



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:20 PM UTC

PDB ID : 7JTY / pdb_00007jty
Title : Co-crystal structure of alpha glucosidase with compound 1
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2020-08-18
Resolution : 2.21 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

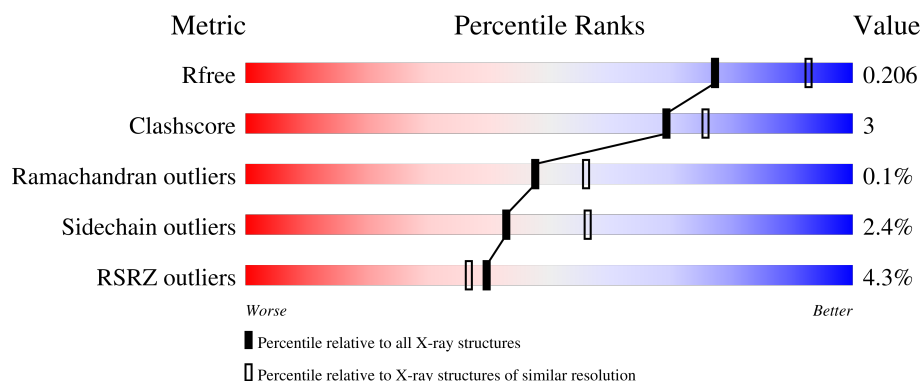
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	977	2% 79% 8% 13%
1	C	977	5% 78% 9% 12%
2	B	547	15% 85%
2	D	547	15% 84%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15943 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 Alpha glucosidase 2 alpha neutral subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	851	Total	C	N	O	S	0	6	0
			6868	4403	1183	1253	29			
1	C	857	Total	C	N	O	S	0	7	0
			6881	4408	1190	1254	29			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP A1A4T2
A	3	GLY	-	expression tag	UNP A1A4T2
A	4	ILE	-	expression tag	UNP A1A4T2
A	5	LEU	-	expression tag	UNP A1A4T2
A	6	PRO	-	expression tag	UNP A1A4T2
A	7	SER	-	expression tag	UNP A1A4T2
A	8	PRO	-	expression tag	UNP A1A4T2
A	9	GLY	-	expression tag	UNP A1A4T2
A	10	MET	-	expression tag	UNP A1A4T2
A	11	PRO	-	expression tag	UNP A1A4T2
A	12	ALA	-	expression tag	UNP A1A4T2
A	13	LEU	-	expression tag	UNP A1A4T2
A	14	LEU	-	expression tag	UNP A1A4T2
A	15	SER	-	expression tag	UNP A1A4T2
A	16	LEU	-	expression tag	UNP A1A4T2
A	17	VAL	-	expression tag	UNP A1A4T2
A	18	SER	-	expression tag	UNP A1A4T2
A	19	LEU	-	expression tag	UNP A1A4T2
A	20	LEU	-	expression tag	UNP A1A4T2
A	21	SER	-	expression tag	UNP A1A4T2
A	22	VAL	-	expression tag	UNP A1A4T2
A	23	LEU	-	expression tag	UNP A1A4T2
A	24	LEU	-	expression tag	UNP A1A4T2
A	25	MET	-	expression tag	UNP A1A4T2
A	26	GLY	-	expression tag	UNP A1A4T2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	CYS	-	expression tag	UNP A1A4T2
A	28	VAL	-	expression tag	UNP A1A4T2
A	29	ALA	-	expression tag	UNP A1A4T2
A	30	GLU	-	expression tag	UNP A1A4T2
A	31	THR	-	expression tag	UNP A1A4T2
A	32	GLY	-	expression tag	UNP A1A4T2
A	97	ASP	ASN	engineered mutation	UNP A1A4T2
A	967	SER	-	expression tag	UNP A1A4T2
A	968	ALA	-	expression tag	UNP A1A4T2
A	969	TRP	-	expression tag	UNP A1A4T2
A	970	SER	-	expression tag	UNP A1A4T2
A	971	HIS	-	expression tag	UNP A1A4T2
A	972	PRO	-	expression tag	UNP A1A4T2
A	973	GLN	-	expression tag	UNP A1A4T2
A	974	PHE	-	expression tag	UNP A1A4T2
A	975	GLU	-	expression tag	UNP A1A4T2
A	976	LYS	-	expression tag	UNP A1A4T2
A	977	LEU	-	expression tag	UNP A1A4T2
A	978	GLU	-	expression tag	UNP A1A4T2
C	2	MET	-	initiating methionine	UNP A1A4T2
C	3	GLY	-	expression tag	UNP A1A4T2
C	4	ILE	-	expression tag	UNP A1A4T2
C	5	LEU	-	expression tag	UNP A1A4T2
C	6	PRO	-	expression tag	UNP A1A4T2
C	7	SER	-	expression tag	UNP A1A4T2
C	8	PRO	-	expression tag	UNP A1A4T2
C	9	GLY	-	expression tag	UNP A1A4T2
C	10	MET	-	expression tag	UNP A1A4T2
C	11	PRO	-	expression tag	UNP A1A4T2
C	12	ALA	-	expression tag	UNP A1A4T2
C	13	LEU	-	expression tag	UNP A1A4T2
C	14	LEU	-	expression tag	UNP A1A4T2
C	15	SER	-	expression tag	UNP A1A4T2
C	16	LEU	-	expression tag	UNP A1A4T2
C	17	VAL	-	expression tag	UNP A1A4T2
C	18	SER	-	expression tag	UNP A1A4T2
C	19	LEU	-	expression tag	UNP A1A4T2
C	20	LEU	-	expression tag	UNP A1A4T2
C	21	SER	-	expression tag	UNP A1A4T2
C	22	VAL	-	expression tag	UNP A1A4T2
C	23	LEU	-	expression tag	UNP A1A4T2
C	24	LEU	-	expression tag	UNP A1A4T2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	25	MET	-	expression tag	UNP A1A4T2
C	26	GLY	-	expression tag	UNP A1A4T2
C	27	CYS	-	expression tag	UNP A1A4T2
C	28	VAL	-	expression tag	UNP A1A4T2
C	29	ALA	-	expression tag	UNP A1A4T2
C	30	GLU	-	expression tag	UNP A1A4T2
C	31	THR	-	expression tag	UNP A1A4T2
C	32	GLY	-	expression tag	UNP A1A4T2
C	97	ASP	ASN	engineered mutation	UNP A1A4T2
C	967	SER	-	expression tag	UNP A1A4T2
C	968	ALA	-	expression tag	UNP A1A4T2
C	969	TRP	-	expression tag	UNP A1A4T2
C	970	SER	-	expression tag	UNP A1A4T2
C	971	HIS	-	expression tag	UNP A1A4T2
C	972	PRO	-	expression tag	UNP A1A4T2
C	973	GLN	-	expression tag	UNP A1A4T2
C	974	PHE	-	expression tag	UNP A1A4T2
C	975	GLU	-	expression tag	UNP A1A4T2
C	976	LYS	-	expression tag	UNP A1A4T2
C	977	LEU	-	expression tag	UNP A1A4T2
C	978	GLU	-	expression tag	UNP A1A4T2

