



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2026 – 12:17 PM EDT

PDB ID : 36GK / pdb_000036gk
Title : D-GlcNAc-bound structure of Vibrio vulnificus putative carbohydrate binding module and split domain
Authors : Soares, B.P.; Allingham, J.S.; Davies, P.L.
Deposited on : 2026-06-08
Resolution : 2.28 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

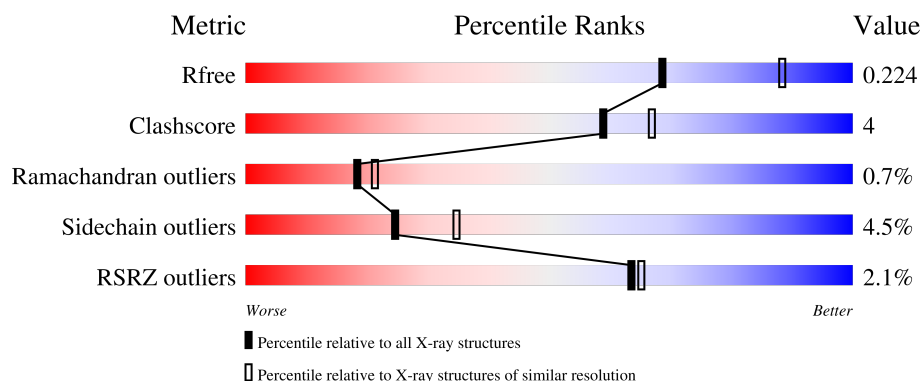
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	308	0% 75% 14% • • 6%
1	B	308	2% 77% 14% • • 6%
1	C	308	80% 11% • • 6%
1	D	308	4% 77% 12% • • 6%
1	E	308	3% 79% 11% • • 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11128 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 RTX protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2150	1323	348	476	3			
1	B	288	Total	C	N	O	S	0	0	0
			2150	1323	348	476	3			
1	C	288	Total	C	N	O	S	0	1	0
			2155	1326	348	478	3			
1	D	288	Total	C	N	O	S	0	0	0
			2150	1323	348	476	3			
1	E	287	Total	C	N	O	S	0	0	0
			2142	1319	346	474	3			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Ca	0	0
			7	7		
2	B	6	Total	Ca	0	0
			6	6		
2	C	6	Total	Ca	0	0
			6	6		
2	D	6	Total	Ca	0	0
			6	6		
2	E	6	Total	Ca	0	0
			6	6		

- Molecule 3 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
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	D	1	Total	C	N	O	0	0
			15	8	1	6		
3	E	1	Total	C	N	O	0	0
			15	8	1	6		

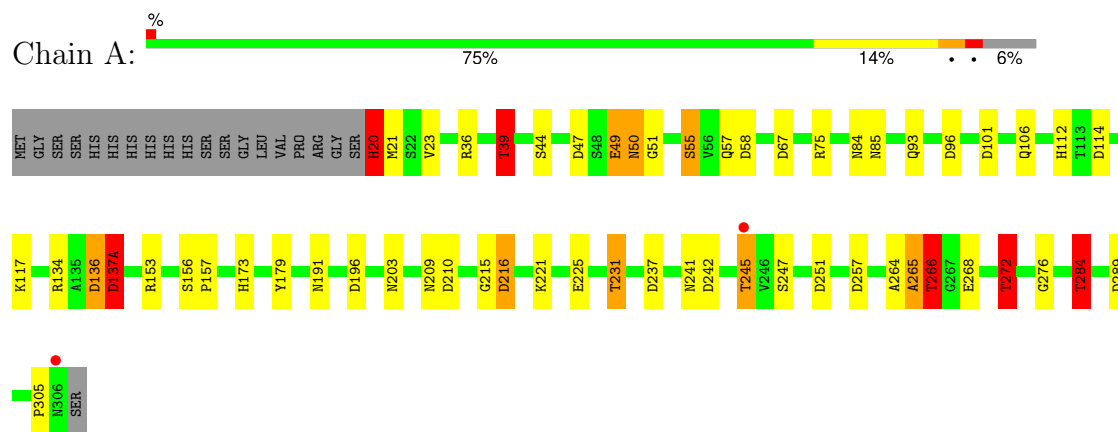
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	30	Total	O	0	0
			30	30		
4	C	134	Total	O	0	0
			134	134		
4	D	31	Total	O	0	0
			31	31		
4	E	36	Total	O	0	0
			36	36		

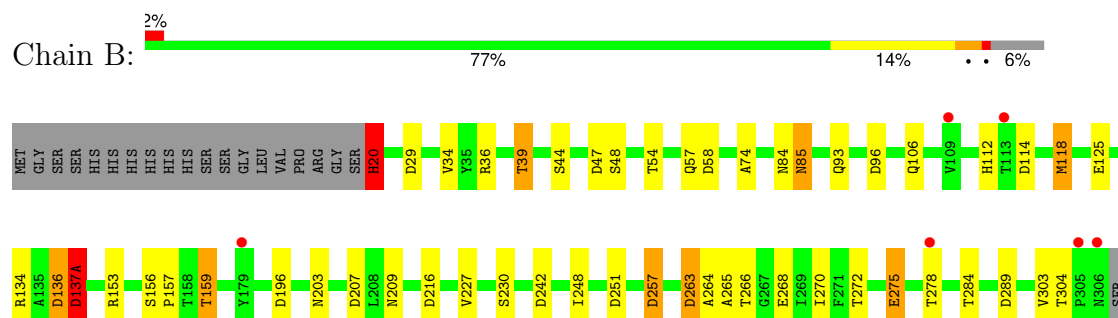
3 Residue-property plots [i](#)

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.

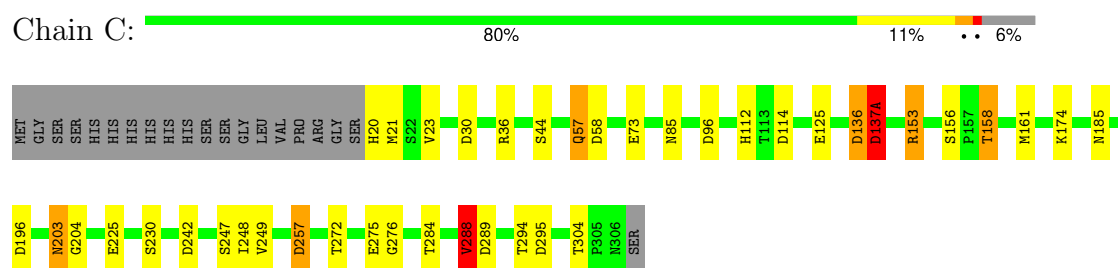
• Molecule 1: RTX protein



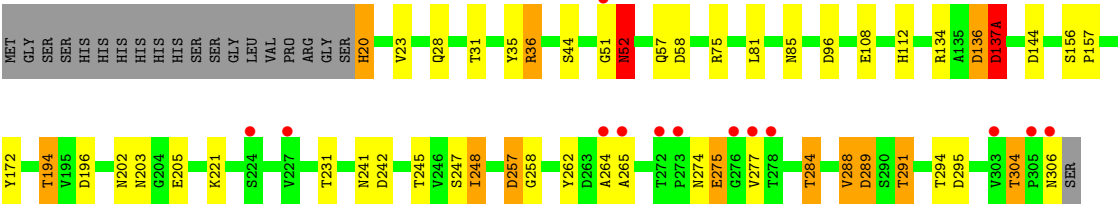
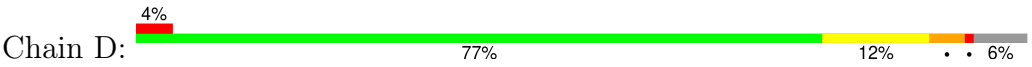
• Molecule 1: RTX protein



