160:VAL:HG23	1.88	0.56
1:B:184:LEU:C	1:B:186:PRO:HD3	2.31	0.55
1:C:157:LEU:HD13	1:C:160:VAL:HG23	1.89	0.55
1:D:98:LEU:HB3	1:D:119:PRO:HB3	1.90	0.54
1:B:172:HIS:HD2	1:B:194:GLN:HB3	1.72	0.54
1:B:162:TRP:HB3	1:B:188:VAL:CG2	2.38	0.54
1:B:18:PRO:HD2	1:B:21:CYS:HB2	1.91	0.52
1:C:171:LEU:HB3	1:C:192:LEU:HD23	1.91	0.52
1:D:85:THR:HG22	1:D:107:ARG:HB2	1.92	0.52
1:A:60:ILE:HG23	1:A:82:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:PRO:HB2	1:B:188:VAL:HG23	1.92	0.51
1:C:106:ASN:HB2	1:C:130:ASN:OD1	2.11	0.50
1:A:98:LEU:HB3	1:A:119:PRO:HB3	1.93	0.50
1:C:30:LEU:HB2	2:C:401:NAG:H82	1.93	0.50
1:D:18:PRO:HD2	1:D:21:CYS:HB2	1.94	0.50
1:B:40:LEU:HD13	1:C:258:ALA:HB2	1.93	0.49
1:A:68:PHE:HA	1:A:71:MET:HE3	1.95	0.49
1:C:68:PHE:HA	1:C:71:MET:HE3	1.95	0.49
1:B:68:PHE:HA	1:B:71:MET:HE3	1.95	0.49
1:C:119:PRO:HB2	1:C:122:LEU:HB2	1.95	0.49
1:A:18:PRO:HD2	1:A:21:CYS:HB2	1.95	0.48
1:D:34:CYS:HB2	1:D:55:LEU:HD23	1.95	0.48
1:D:68:PHE:HA	1:D:71:MET:HE3	1.95	0.48
1:C:18:PRO:HD2	1:C:21:CYS:HB2	1.96	0.48
1:A:40:LEU:HD13	1:D:258:ALA:HB2	1.96	0.48
1:B:34:CYS:HB2	1:B:55:LEU:HD23	1.97	0.46
1:C:34:CYS:HB2	1:C:55:LEU:HD23	1.97	0.46
1:C:68:PHE:HB3	1:C:95:LEU:HD21	1.96	0.46
1:C:166:GLY:HA2	1:C:192:LEU:HD11	1.97	0.46
1:D:185:PRO:HB2	1:D:188:VAL:HG23	1.98	0.46
1:A:34:CYS:HB2	1:A:55:LEU:HD23	1.97	0.45
1:C:98:LEU:HB3	1:C:119:PRO:HB3	1.97	0.45
1:B:68:PHE:HB3	1:B:95:LEU:HD21	1.97	0.45