- Molecule 2 is a protein called Glucosidase 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			592	351	98	133	10			
2	D	85	Total	C	N	O	S	0	0	0
			606	361	98	137	10			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP O08795
B	-15	GLY	-	expression tag	UNP O08795
B	-14	ILE	-	expression tag	UNP O08795
B	-13	LEU	-	expression tag	UNP O08795
B	-12	PRO	-	expression tag	UNP O08795
B	-11	SER	-	expression tag	UNP O08795
B	-10	PRO	-	expression tag	UNP O08795
B	-9	GLY	-	expression tag	UNP O08795
B	-8	MET	-	expression tag	UNP O08795

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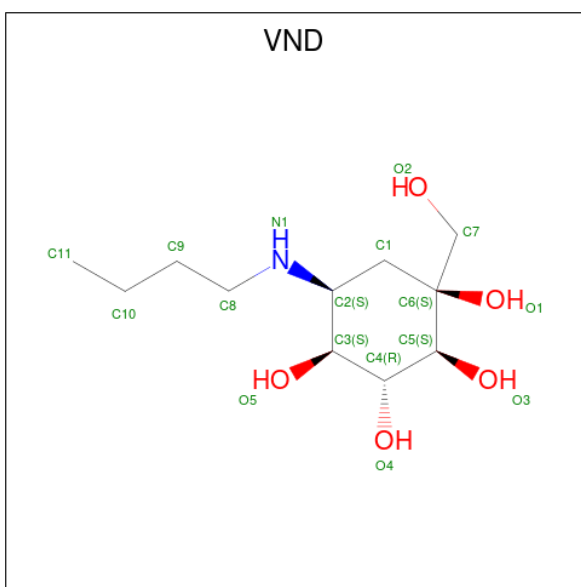
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	PRO	-	expression tag	UNP O08795
B	-6	ALA	-	expression tag	UNP O08795
B	-5	LEU	-	expression tag	UNP O08795
B	-4	LEU	-	expression tag	UNP O08795
B	-3	SER	-	expression tag	UNP O08795
B	-2	LEU	-	expression tag	UNP O08795
B	-1	VAL	-	expression tag	UNP O08795
B	0	SER	-	expression tag	UNP O08795
B	1	LEU	-	expression tag	UNP O08795
B	2	LEU	-	expression tag	UNP O08795
B	3	SER	-	expression tag	UNP O08795
B	4	VAL	-	expression tag	UNP O08795
B	5	LEU	-	expression tag	UNP O08795
B	6	LEU	-	expression tag	UNP O08795
B	7	MET	-	expression tag	UNP O08795
B	8	GLY	-	expression tag	UNP O08795
B	9	CYS	-	expression tag	UNP O08795
B	10	VAL	-	expression tag	UNP O08795
B	11	ALA	-	expression tag	UNP O08795
B	12	GLU	-	expression tag	UNP O08795
B	13	THR	-	expression tag	UNP O08795
B	14	GLY	-	expression tag	UNP O08795
B	518	SER	-	expression tag	UNP O08795
B	519	ALA	-	expression tag	UNP O08795
B	520	TRP	-	expression tag	UNP O08795
B	521	LEU	-	expression tag	UNP O08795
B	522	GLU	-	expression tag	UNP O08795
B	523	THR	-	expression tag	UNP O08795
B	524	LYS	-	expression tag	UNP O08795
B	525	HIS	-	expression tag	UNP O08795
B	526	HIS	-	expression tag	UNP O08795
B	527	HIS	-	expression tag	UNP O08795
B	528	HIS	-	expression tag	UNP O08795
B	529	HIS	-	expression tag	UNP O08795
B	530	HIS	-	expression tag	UNP O08795
D	-16	MET	-	initiating methionine	UNP O08795
D	-15	GLY	-	expression tag	UNP O08795
D	-14	ILE	-	expression tag	UNP O08795
D	-13	LEU	-	expression tag	UNP O08795
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression tag	UNP O08795