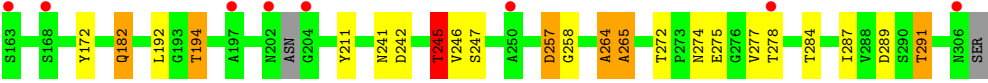
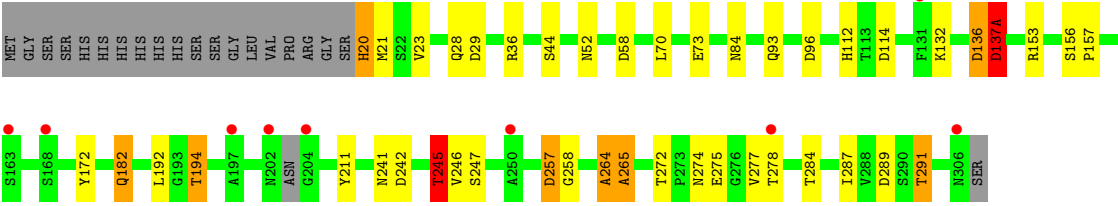
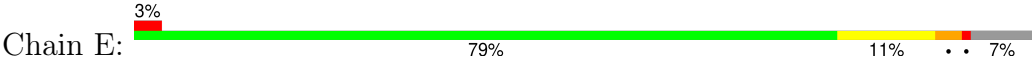
• Molecule 1: RTX protein



• Molecule 1: RTX protein



• Molecule 1: RTX protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.58Å 189.49Å 199.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.28 48.81 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.81-2.28) 100.0 (48.81-2.28)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.192 , 0.223 0.196 , 0.224	Depositor DCC
R_{free} test set	5270 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11128	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: CA, 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	1.10	3/2184 (0.1%)	1.65	36/2985 (1.2%)
1	B	0.84	0/2184	1.40	23/2985 (0.8%)
1	C	1.13	3/2192 (0.1%)	1.57	33/2996 (1.1%)
1	D	0.88	1/2184 (0.0%)	1.53	30/2985 (1.0%)
1	E	0.87	0/2175	1.48	27/2971 (0.9%)
All	All	0.97	7/10919 (0.1%)	1.53	149/14922 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	2
1	E	0	5
All	All	0	19

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	ARG	NE-CZ	9.29	1.43	1.33
1	C	20	HIS	CG-CD2	8.15	1.44	1.35
1	A	134	ARG	NE-CZ	6.79	1.40	1.33
1	A	137(A)	ASP	CG-OD1	6.17	1.37	1.25
1	C	23	VAL	C-O	-5.96	1.18	1.24
1	C	137(A)	ASP	CG-OD2	5.90	1.36	1.25
1	D	134	ARG	NE-CZ	5.40	1.39	1.33