1:D:232:SER:HA	1:D:255:GLU:HG3	1.98	0.45
1:A:237:HIS:HD2	1:A:239:ASN:ND2	2.15	0.45
1:C:78:THR:HG22	1:C:102:HIS:ND1	2.32	0.45
1:A:237:HIS:CD2	1:A:239:ASN:ND2	2.85	0.45
1:A:173:THR:HG23	1:A:197:ARG:HB3	1.99	0.44
1:B:92:PHE:HB3	1:B:95:LEU:HD12	2.00	0.44
1:A:78:THR:HG22	1:A:102:HIS:ND1	2.33	0.43
1:A:68:PHE:HB3	1:A:95:LEU:HD21	1.99	0.43
1:C:185:PRO:HB2	1:C:188:VAL:HG23	2.00	0.43
1:D:92:PHE:HB3	1:D:95:LEU:HD12	2.00	0.43
1:B:101:LEU:HD11	1:B:103:LEU:HD11	1.99	0.43
1:A:263:LEU:HD22	1:A:271:VAL:HG11	2.00	0.43
1:D:54:ARG:HA	1:D:78:THR:HG23	2.00	0.43
1:B:78:THR:HG22	1:B:102:HIS:ND1	2.33	0.43
1:B:185:PRO:N	1:B:186:PRO:HD3	2.34	0.42
1:A:162:TRP:HB3	1:A:188:VAL:HG12	2.01	0.42
1:C:143:PHE:HD2	1:C:147:LEU:HG	1.84	0.42
1:C:162:TRP:HE3	1:C:188:VAL:HG11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HG13	1:A:99:ARG:HE	1.85	0.41
1:D:68:PHE:HB3	1:D:95:LEU:HD21	2.03	0.41
1:A:63:LEU:HD11	1:A:84:ILE:HD13	2.03	0.40
1:B:78:THR:HA	1:B:102:HIS:HB2	2.03	0.40
1:D:42:VAL:HG22	1:D:55:LEU:HD13	2.03	0.40
1:D:50:THR:HG23	1:D:74:LEU:HD13	2.03	0.40
1:B:42:VAL:HG22	1:B:55:LEU:HD13	2.02	0.40
1:A:42:VAL:HG22	1:A:55:LEU:HD13	2.02	0.40
1:A:92:PHE:HB3	1:A:95:LEU:HD12	2.03	0.40
1:A:245:LEU:HA	1:A:248:LEU:HD12	2.04	0.40
1:B:155:ASN:H	1:B:179:ASN:ND2	2.19	0.40
1:A:146:SER:O	1:A:148:GLU:HG3	2.21	0.40
1:B:119:PRO:HB2	1:B:122:LEU:HB2	2.03	0.40
1:B:137:PRO:HA	1:B:161:PRO:HB3	2.04	0.40