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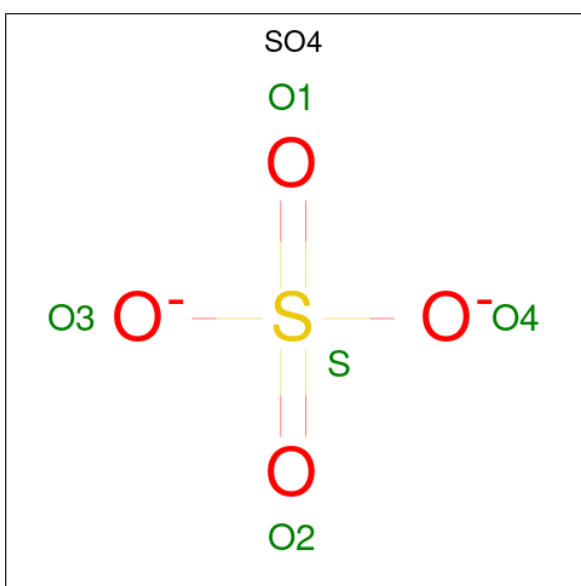
Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP O08795
D	-5	LEU	-	expression tag	UNP O08795
D	-4	LEU	-	expression tag	UNP O08795
D	-3	SER	-	expression tag	UNP O08795
D	-2	LEU	-	expression tag	UNP O08795
D	-1	VAL	-	expression tag	UNP O08795
D	0	SER	-	expression tag	UNP O08795
D	1	LEU	-	expression tag	UNP O08795
D	2	LEU	-	expression tag	UNP O08795
D	3	SER	-	expression tag	UNP O08795
D	4	VAL	-	expression tag	UNP O08795
D	5	LEU	-	expression tag	UNP O08795
D	6	LEU	-	expression tag	UNP O08795
D	7	MET	-	expression tag	UNP O08795
D	8	GLY	-	expression tag	UNP O08795
D	9	CYS	-	expression tag	UNP O08795
D	10	VAL	-	expression tag	UNP O08795
D	11	ALA	-	expression tag	UNP O08795
D	12	GLU	-	expression tag	UNP O08795
D	13	THR	-	expression tag	UNP O08795
D	14	GLY	-	expression tag	UNP O08795
D	518	SER	-	expression tag	UNP O08795
D	519	ALA	-	expression tag	UNP O08795
D	520	TRP	-	expression tag	UNP O08795
D	521	LEU	-	expression tag	UNP O08795
D	522	GLU	-	expression tag	UNP O08795
D	523	THR	-	expression tag	UNP O08795
D	524	LYS	-	expression tag	UNP O08795
D	525	HIS	-	expression tag	UNP O08795
D	526	HIS	-	expression tag	UNP O08795
D	527	HIS	-	expression tag	UNP O08795
D	528	HIS	-	expression tag	UNP O08795
D	529	HIS	-	expression tag	UNP O08795
D	530	HIS	-	expression tag	UNP O08795

- Molecule 3 is (1S,2S,3R,4S,5S)-5-(butylamino)-1-(hydroxymethyl)cyclohexane-1,2,3,4-tetrol (CCD ID: VND) (formula: C₁₁H₂₃NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	11	1	5		
3	C	1	Total	C	N	O	0	0
			17	11	1	5		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