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	194	THR	CA-CB-OG1	-16.35	85.08	109.60
1	A	272	THR	OG1-CB-CG2	-15.99	77.31	109.30
1	A	137(A)	ASP	CB-CA-C	14.51	139.29	110.42
1	C	158	THR	OG1-CB-CG2	-14.46	80.37	109.30
1	C	137(A)	ASP	CB-CA-C	14.45	139.17	110.42
1	D	137(A)	ASP	CB-CA-C	13.74	137.77	110.42
1	A	231	THR	CA-CB-OG1	-13.73	89.00	109.60
1	E	137(A)	ASP	CB-CA-C	13.36	137.00	110.42
1	B	137(A)	ASP	CB-CA-C	13.34	136.97	110.42
1	D	35	TYR	CA-C-N	-11.91	98.78	121.54
1	D	35	TYR	C-N-CA	-11.91	98.78	121.54
1	A	245	THR	CA-CB-OG1	-11.58	92.22	109.60
1	A	284	THR	CA-CB-OG1	-10.05	94.52	109.60
1	E	20	HIS	CA-CB-CG	9.94	123.74	113.80
1	D	20	HIS	CA-CB-CG	9.80	123.60	113.80
1	A	257	ASP	CA-CB-CG	9.68	122.28	112.60
1	C	96	ASP	CA-CB-CG	9.33	121.93	112.60
1	D	284	THR	CA-CB-OG1	-9.30	95.66	109.60
1	E	275	GLU	N-CA-CB	9.04	123.53	110.16
1	A	266	THR	CA-CB-OG1	-8.98	96.14	109.60
1	D	136	ASP	CA-C-N	8.90	138.54	121.54
1	D	136	ASP	C-N-CA	8.90	138.54	121.54
1	C	136	ASP	CA-C-N	8.87	138.48	121.54
1	C	136	ASP	C-N-CA	8.87	138.48	121.54
1	B	257	ASP	CA-CB-CG	8.45	121.05	112.60
1	C	125	GLU	CB-CG-CD	8.34	126.77	112.60
1	A	136	ASP	CA-C-N	8.28	137.36	121.54
1	A	136	ASP	C-N-CA	8.28	137.36	121.54
1	A	20	HIS	CA-CB-CG	8.23	122.03	113.80
1	B	275	GLU	N-CA-CB	8.18	121.88	110.01
1	D	291	THR	CA-CB-OG1	8.11	121.76	109.60
1	E	194	THR	N-CA-CB	-8.09	98.53	110.17
1	D	96	ASP	CA-CB-CG	7.97	120.57	112.60
1	B	118	MET	CG-SD-CE	-7.96	83.39	100.90
1	C	57	GLN	N-CA-CB	7.95	121.81	110.12
1	E	132	LYS	CG-CD-CE	7.94	129.57	111.30
1	E	136	ASP	CA-C-N	7.93	136.69	121.54
1	E	136	ASP	C-N-CA	7.93	136.69	121.54
1	B	136	ASP	CA-C-N	7.90	136.63	121.54
1	B	136	ASP	C-N-CA	7.90	136.63	121.54
1	B	304	THR	CB-CA-C	7.79	118.90	109.31
1	B	275	GLU	CB-CA-C	-7.79	98.65	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	HIS	CA-CB-CG	7.79	121.58	113.80
1	A	242	ASP	CB-CA-C	-7.71	97.55	109.89
1	D	31	THR	OG1-CB-CG2	-7.69	93.93	109.30
1	D	203	ASN	CB-CA-C	-7.53	98.49	111.45
1	B	96	ASP	CA-CB-CG	7.48	120.08	112.60
1	C	242	ASP	CB-CA-C	-7.41	98.34	109.90
1	E	194	THR	OG1-CB-CG2	7.33	123.96	109.30
1	E	289	ASP	CA-CB-CG	7.30	119.90	112.60
1	E	96	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	96	ASP	CA-CB-CG	7.16	119.76	112.60
1	C	136	ASP	CA-CB-CG	7.09	119.69	112.60
1	E	257	ASP	CA-CB-CG	7.01	119.61	112.60
1	D	52	ASN	N-CA-CB	6.90	122.15	110.49
1	B	284	THR	CA-CB-OG1	-6.86	99.31	109.60
1	C	73	GLU	CG-CD-OE2	-6.86	102.62	118.40
1	E	245	THR	CA-CB-OG1	-6.81	99.39	109.60
1	B	251	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	272	THR	CA-CB-CG2	6.76	121.99	110.50
1	D	304	THR	CB-CA-C	6.66	117.89	108.76
1	D	289	ASP	CA-CB-CG	6.62	119.22	112.60
1	D	275	GLU	CB-CA-C	-6.61	100.24	110.81
1	E	291	THR	OG1-CB-CG2	6.60	122.50	109.30
1	E	136	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	289	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	117	LYS	CG-CD-CE	6.57	126.42	111.30
1	C	161	MET	CG-SD-CE	-6.54	86.51	100.90
1	C	203	ASN	CB-CA-C	6.53	123.40	110.42
1	D	194	THR	CA-CB-OG1	-6.51	99.84	109.60
1	E	58	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	50	ASN	CB-CA-C	-6.50	97.49	110.42
1	C	289	ASP	CA-CB-CG	6.49	119.09	112.60
1	D	257	ASP	CA-CB-CG	6.47	119.07	112.60
1	D	295	ASP	CA-CB-CG	6.46	119.06	112.60
1	D	291	THR	OG1-CB-CG2	-6.42	96.46	109.30
1	B	289	ASP	CA-CB-CG	6.41	119.01	112.60
1	B	136	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	210	ASP	CA-CB-CG	6.35	118.95	112.60
1	D	275	GLU	N-CA-CB	6.34	119.38	109.94
1	C	20	HIS	N-CA-CB	6.33	121.25	110.50
1	C	225	GLU	CG-CD-OE2	-6.29	103.92	118.40
1	C	20	HIS	CB-CA-C	-6.16	98.39	110.10
1	D	136	ASP	CA-CB-CG	6.16	118.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	THR	N-CA-CB	-6.10	101.56	110.47
1	A	153	ARG	NE-CZ-NH2	6.04	124.64	119.20
1	E	284	THR	CA-CB-OG1	-6.03	100.55	109.60
1	C	58	ASP	CA-CB-CG	6.03	118.63	112.60
1	D	242	ASP	CB-CA-C	-5.96	100.61	109.90
1	B	196	ASP	CA-CB-CG	5.93	118.53	112.60
1	C	284	THR	OG1-CB-CG2	-5.92	97.47	109.30
1	A	266	THR	CA-CB-CG2	5.88	120.49	110.50
1	C	57	GLN	CB-CA-C	-5.84	101.09	110.79
1	E	29	ASP	CA-CB-CG	5.82	118.42	112.60
1	E	242	ASP	CB-CA-C	-5.81	100.08	109.72
1	B	29	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	191	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	D	144	ASP	CB-CA-C	5.73	120.16	111.80
1	E	21	MET	CG-SD-CE	5.69	113.42	100.90
1	D	196	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	114	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	39	THR	CB-CA-C	5.67	119.10	109.80
1	E	28	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	A	216	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	58	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	225	GLU	CB-CA-C	5.58	119.72	109.46
1	E	73	GLU	CG-CD-OE2	-5.58	105.58	118.40
1	C	20	HIS	CA-CB-CG	5.57	119.37	113.80
1	B	58	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	114	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	284	THR	CA-CB-OG1	-5.48	101.38	109.60
1	D	194	THR	N-CA-CB	-5.47	102.13	110.45
1	C	153	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	251	ASP	N-CA-CB	-5.45	102.58	110.70
1	A	50	ASN	N-CA-CB	5.45	119.70	110.49
1	B	159	THR	CA-CB-CG2	5.44	119.75	110.50
1	A	47	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	21	MET	CB-CA-C	-5.43	99.12	109.66
1	B	207	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	305	PRO	CB-CA-C	5.42	118.05	110.95
1	C	288	VAL	CB-CA-C	-5.40	101.04	110.71
1	C	196	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	55	SER	N-CA-CB	-5.37	102.69	111.66
1	A	237	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	36	ARG	CD-NE-CZ	5.36	131.90	124.40
1	A	49	GLU	N-CA-C	-5.34	102.11	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	264	ALA	CA-C-N	-5.32	111.39	121.54
1	E	264	ALA	C-N-CA	-5.32	111.39	121.54
1	A	173	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	D	28	GLN	OE1-CD-NE2	5.28	127.88	122.60
1	E	194	THR	CB-CA-C	5.28	119.26	109.54
1	C	295	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	209	ASN	CA-CB-CG	-5.22	107.38	112.60
1	C	174	LYS	CB-CA-C	5.22	118.04	109.90
1	B	263	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	58	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	114	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	30	ASP	CB-CA-C	5.18	118.43	110.14
1	D	205	GLU	N-CA-CB	-5.17	101.99	110.68
1	C	185	ASN	OD1-CG-ND2	5.14	127.74	122.60
1	A	101	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	231	THR	OG1-CB-CG2	-5.13	99.03	109.30
1	A	196	ASP	CA-CB-CG	5.13	117.73	112.60
1	E	114	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	257	ASP	CA-CB-CG	5.05	117.65	112.60
1	D	36	ARG	CA-C-O	-5.05	113.29	120.51
1	E	20	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	C	272	THR	CA-CB-OG1	-5.02	102.07	109.60
1	B	47	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ASP	Peptide,Mainchain
1	A	276	GLY	Peptide
1	A	75	ARG	Sidechain
1	B	136	ASP	Peptide,Mainchain
1	B	153	ARG	Sidechain
1	B	36	ARG	Sidechain
1	C	136	ASP	Peptide,Mainchain
1	C	276	GLY	Peptide
1	C	36	ARG	Sidechain
1	D	136	ASP	Peptide,Mainchain
1	E	136	ASP	Peptide,Mainchain
1	E	153	ARG	Sidechain
1	E	277	VAL	Peptide
1	E	36	ARG	Sidechain

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	2150	0	1996	21	0
1	B	2150	0	1997	23	0
1	C	2155	0	2001	8	0
1	D	2150	0	1996	20	0
1	E	2142	0	1989	22	0
2	A	7	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	E	6	0	0	0	0
3	B	15	0	14	0	0
3	D	15	0	13	0	0
3	E	15	0	14	4	0
4	A	74	0	0	4	0
4	B	30	0	0	1	0
4	C	134	0	0	2	0
4	D	31	0	0	2	0
4	E	36	0	0	2	0
All	All	11128	0	10020	92	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 4.