1:D:124:HIS:CE1	1:D:149:ASP:OD2	2.75	0.40
1:D:149:ASP:OD1	1:D:172:HIS:CD2	2.75	0.40
1:B:245:LEU:HA	1:B:248:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/299 (83%)	226 (92%)	18 (7%)	3 (1%)	10	34
1	B	249/299 (83%)	226 (91%)	20 (8%)	3 (1%)	10	34
1	C	249/299 (83%)	226 (91%)	22 (9%)	1 (0%)	30	60
1	D	247/299 (83%)	224 (91%)	23 (9%)	0	100	100
All	All	992/1196 (83%)	902 (91%)	83 (8%)	7 (1%)	18	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	CYS
1	B	185	PRO
1	C	236	LEU
1	A	27	SER
1	B	186	PRO
1	A	147	LEU
1	A	212	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	183/255 (72%)	173 (94%)	10 (6%)	19	51
1	B	183/255 (72%)	170 (93%)	13 (7%)	13	39
1	C	188/255 (74%)	178 (95%)	10 (5%)	20	52
1	D	186/255 (73%)	174 (94%)	12 (6%)	15	43
All	All	740/1020 (72%)	695 (94%)	45 (6%)	17	46

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	28	GLU
1	A	30	LEU
1	A	109	VAL
1	A	116	LEU
1	A	120	VAL
1	A	147	LEU
1	A	239	ASN
1	A	240	CYS
1	A	262	THR
1	B	16	LEU
1	B	27	SER
1	B	54	ARG
1	B	69	ARG
1	B	90	ARG

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Mol	Chain	Res	Type
1	B	100	SER
1	B	101	LEU
1	B	109	VAL
1	B	147	LEU
1	B	153	SER
1	B	160	VAL
1	B	184	LEU
1	B	197	ARG
1	C	16	LEU
1	C	61	GLN
1	C	108	LEU
1	C	120	VAL
1	C	142	ASP
1	C	147	LEU
1	C	150	LEU
1	C	160	VAL
1	C	184	LEU
1	C	262	THR
1	D	16	LEU
1	D	30	LEU
1	D	109	VAL
1	D	111	LEU
1	D	160	VAL