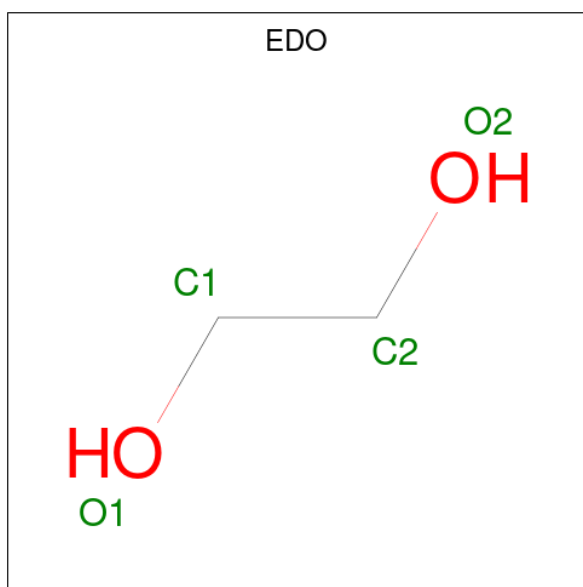
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



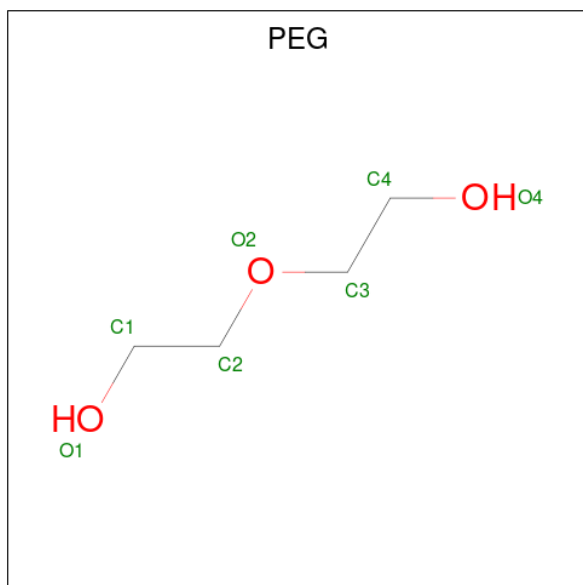
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	D	2	Total	Ca	0	0
			2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	462	Total	O	0	0
			462	462		

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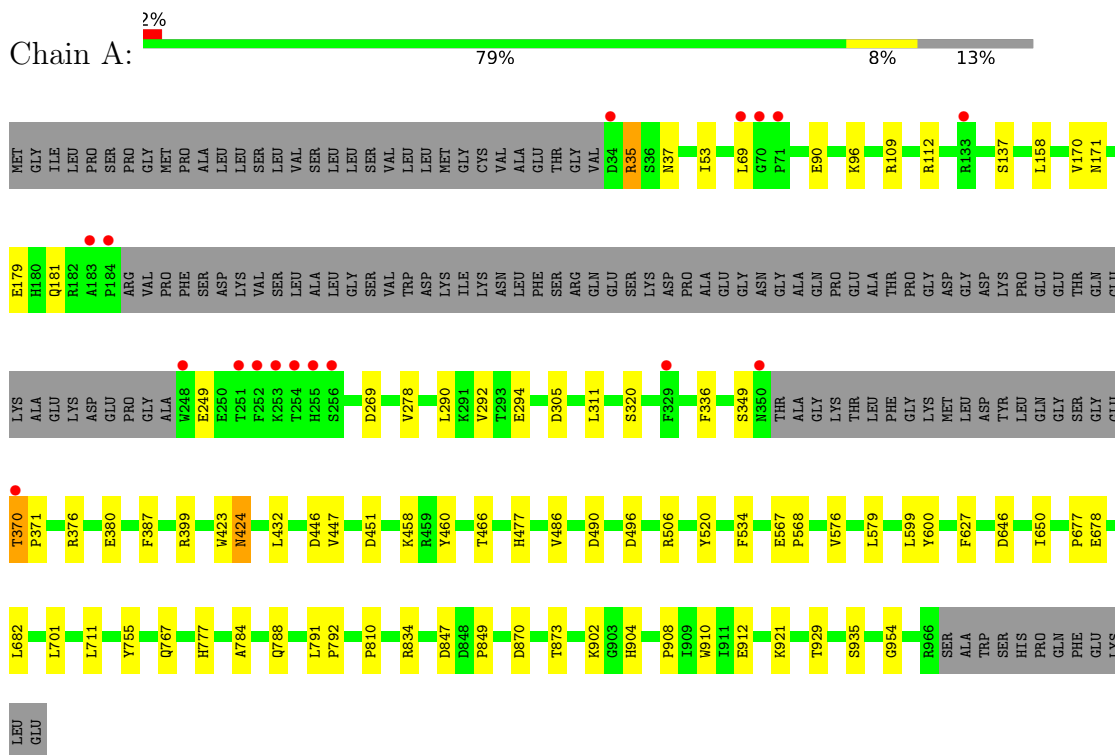
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	30	Total 30	O 30	0	0
8	C	369	Total 369	O 369	0	0
8	D	21	Total 21	O 21	0	0