All (92) 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:E:52:ASN:HD21	1:E:182:GLN:HG3	1.30	0.94
1:A:284:THR:HG22	4:A:511:HOH:O	1.72	0.89
1:D:23:VAL:H	1:D:241:ASN:HD21	1.20	0.89
1:E:23:VAL:H	1:E:241:ASN:HD21	1.22	0.88
1:E:264:ALA:O	1:E:265:ALA:HB3	1.74	0.88
1:A:39:THR:CG2	1:A:216:ASP:H	1.87	0.88
1:A:23:VAL:H	1:A:241:ASN:HD21	1.21	0.86
1:D:289:ASP:OD1	1:D:291:THR:HG22	1.76	0.85
1:A:50:ASN:ND2	4:A:502:HOH:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:HH11	1:B:159:THR:HG23	1.45	0.82
1:C:156:SER:O	1:C:158:THR:HG23	1.82	0.80
1:A:264:ALA:O	1:A:265:ALA:HB3	1.81	0.80
1:A:85:ASN:OD1	4:A:501:HOH:O	2.02	0.78
1:E:156:SER:HB2	3:E:401:NAG:H83	1.68	0.75
1:B:39:THR:HG23	1:B:216:ASP:H	1.52	0.74
1:C:153:ARG:HD3	4:C:513:HOH:O	1.88	0.74
1:D:81:LEU:O	4:D:501:HOH:O	2.07	0.72
1:D:248:ILE:HG21	1:D:262:TYR:CZ	2.26	0.71
1:E:182:GLN:O	1:E:182:GLN:HG2	1.90	0.70
1:A:266:THR:HG22	1:A:268:GLU:H	1.58	0.69
1:B:39:THR:CG2	1:B:216:ASP:H	2.05	0.69
1:D:194:THR:HG23	1:D:202:ASN:OD1	1.93	0.69
1:A:84:ASN:HD21	1:A:93:GLN:HE22	1.39	0.68
1:E:84:ASN:HD21	1:E:93:GLN:HE22	1.42	0.68
1:A:39:THR:HG22	1:A:216:ASP:H	1.58	0.67
1:B:20:HIS:N	4:B:502:HOH:O	2.26	0.67
1:D:274:ASN:O	1:D:277:VAL:HG12	1.95	0.67
1:E:264:ALA:O	1:E:265:ALA:CB	2.35	0.67
1:C:85:ASN:OD1	4:C:501:HOH:O	2.12	0.66
1:A:264:ALA:O	1:A:265:ALA:CB	2.41	0.65
1:B:84:ASN:HD21	1:B:93:GLN:HE22	1.45	0.65
1:D:258:GLY:HA2	1:D:274:ASN:ND2	2.11	0.65
1:C:288:VAL:HG13	1:C:294:THR:HG22	1.79	0.64
1:B:134:ARG:HB2	1:B:159:THR:HG22	1.78	0.64
1:B:278:THR:O	1:B:303:VAL:HG23	1.98	0.64
1:D:51:GLY:O	1:D:52:ASN:O	2.17	0.63
1:E:137(A):ASP:OD1	1:E:137(A):ASP:N	2.32	0.61
1:D:289:ASP:CG	1:D:291:THR:HG22	2.25	0.61
1:E:258:GLY:HA2	1:E:274:ASN:ND2	2.15	0.61
1:B:266:THR:HG23	1:B:268:GLU:H	1.66	0.60
1:B:34:VAL:HG23	1:B:39:THR:HG22	1.84	0.59
1:A:39:THR:HG21	1:A:216:ASP:H	1.66	0.58
1:C:203:ASN:OD1	1:C:204:GLY:N	2.38	0.56
1:A:209:ASN:ND2	1:A:209:ASN:H	2.03	0.55
1:B:84:ASN:C	1:B:85:ASN:HD22	2.14	0.55
1:B:74:ALA:HB1	1:B:118:MET:CE	2.36	0.54
1:A:49:GLU:O	1:A:51:GLY:N	2.39	0.54
1:D:85:ASN:OD1	4:D:501:HOH:O	2.18	0.54
1:E:246:VAL:CG2	1:E:287:ILE:HD12	2.38	0.54
1:D:36:ARG:H	1:D:75:ARG:HH12	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:OD2	1:A:221:LYS:NZ	2.42	0.53
1:B:263:ASP:CG	1:B:266:THR:HG22	2.34	0.53
1:E:156:SER:CB	3:E:401:NAG:H83	2.37	0.52
1:E:157:PRO:HD3	3:E:401:NAG:H82	1.92	0.52
1:E:137(A):ASP:OD2	1:E:182:GLN:HB3	2.11	0.51
1:B:134:ARG:NH1	1:B:159:THR:HG23	2.21	0.51
1:E:246:VAL:HG21	1:E:287:ILE:HD12	1.91	0.51
1:E:291:THR:O	4:E:501:HOH:O	2.19	0.50
1:B:264:ALA:O	1:B:265:ALA:HB3	2.12	0.50
1:A:20:HIS:HB2	1:D:172:TYR:CD2	2.46	0.50
1:E:52:ASN:ND2	1:E:182:GLN:HG3	2.13	0.49
1:E:156:SER:HB2	1:E:157:PRO:CD	2.43	0.49
1:D:156:SER:HB2	1:D:157:PRO:CD	2.43	0.48
1:A:284:THR:CG2	4:A:511:HOH:O	2.46	0.48
1:B:227:VAL:HG22	1:B:270:ILE:HD13	1.95	0.48
1:D:288:VAL:CG1	1:D:294:THR:HG22	2.44	0.48
1:D:264:ALA:O	1:D:265:ALA:HB3	2.14	0.47
1:E:44:SER:HB2	1:E:112:HIS:CG	2.49	0.47
1:A:44:SER:HB2	1:A:112:HIS:CG	2.49	0.47
1:C:44:SER:HB2	1:C:112:HIS:CG	2.49	0.47
1:B:74:ALA:CB	1:B:118:MET:CE	2.93	0.47
1:E:192:LEU:HD23	1:E:211:TYR:CE2	2.50	0.46
1:D:44:SER:HB2	1:D:112:HIS:CG	2.51	0.46
1:B:44:SER:HB2	1:B:112:HIS:CG	2.51	0.46
1:C:230:SER:HB2	1:C:248:ILE:HG13	1.97	0.45
1:E:157:PRO:HD3	3:E:401:NAG:C8	2.47	0.45
1:B:156:SER:HB2	1:B:157:PRO:CD	2.47	0.44
1:A:156:SER:HB2	1:A:157:PRO:CD	2.47	0.44
1:B:230:SER:HB2	1:B:248:ILE:HG13	1.99	0.44
1:D:288:VAL:HG13	1:D:294:THR:HG22	2.01	0.43
1:C:249:VAL:HG22	1:C:288:VAL:HG22	2.01	0.42
1:D:258:GLY:HA2	1:D:274:ASN:HD21	1.82	0.42
1:A:225:GLU:HB3	1:A:272:THR:HG22	2.01	0.42
1:D:245:THR:O	1:D:289:ASP:HA	2.20	0.42
1:B:227:VAL:HG22	1:B:270:ILE:CD1	2.50	0.41
1:B:85:ASN:HD22	1:B:85:ASN:N	2.19	0.41
1:A:39:THR:HG22	1:A:215:GLY:CA	2.51	0.41
1:B:20:HIS:HB2	1:E:172:TYR:CD1	2.55	0.41
1:B:263:ASP:OD1	1:B:266:THR:HG22	2.21	0.41
1:E:245:THR:HG22	4:E:508:HOH:O	2.20	0.41
1:A:179:TYR:CD1	1:A:179:TYR:C	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:LYS:HE3	1:D:304:THR:HG23	2.02	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	286/308 (93%)	271 (95%)	12 (4%)	3 (1%)	12	13
1	B	286/308 (93%)	273 (96%)	11 (4%)	2 (1%)	18	21
1	C	287/308 (93%)	274 (96%)	12 (4%)	1 (0%)	36	44
1	D	286/308 (93%)	269 (94%)	15 (5%)	2 (1%)	18	21
1	E	283/308 (92%)	268 (95%)	13 (5%)	2 (1%)	18	21
All	All	1428/1540 (93%)	1355 (95%)	63 (4%)	10 (1%)	18	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137(A)	ASP
1	B	137(A)	ASP
1	C	137(A)	ASP
1	D	52	ASN
1	D	137(A)	ASP
1	E	137(A)	ASP
1	A	265	ALA
1	A	203	ASN
1	B	203	ASN
1	E	265	ALA