1	D	172	HIS
1	D	184	LEU
1	D	191	GLN
1	D	197	ARG
1	D	207	THR
1	D	262	THR
1	D	266	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	156	ASN
1	A	239	ASN
1	B	131	GLN
1	B	156	ASN
1	B	179	ASN
1	C	36	HIS
1	C	131	GLN

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Mol	Chain	Res	Type
1	C	156	ASN
1	D	131	GLN
1	D	156	ASN
1	D	172	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	NAG	C	401	1	14,14,15	0.28	0	17,19,21	0.50	0
2	NAG	D	401	1	14,14,15	0.26	0	17,19,21	0.46	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	NAG	C	401	1	-	0/6/23/26	0/1/1/1
2	NAG	D	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

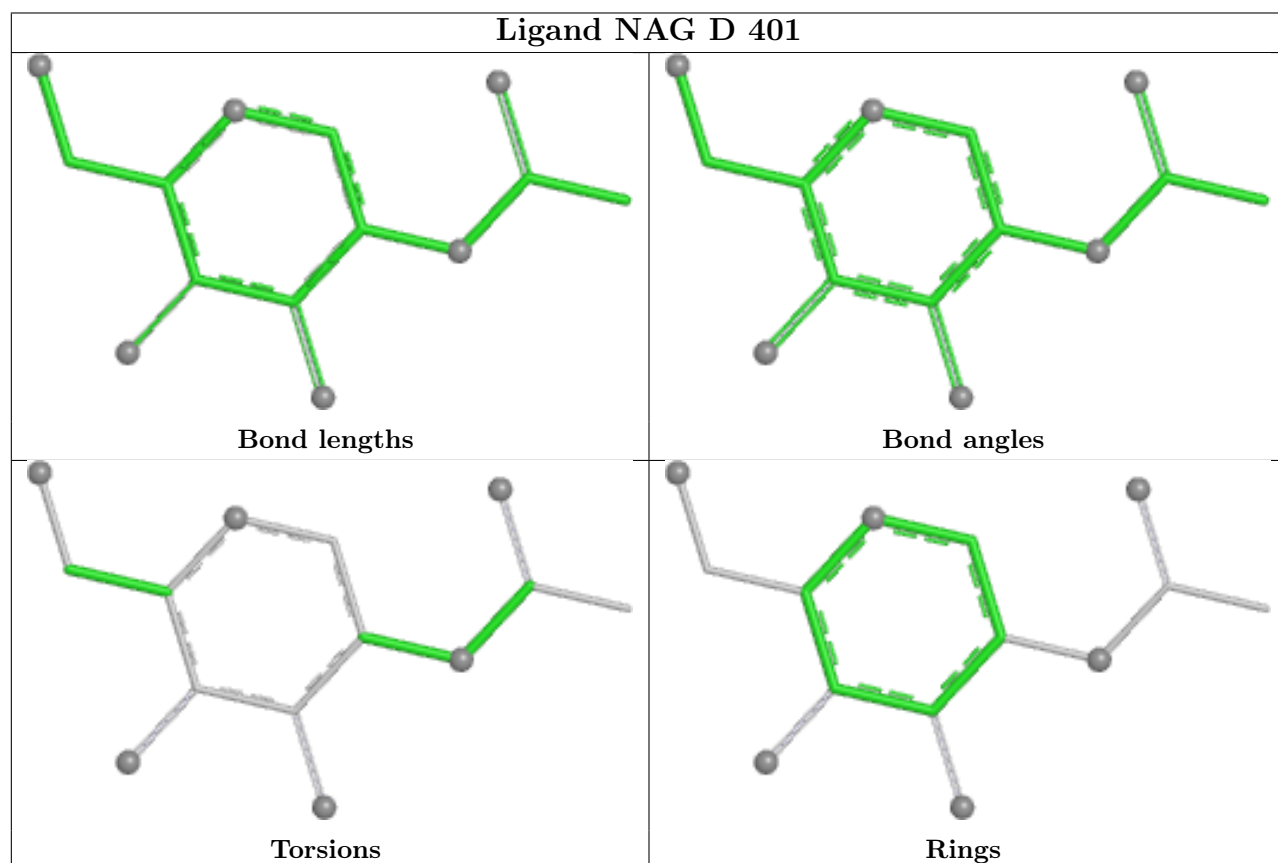
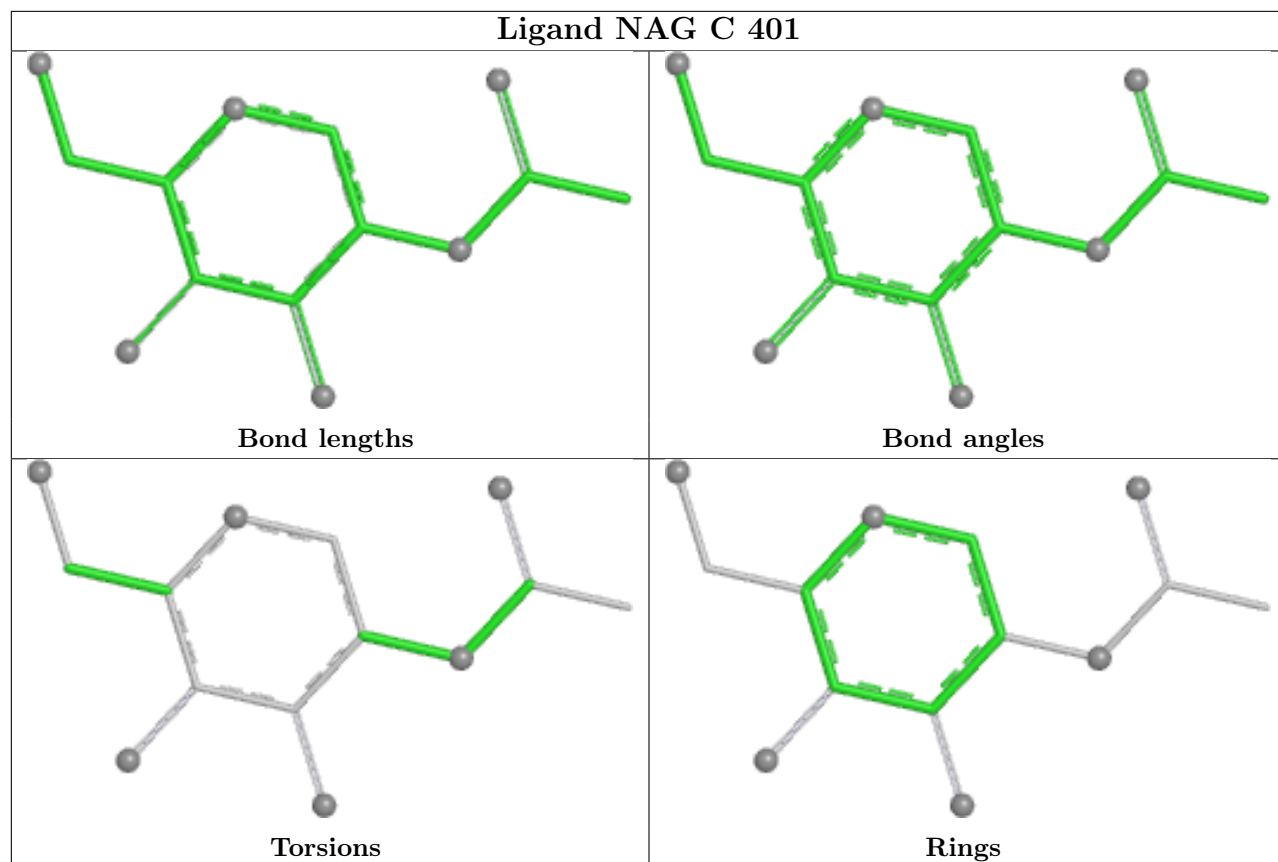
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	251/299 (83%)	1.55	73 (29%) 1 1	60, 84, 107, 115	0
1	B	253/299 (84%)	1.49	62 (24%) 2 1	66, 88, 109, 120	0
1	C	253/299 (84%)	1.48	59 (23%) 2 1	67, 87, 110, 125	0
1	D	253/299 (84%)	1.51	58 (22%) 2 1	62, 88, 111, 130	0
All	All	1010/1196 (84%)	1.51	252 (24%) 2 1	60, 87, 109, 130	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	208	LEU	7.2
1	D	76	ASP	6.5
1	A	187	GLY	5.9
1	A	56	ALA	5.5
1	B	28	GLU	5.5
1	A	32	THR	5.4
1	D	173	THR	5.1
1	B	45	ASN	5.1
1	B	145	ASP	4.5
1	B	24	GLN	4.5
1	B	231	PHE	4.5
1	C	169	PRO	4.4
1	B	140	PHE	4.4
1	C	274	GLY	4.3
1	B	36	HIS	4.2
1	A	112	GLY	4.1
1	A	25	ASN	4.1