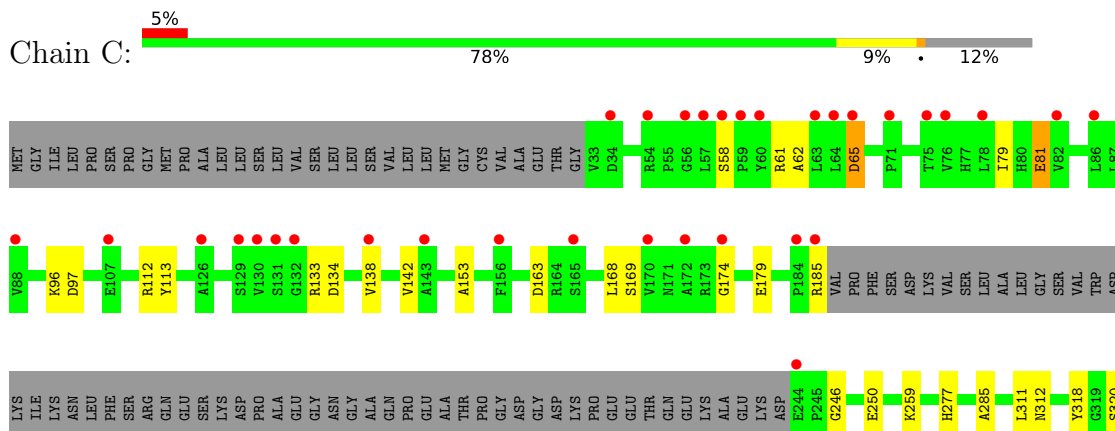
3 Residue-property plots

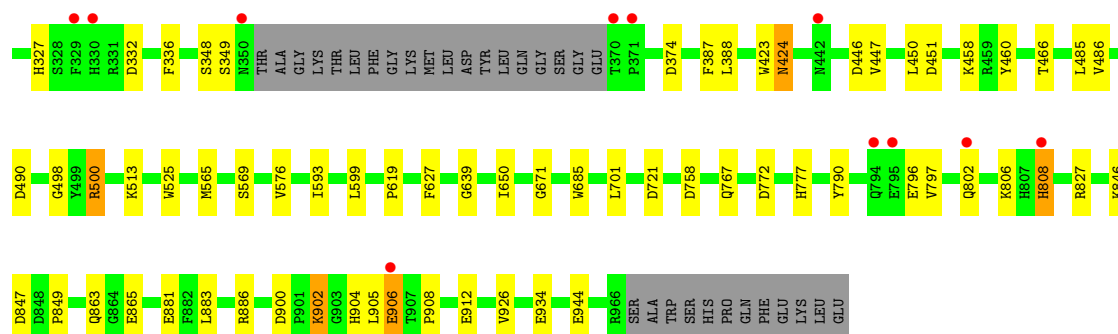
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha glucosidase 2 alpha neutral subunit