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	240/257 (93%)	227 (95%)	13 (5%)	20	27
1	B	240/257 (93%)	227 (95%)	13 (5%)	20	27
1	C	241/257 (94%)	234 (97%)	7 (3%)	37	52
1	D	240/257 (93%)	229 (95%)	11 (5%)	24	34
1	E	239/257 (93%)	229 (96%)	10 (4%)	26	37
All	All	1200/1285 (93%)	1146 (96%)	54 (4%)	24	35

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

Mol	Chain	Res	Type
1	A	20	HIS
1	A	21	MET
1	A	39	THR
1	A	55	SER
1	A	57	GLN
1	A	106	GLN
1	A	137(A)	ASP
1	A	231	THR
1	A	245	THR
1	A	247	SER
1	A	266	THR
1	A	272	THR
1	A	284	THR
1	B	20	HIS
1	B	39	THR
1	B	48	SER
1	B	54	THR
1	B	57	GLN
1	B	85	ASN
1	B	106	GLN
1	B	125	GLU
1	B	137(A)	ASP
1	B	242	ASP

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Mol	Chain	Res	Type
1	B	257	ASP
1	B	272	THR
1	B	275	GLU
1	C	57	GLN
1	C	137(A)	ASP
1	C	247	SER
1	C	257	ASP
1	C	275	GLU
1	C	288	VAL
1	C	304	THR
1	D	20	HIS
1	D	57	GLN
1	D	108	GLU
1	D	137(A)	ASP
1	D	247	SER
1	D	248	ILE
1	D	257	ASP
1	D	275	GLU
1	D	284	THR
1	D	288	VAL
1	D	306	ASN
1	E	20	HIS
1	E	70	LEU
1	E	137(A)	ASP
1	E	182	GLN
1	E	194	THR
1	E	245	THR
1	E	247	SER
1	E	257	ASP
1	E	272	THR
1	E	278	THR

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	20	HIS
1	A	28	GLN
1	A	57	GLN
1	A	93	GLN
1	A	100	ASN
1	A	128	ASN
1	A	198	ASN

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Mol	Chain	Res	Type
1	A	209	ASN
1	B	20	HIS
1	B	85	ASN
1	B	93	GLN
1	C	20	HIS
1	C	111	ASN
1	C	128	ASN
1	C	173	HIS
1	D	128	ASN
1	D	173	HIS
1	D	274	ASN
1	E	28	GLN
1	E	93	GLN
1	E	274	ASN

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 34 ligands modelled in this entry, 31 are monoatomic - leaving 3 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	NAG	B	401	2	15,15,15	0.68	0	21,21,21	1.62	5 (23%)
3	NAG	D	401	2	15,15,15	0.70	0	21,21,21	2.91	8 (38%)
3	NAG	E	401	2	15,15,15	1.04	0	21,21,21	3.32	10 (47%)

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	NAG	B	401	2	-	2/6/26/26	0/1/1/1
3	NAG	D	401	2	-	0/6/26/26	0/1/1/1
3	NAG	E	401	2	-	4/6/26/26	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	NAG	O5-C1-C2	8.93	118.49	109.52
3	E	401	NAG	C1-C2-C3	-6.81	101.25	110.54
3	D	401	NAG	C1-C2-N2	6.57	118.34	110.73
3	E	401	NAG	C1-C2-N2	6.09	117.78	110.73
3	E	401	NAG	C3-C2-N2	5.47	120.69	110.62
3	E	401	NAG	O3-C3-C2	4.77	119.07	109.58
3	E	401	NAG	C2-N2-C7	4.57	133.80	123.11
3	E	401	NAG	C6-C5-C4	4.10	123.08	113.02
3	E	401	NAG	C8-C7-N2	3.58	122.05	116.12
3	B	401	NAG	C3-C2-N2	3.32	116.74	110.62
3	D	401	NAG	C3-C2-N2	3.18	116.47	110.62
3	E	401	NAG	O6-C6-C5	3.16	122.09	111.33
3	B	401	NAG	O5-C1-C2	3.07	112.60	109.52
3	E	401	NAG	O7-C7-C8	-3.00	116.71	122.05
3	D	401	NAG	C1-C2-C3	-2.99	106.47	110.54
3	D	401	NAG	O1-C1-C2	-2.65	103.70	109.22
3	D	401	NAG	O4-C4-C3	-2.50	104.48	110.38
3	D	401	NAG	O3-C3-C2	2.46	114.48	109.58
3	B	401	NAG	O3-C3-C2	2.44	114.44	109.58
3	D	401	NAG	O1-C1-O5	-2.26	103.71	110.41
3	E	401	NAG	C3-C4-C5	-2.23	106.19	110.23
3	B	401	NAG	C1-C2-C3	-2.08	107.71	110.54
3	B	401	NAG	O4-C4-C3	-2.04	105.57	110.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