1	C	133	GLY	4.1
1	A	198	LEU	4.0
1	D	209	ALA	4.0
1	A	38	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	105	GLY	4.0
1	A	195	LEU	3.9
1	B	244	TRP	3.9
1	A	53	LEU	3.8
1	D	238	CYS	3.8
1	B	236	LEU	3.7
1	A	27	SER	3.7
1	C	253	ASP	3.7
1	C	193	SER	3.7
1	D	201	THR	3.7
1	A	169	PRO	3.6
1	C	261	PRO	3.6
1	C	189	PHE	3.6
1	A	183	ALA	3.5
1	D	31	SER	3.5
1	D	184	LEU	3.5
1	C	275	GLU	3.5
1	D	172	HIS	3.5
1	C	24	GLN	3.4
1	A	242	LEU	3.4
1	A	186	PRO	3.4
1	C	163	ALA	3.4
1	D	239	ASN	3.4
1	B	23	CYS	3.3
1	B	230	SER	3.3
1	B	232	SER	3.3
1	D	23	CYS	3.3
1	D	63	LEU	3.2
1	C	276	PHE	3.2
1	D	137	PRO	3.2
1	C	230	SER	3.2
1	D	135	ILE	3.2
1	A	83	ALA	3.2
1	D	284	ALA	3.2
1	A	131	GLN	3.2
1	D	91	SER	3.1
1	B	163	ALA	3.1
1	D	271	VAL	3.1
1	A	54	ARG	3.1
1	D	27	SER	3.1
1	D	207	THR	3.1
1	A	39	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	57	ASP	3.1
1	D	232	SER	3.1
1	A	93	GLY	3.1
1	A	109	VAL	3.1
1	B	114	SER	3.1
1	C	138	GLY	3.0
1	A	78	THR	3.0
1	B	113	SER	3.0
1	A	185	PRO	3.0
1	B	119	PRO	3.0
1	B	197	ARG	3.0
1	C	241	GLU	3.0
1	B	258	ALA	2.9
1	C	256	THR	2.9
1	D	193	SER	2.9
1	D	254	LEU	2.9
1	A	265	GLY	2.9
1	D	139	ALA	2.9
1	B	40	LEU	2.9
1	B	65	PRO	2.9
1	D	151	ASP	2.9
1	C	53	LEU	2.9
1	C	245	LEU	2.9
1	D	277	SER	2.8
1	D	136	ALA	2.8
1	D	231	PHE	2.8
1	D	101	LEU	2.8
1	B	265	GLY	2.8
1	A	268	PHE	2.8
1	C	171	LEU	2.8
1	B	31	SER	2.8
1	C	214	PHE	2.7
1	B	102	HIS	2.7
1	A	88	GLY	2.7
1	B	187	GLY	2.7