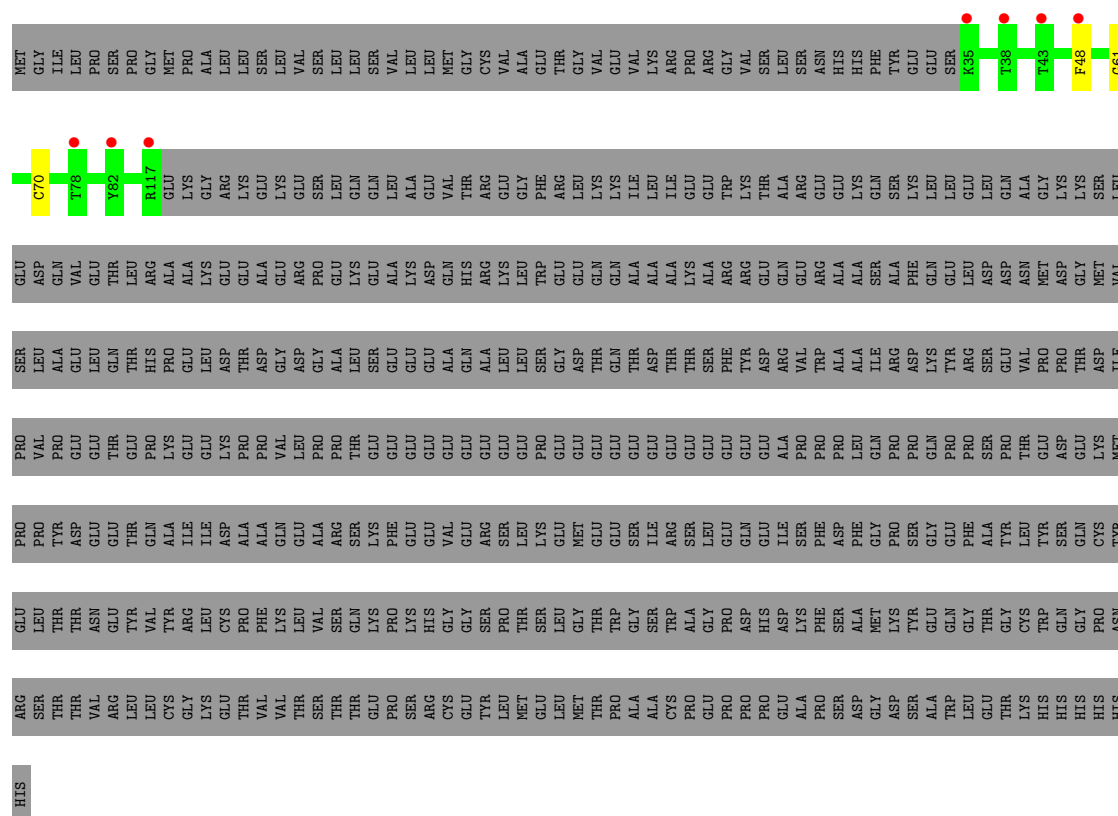


- Molecule 1: Alpha glucosidase 2 alpha neutral subunit

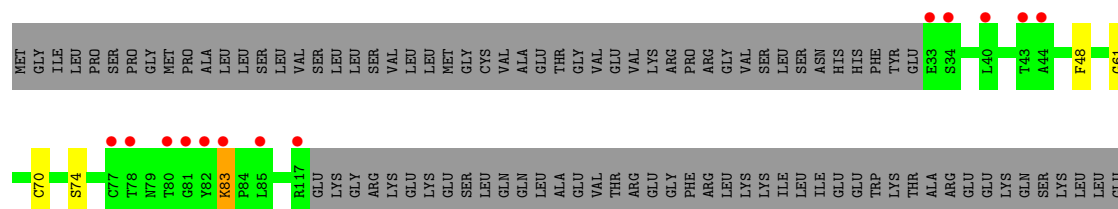




- Molecule 2: Glucosidase 2 subunit beta



- Molecule 2: Glucosidase 2 subunit beta



GLU	THR	ALA	SER	SER	ASP	LEU
THR	GLY	THR	PRO	GLY	ASP	GLN
LYS	CYS	LEU	THR	VAL	ASN	ALA
HIS	TRP	TYR	GLU	PRO	MET	GLY
HIS	GLN	SER	ASP	PRO	ASP	LYS
HIS	GLY	GLN	GLU	THR	GLY	LYS
HIS	PRO	CYS	LYS	LYS	MET	SER
HIS	ASN	TYR	MET	ILE	VAL	LEU
HIS	ARG	GLU	PRO	PRO	SER	GLU
	SER	LEU	PRO	VAL	LEU	ASP
	THR	THR	TYR	PRO	ALA	GLN
	THR	THR	ASP	GLU	GLU	VAL
	VAL	ASN	GLU	GLU	LEU	GLU
	ARG	GLU	GLU	THR	GLN	THR
	LEU	TYR	THR	GLU	THR	LEU
	LEU	VAL	GLN	PRO	HIS	ARG
	CYS	TYR	ALA	LYS	PRO	ALA
	GLY	ARG	ILE	GLU	GLU	ALA
	LYS	LEU	ILE	GLU	LEU	LYS
	GLU	CYS	ASP	LYS	ASP	GLU
	THR	PRO	ALA	PRO	THR	GLU
	VAL	PHE	VAL	PRO	ASP	ALA
	VAL	LYS	GLN	VAL	GLY	GLU
	THR	LEU	GLU	LEU	ASP	ARG
	SER	VAL	ALA	PRO	GLY	PRO
	THR	GLN	ARG	PRO	ALA	GLU
	THR	SER	SER	THR	LEU	LYS
	GLU	LYS	LYS	GLU	SER	GLU
	PRO	PRO	PHE	GLU	GLU	ALA
	SER	LYS	GLU	GLU	GLU	LYS
	ARG	HIS	GLU	GLU	GLU	ASP
	CYS	GLY	VAL	GLU	ALA	GLN
	GLU	GLY	GLU	GLU	GLN	HIS
	TYR	SER	ARG	GLU	ALA	ARG
	LEU	PRO	SER	GLU	LEU	LYS
	MET	THR	LEU	GLU	LEU	LEU