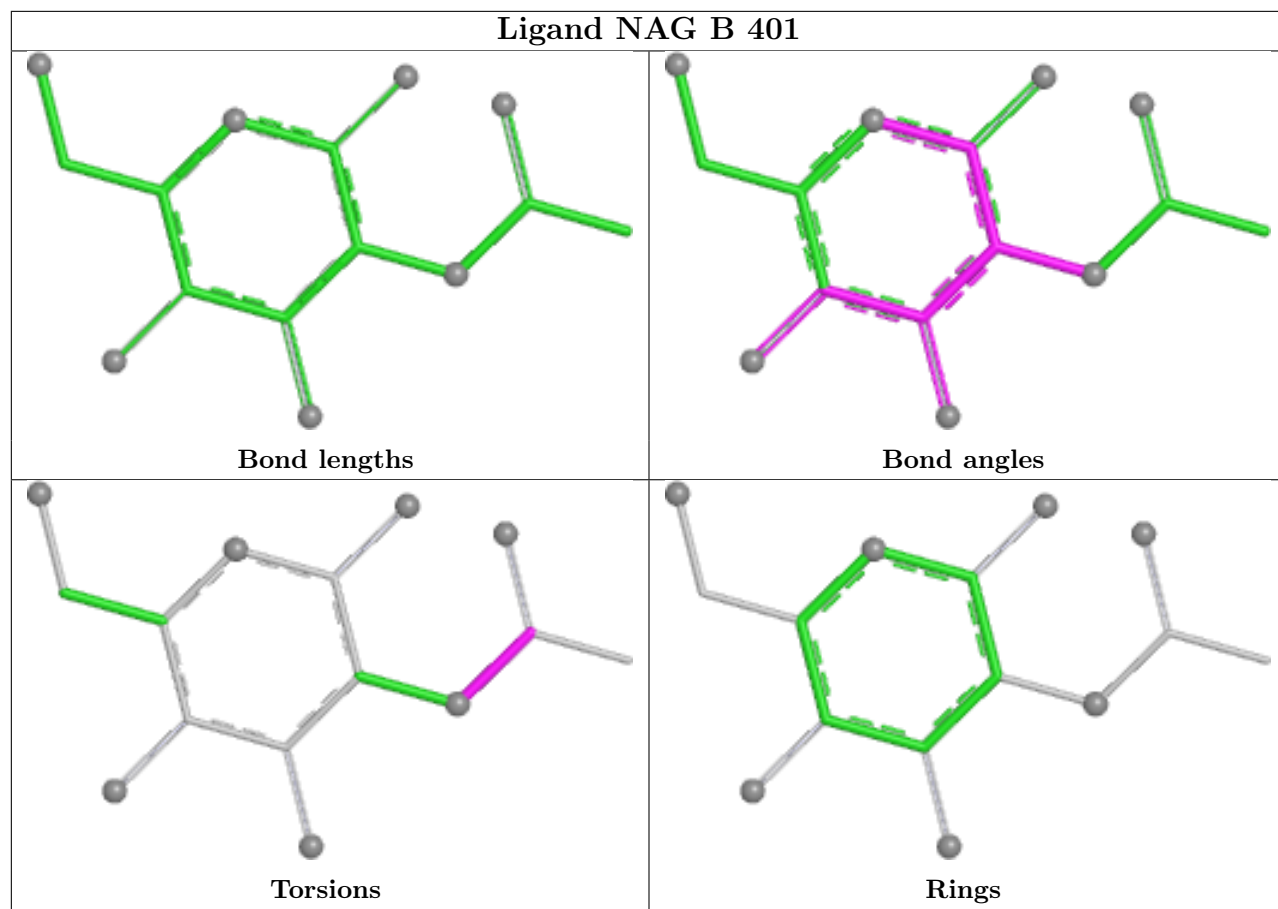
Mol	Chain	Res	Type	Atoms
3	B	401	NAG	C8-C7-N2-C2
3	B	401	NAG	O7-C7-N2-C2
3	E	401	NAG	C8-C7-N2-C2
3	E	401	NAG	O7-C7-N2-C2
3	E	401	NAG	O5-C5-C6-O6
3	E	401	NAG	C4-C5-C6-O6

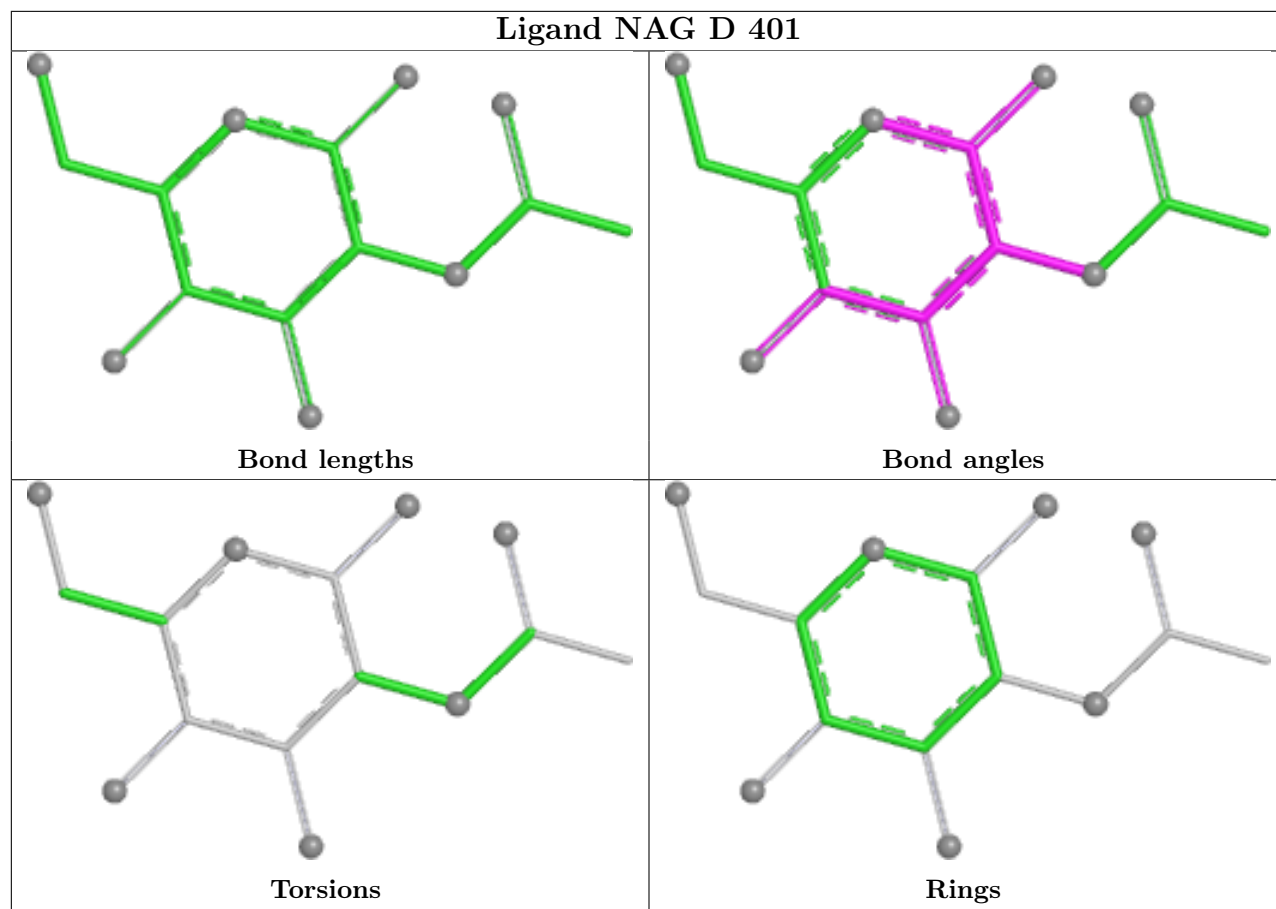
There are no ring outliers.