1	C	260	PRO	2.7
1	C	255	GLU	2.7
1	D	109	VAL	2.7
1	A	103	LEU	2.7
1	D	181	ILE	2.7
1	A	34	CYS	2.7
1	C	110	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	55	LEU	2.7
1	C	252	ASP	2.7
1	D	28	GLU	2.7
1	A	238	CYS	2.6
1	B	81	ARG	2.6
1	A	68	PHE	2.6
1	B	29	SER	2.6
1	B	184	LEU	2.6
1	D	68	PHE	2.6
1	C	36	HIS	2.6
1	A	33	LEU	2.6
1	C	167	SER	2.6
1	B	138	GLY	2.6
1	C	254	LEU	2.6
1	C	143	PHE	2.6
1	D	177	ASP	2.6
1	A	96	GLU	2.5
1	C	131	GLN	2.5
1	C	238	CYS	2.5
1	C	268	PHE	2.5
1	A	104	ASP	2.5
1	A	63	LEU	2.5
1	C	186	PRO	2.5
1	D	22	VAL	2.5
1	B	177	ASP	2.5
1	B	75	VAL	2.5
1	C	207	THR	2.5
1	B	86	ARG	2.5
1	C	257	CYS	2.5
1	B	141	ASP	2.5
1	C	208	LEU	2.5
1	A	115	SER	2.5
1	B	44	PRO	2.5
1	B	38	GLY	2.5
1	A	134	ARG	2.5
1	A	116	LEU	2.4
1	A	263	LEU	2.4
1	C	263	LEU	2.4
1	C	29	SER	2.4
1	D	75	VAL	2.4
1	A	81	ARG	2.4
1	A	264	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	213	LEU	2.4
1	D	29	SER	2.4
1	A	62	ALA	2.4
1	A	19	LEU	2.4
1	D	206	ALA	2.4
1	C	227	LEU	2.4
1	D	242	LEU	2.4
1	A	57	ASP	2.4
1	B	100	SER	2.4
1	B	215	SER	2.4
1	B	72	THR	2.4
1	B	262	THR	2.4
1	B	39	LEU	2.4
1	B	171	LEU	2.4
1	D	138	GLY	2.3
1	A	24	GLN	2.3
1	B	79	LEU	2.3
1	D	256	THR	2.3
1	D	45	ASN	2.3
1	A	180	LEU	2.3
1	B	33	LEU	2.3
1	C	242	LEU	2.3
1	B	169	PRO	2.3
1	B	152	VAL	2.3
1	A	139	ALA	2.3
1	B	168	MET	2.3
1	C	198	LEU	2.3
1	B	167	SER	2.3
1	B	193	SER	2.3
1	D	244	TRP	2.3
1	A	85	THR	2.3
1	A	154	TYR	2.3
1	C	48	ARG	2.3