	GLU	SER	LYS	PRO	SER	TRP
	LEU	SER	LYS	GLU	GLY	GLU
	THR	THR	GLU	GLU	THR	GLN
	PRO	TRP	GLU	GLU	GLN	GLN
	ALA	GLY	SER	GLU	THR	ALA
	ALA	SER	ILE	GLU	ASP	ALA
	CYS	TRP	ARG	GLU	THR	ALA
	PRO	ALA	SER	GLU	THR	LYS
	GLU	GLY	LEU	GLU	SER	ALA
	PRO	PRO	GLU	GLU	PHE	ARG
	PRO	ASP	GLN	GLU	TYR	ARG
	PRO	HIS	GLU	GLU	ASP	GLU
	GLU	ASP	ILE	ALA	ARG	GLN
	ALA	LYS	SER	PRO	VAL	GLU
	PRO	PHE	PHE	PRO	TRP	ARG
	SER	SER	ASP	PRO	ALA	ALA
	ASP	ALA	PHE	LEU	ALA	ALA
	GLY	MET	GLY	GLN	ILE	SER
	ASP	LYS	PRO	PRO	ARG	ALA
	SER	TYR	SER	PRO	TYR	PHE
	ALA	GLU	GLY	GLN	LYS	GLN
	TRP	GLN	GLU	PRO	THR	LYS
	LEU	CYS	PHE	PRO	ASP	ASP
	THR	GLY	THR	PRO	GLU	LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.56Å 102.56Å 239.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.17 – 2.21 42.17 – 2.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.17-2.21) 96.5 (42.17-2.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.170 , 0.203 0.171 , 0.206	Depositor DCC
R_{free} test set	1992 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.085 for h,-h-k,-l 0.037 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15943	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VND, SO4, EDO, PEG, CA