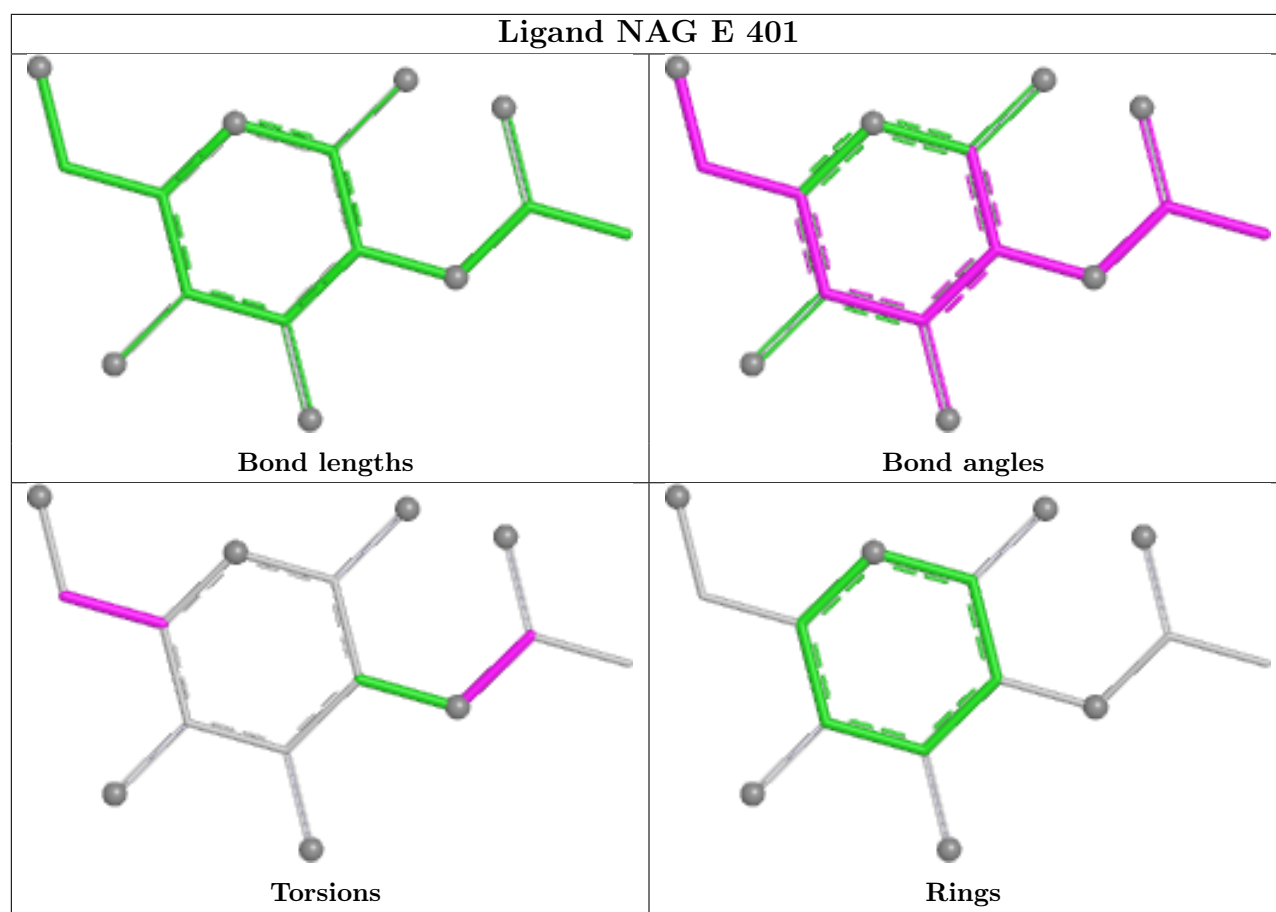
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	NAG	4	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 [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	288/308 (93%)	-0.08	2 (0%) 84 85	49, 67, 97, 122	0
1	B	288/308 (93%)	0.21	6 (2%) 63 65	55, 86, 120, 147	0
1	C	288/308 (93%)	-0.36	0 100 100	42, 57, 83, 116	1 (0%)
1	D	288/308 (93%)	0.36	13 (4%) 38 39	59, 84, 124, 152	0
1	E	287/308 (93%)	0.28	9 (3%) 51 53	51, 84, 129, 156	0
All	All	1439/1540 (93%)	0.08	30 (2%) 63 65	42, 74, 119, 156	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	265	ALA	3.7
1	E	278	THR	3.7
1	D	277	VAL	3.4
1	D	306	ASN	3.3
1	E	204	GLY	3.2
1	D	278	THR	3.2
1	D	227	VAL	2.9
1	D	305	PRO	2.8
1	E	202	ASN	2.8
1	D	224	SER	2.8
1	A	306	ASN	2.7
1	A	245	THR	2.7
1	D	276	GLY	2.6
1	B	305	PRO	2.6
1	E	197	ALA	2.5
1	B	306	ASN	2.5
1	E	168	SER	2.4
1	D	273	PRO	2.3
1	E	306	ASN	2.3
1	B	179	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	51	GLY	2.2
1	E	250	ALA	2.2
1	B	109	VAL	2.1
1	D	303	VAL	2.1
1	E	131	PHE	2.1
1	B	278	THR	2.0
1	D	272	THR	2.0
1	E	163	SER	2.0
1	B	113	THR	2.0
1	D	264	ALA	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(Å ²)	Q<0.9
3	NAG	E	401	15/15	0.83	0.12	87,121,153,157	0
3	NAG	B	401	15/15	0.86	0.11	96,125,152,160	0
2	CA	B	406	1/1	0.90	0.11	98,98,98,98	0
2	CA	B	404	1/1	0.93	0.07	103,103,103,103	0
2	CA	A	407	1/1	0.93	0.07	98,98,98,98	0
3	NAG	D	401	15/15	0.94	0.09	62,86,111,114	0
2	CA	D	403	1/1	0.96	0.07	93,93,93,93	0
2	CA	C	406	1/1	0.96	0.04	57,57,57,57	0
2	CA	D	405	1/1	0.97	0.05	87,87,87,87	0
2	CA	A	405	1/1	0.98	0.03	62,62,62,62	0
2	CA	A	404	1/1	0.99	0.04	64,64,64,64	0
2	CA	C	403	1/1	0.99	0.05	60,60,60,60	0
2	CA	C	405	1/1	0.99	0.04	65,65,65,65	0