1	A	157	LEU	2.3
1	A	165	ILE	2.3
1	C	162	TRP	2.3
1	B	233	GLY	2.3
1	B	156	ASN	2.2
1	B	209	ALA	2.2
1	A	132	LEU	2.2
1	A	254	LEU	2.2
1	A	44	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	73	GLY	2.2
1	B	189	PHE	2.2
1	B	214	PHE	2.2
1	A	184	LEU	2.2
1	B	47	ASP	2.2
1	A	80	SER	2.2
1	C	192	LEU	2.2
1	B	261	PRO	2.2
1	D	202	SER	2.2
1	B	16	LEU	2.2
1	A	275	GLU	2.2
1	B	87	ILE	2.2
1	C	126	ILE	2.2
1	C	25	ASN	2.2
1	A	119	PRO	2.2
1	D	265	GLY	2.2
1	D	274	GLY	2.2
1	D	113	SER	2.2
1	D	268	PHE	2.2
1	A	40	LEU	2.2
1	A	205	LEU	2.2
1	C	270	ALA	2.2
1	D	126	ILE	2.1
1	D	42	VAL	2.1
1	A	233	GLY	2.1
1	B	201	THR	2.1
1	C	259	SER	2.1
1	D	196	SER	2.1
1	A	199	ASP	2.1
1	B	76	ASP	2.1
1	A	111	LEU	2.1
1	A	23	CYS	2.1
1	A	60	ILE	2.1
1	A	193	SER	2.1
1	C	22	VAL	2.1
1	C	179	ASN	2.1
1	A	127	LEU	2.1
1	A	171	LEU	2.1
1	A	245	LEU	2.1
1	C	248	LEU	2.1
1	C	139	ALA	2.1
1	C	80	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	226	PRO	2.1
1	D	272	PRO	2.1
1	B	55	LEU	2.1
1	D	236	LEU	2.1
1	A	133	GLY	2.1
1	D	50	THR	2.1
1	B	84	ILE	2.1
1	D	161	PRO	2.0
1	C	38	GLY	2.0
1	D	85	THR	2.0
1	C	149	ASP	2.0
1	C	165	ILE	2.0
1	D	154	TYR	2.0
1	B	146	SER	2.0
1	C	194	GLN	2.0
1	A	30	LEU	2.0
1	C	95	LEU	2.0
1	D	229	LEU	2.0
1	A	209	ALA	2.0
1	C	104	ASP	2.0
1	C	188	VAL	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](#)

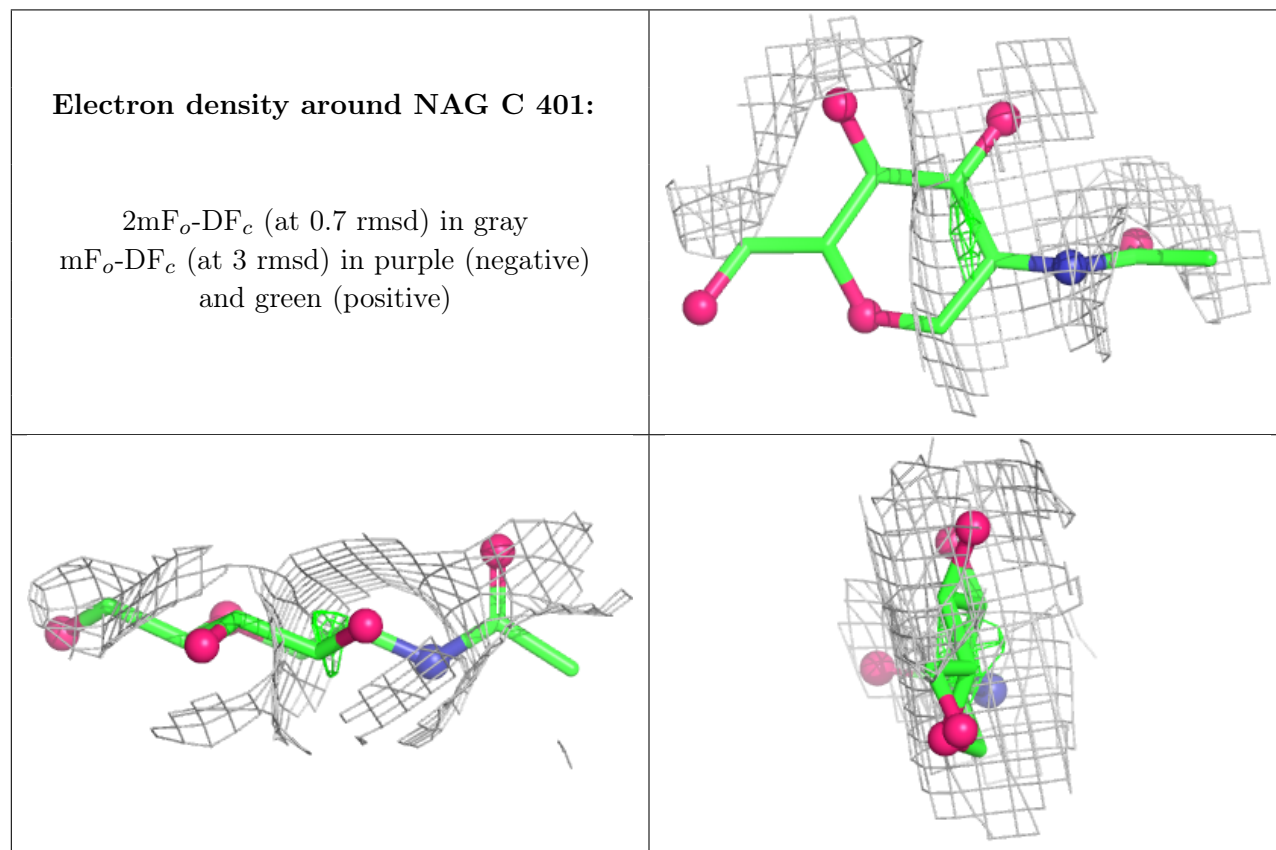
There are no oligosaccharides in this entry.