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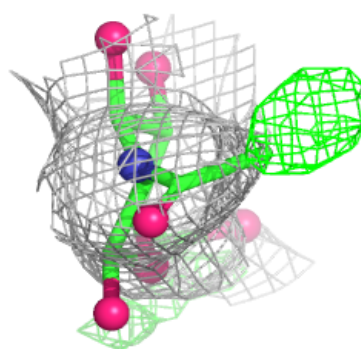
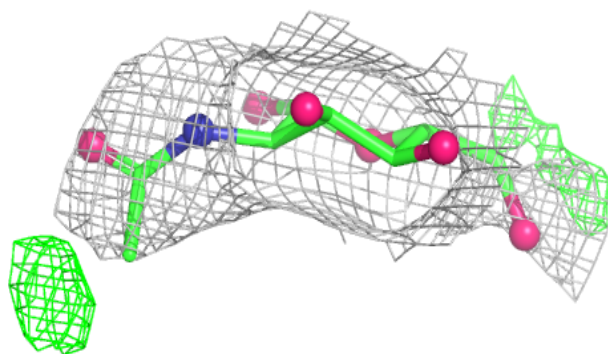
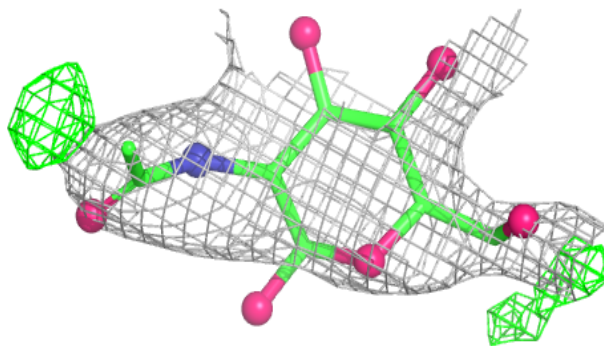
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	401	1/1	0.99	0.04	63,63,63,63	0
2	CA	D	402	1/1	0.99	0.02	79,79,79,79	0
2	CA	A	406	1/1	0.99	0.08	75,75,75,75	0
2	CA	D	404	1/1	0.99	0.04	69,69,69,69	0
2	CA	A	402	1/1	0.99	0.03	61,61,61,61	0
2	CA	D	406	1/1	0.99	0.05	66,66,66,66	0
2	CA	D	407	1/1	0.99	0.03	71,71,71,71	0
2	CA	E	402	1/1	0.99	0.02	95,95,95,95	0
2	CA	E	403	1/1	0.99	0.10	76,76,76,76	0
2	CA	E	404	1/1	0.99	0.02	59,59,59,59	0
2	CA	E	406	1/1	0.99	0.04	105,105,105,105	0
2	CA	E	407	1/1	0.99	0.05	81,81,81,81	0
2	CA	B	402	1/1	0.99	0.04	97,97,97,97	0
2	CA	A	403	1/1	0.99	0.04	64,64,64,64	0
2	CA	B	405	1/1	0.99	0.03	75,75,75,75	0
2	CA	E	405	1/1	1.00	0.02	59,59,59,59	0
2	CA	C	401	1/1	1.00	0.01	48,48,48,48	0
2	CA	C	402	1/1	1.00	0.01	47,47,47,47	0
2	CA	B	403	1/1	1.00	0.06	62,62,62,62	0
2	CA	C	404	1/1	1.00	0.02	54,54,54,54	0
2	CA	B	407	1/1	1.00	0.03	59,59,59,59	0

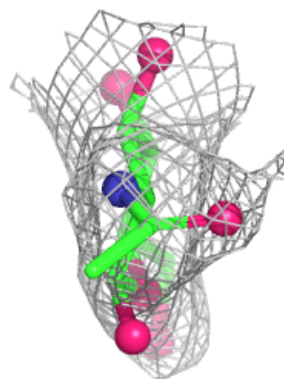
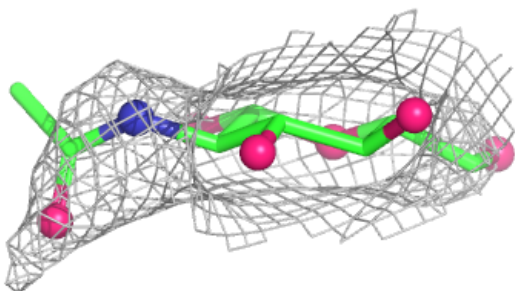
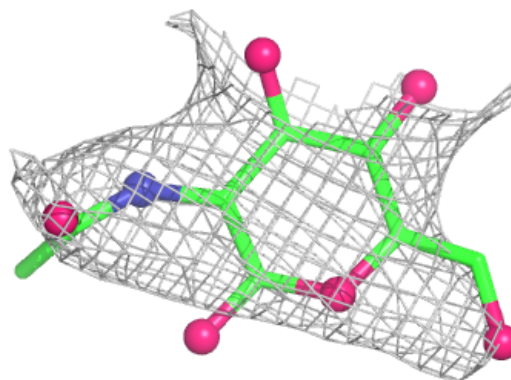
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG E 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

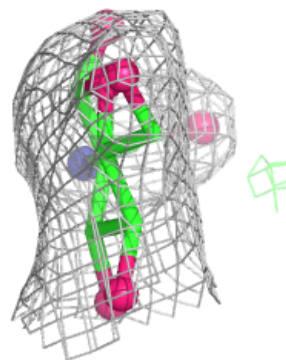
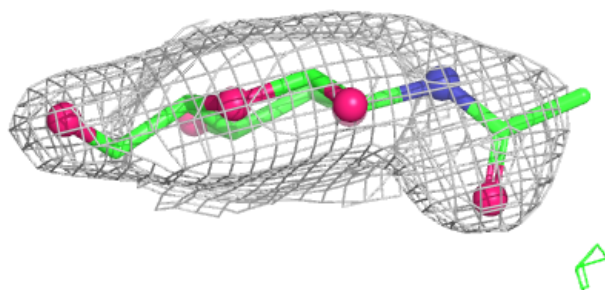
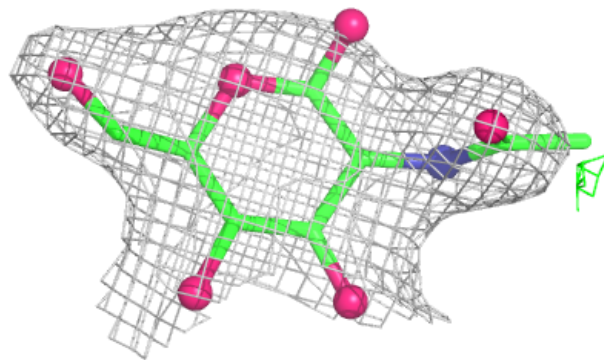
**Electron density around NAG B 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAG D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.