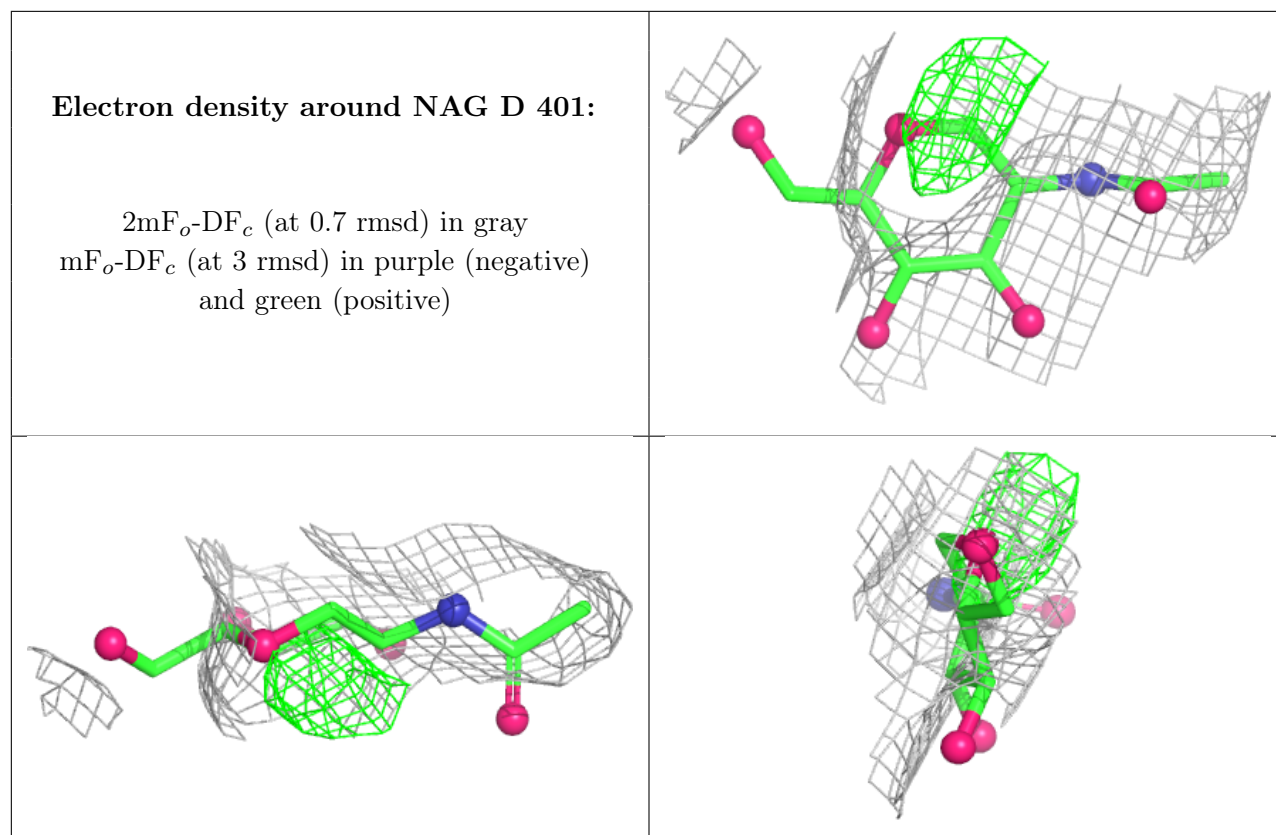
6.4 Ligands [i](#)

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
2	NAG	C	401	14/15	0.90	0.18	111,111,112,112	0
2	NAG	D	401	14/15	0.94	0.17	105,106,106,106	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.