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	0.28	0/7096	0.51	0/9664
1	C	0.26	0/7112	0.51	0/9687
2	B	0.25	0/603	0.53	0/826
2	D	0.25	0/618	0.50	0/846
All	All	0.27	0/15429	0.51	0/21023

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6868	0	6601	47	0
1	C	6881	0	6587	51	0
2	B	592	0	489	1	0
2	D	606	0	490	3	0
3	A	17	0	0	0	0
3	C	17	0	0	0	0
4	A	10	0	0	1	0
4	C	15	0	0	1	0
5	A	12	0	18	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	6	0	0
5	C	28	0	42	1	0
6	B	7	0	10	0	0
7	B	2	0	0	0	0
7	D	2	0	0	0	0
8	A	462	0	0	10	0
8	B	30	0	0	0	0
8	C	369	0	0	11	0
8	D	21	0	0	0	0
All	All	15943	0	14243	101	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 3.

All (101) 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:C:721:ASP:OD1	8:C:1101:HOH:O	1.88	0.90
2:D:83:LYS:HD3	2:D:83:LYS:H	1.44	0.83
1:A:90:GLU:OE2	8:A:1101:HOH:O	2.03	0.76
1:A:646[B]:ASP:OD2	8:A:1102:HOH:O	2.07	0.73
1:C:796:GLU:OE1	8:C:1103:HOH:O	2.08	0.72
4:C:1002:SO4:O2	8:C:1102:HOH:O	2.07	0.70
1:C:112:ARG:NH2	1:C:179:GLU:O	2.26	0.68
1:C:900:ASP:OD1	1:C:902:LYS:HG3	1.96	0.66
1:C:65:ASP:OD1	8:C:1104:HOH:O	2.14	0.65
1:A:399:ARG:NE	8:A:1108:HOH:O	2.28	0.64
1:A:399:ARG:NH1	8:A:1109:HOH:O	2.30	0.63
1:A:380:GLU:OE1	8:A:1103:HOH:O	2.16	0.61
1:C:806:LYS:NZ	1:C:808:HIS:HD2	1.99	0.61
1:C:423:TRP:O	1:C:701:LEU:HA	2.02	0.59
1:C:865:GLU:OE2	1:C:886:ARG:NH2	2.35	0.58
1:C:847:ASP:HB3	1:C:908:PRO:HG2	1.88	0.55
1:A:904:HIS:HB2	4:A:1003:SO4:O3	2.05	0.55
1:C:450:LEU:HG	1:C:485:LEU:HD21	1.89	0.55
1:A:423:TRP:O	1:A:701:LEU:HA	2.07	0.55
1:C:513:LYS:NZ	8:C:1113:HOH:O	2.39	0.55
1:A:311:LEU:HD22	1:A:650:ILE:HD13	1.88	0.54
1:C:277:HIS:HD2	8:C:1241:HOH:O	1.91	0.53
1:A:292:VAL:HG12	1:A:294:GLU:H	1.74	0.53
1:A:171:ASN:HA	1:A:269:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LYS:HE2	1:C:466:THR:HB	1.90	0.53
1:A:447:VAL:HG11	1:A:486:VAL:HG23	1.92	0.52
1:A:112:ARG:NH2	1:A:179:GLU:O	2.42	0.52
1:A:682:LEU:HD23	1:A:711:LEU:HD11	1.92	0.52
1:C:336:PHE:HB3	1:C:387:PHE:HB2	1.91	0.52
1:A:788:GLN:NE2	8:A:1121:HOH:O	2.43	0.52
1:A:847:ASP:HB3	1:A:908:PRO:HG2	1.91	0.51
1:A:784:ALA:HA	5:A:1005:EDO:H11	1.91	0.51
1:C:447:VAL:HG11	1:C:486:VAL:HG23	1.93	0.51
1:C:424:ASN:OD1	1:C:451:ASP:HB3	2.10	0.50
1:A:466:THR:HB	1:C:458:LYS:HE2	1.94	0.49
1:A:767:GLN:HG3	1:A:777:HIS:ND1	2.27	0.49
1:A:305:ASP:OD2	5:A:1006:EDO:O1	2.29	0.49
1:A:432:LEU:HD22	1:A:477[A]:HIS:ND1	2.28	0.49
1:C:906:GLU:OE2	1:C:906:GLU:HA	2.12	0.48
1:A:35:ARG:HG2	8:A:1561:HOH:O	2.12	0.48
1:A:834:ARG:NH1	8:A:1106:HOH:O	2.26	0.47
1:A:370:THR:N	1:A:371:PRO:HD2	2.28	0.47
1:A:755:TYR:CE2	1:A:792:PRO:HG2	2.48	0.47
1:C:327:HIS:ND1	1:C:332:ASP:OD1	2.38	0.47
1:A:320:SER:O	1:A:627:PHE:HA	2.15	0.47
1:C:133:ARG:HD2	1:C:138:VAL:HG22	1.97	0.47
1:A:424:ASN:OD1	1:A:451:ASP:HB3	2.14	0.47
1:C:772:ASP:OD2	1:C:827:ARG:NH2	2.37	0.47
1:C:311:LEU:HD22	1:C:650:ILE:HD13	1.97	0.46
2:B:61:GLY:HA2	2:B:70:CYS:SG	2.55	0.46
1:C:846:LYS:NZ	8:C:1128:HOH:O	2.48	0.46
1:C:62:ALA:HB3	1:C:153:ALA:HA	1.98	0.46
1:A:506:ARG:NH2	8:A:1113:HOH:O	2.34	0.45
1:C:318:TYR:CE2	1:C:639:GLY:HA3	2.52	0.45
1:A:109:ARG:NH1	1:A:181:GLN:O	2.48	0.45
1:C:246:GLY:O	1:C:259:LYS:NZ	2.49	0.45
1:C:758:ASP:OD2	1:C:790:TYR:OH	2.34	0.45
5:C:1007:EDO:O1	8:C:1106:HOH:O	2.21	0.45
1:A:870:ASP:OD2	1:A:873:THR:OG1	2.34	0.45
1:C:133:ARG:NH1	1:C:134:ASP:O	2.50	0.44
1:C:849:PRO:HB2	1:C:912:GLU:HB3	1.98	0.44
1:C:134:ASP:OD2	8:C:1107:HOH:O	2.21	0.44
1:C:348:SER:OG	1:C:374:ASP:HB2	2.17	0.44
1:C:285:ALA:O	1:C:312:ASN:N	2.48	0.43
1:C:926:VAL:HG13	1:C:934:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:GLY:HA2	2:D:70:CYS:SG	2.57	0.43
1:A:567:GLU:N	1:A:568:PRO:HA	2.33	0.43
1:A:496:ASP:OD1	1:C:498:GLY:HA3	2.18	0.43
1:A:278:VAL:HG23	1:A:290:LEU:HB2	2.00	0.43
1:A:834:ARG:NH2	8:A:1106:HOH:O	2.46	0.43
1:C:500:ARG:HG2	8:C:1454:HOH:O	2.18	0.42
1:C:806:LYS:HZ2	1:C:808:HIS:HD2	1.66	0.42
1:C:113:TYR:CZ	1:C:593:ILE:HG22	2.55	0.42
1:C:883:LEU:HG	1:C:905:LEU:HB3	2.02	0.42
1:C:460:TYR:CE2	1:C:490:ASP:HB2	2.54	0.42
1:A:460:TYR:CE2	1:A:490:ASP:HB2	2.55	0.42
1:C:320:SER:O	1:C:627:PHE:HA	2.20	0.42
1:A:677:PRO:HA	5:A:1004:EDO:H11	2.00	0.42
1:C:671:GLY:H	1:C:685:TRP:CG	2.38	0.42
1:C:599:LEU:C	1:C:599:LEU:HD23	2.45	0.41
1:C:767:GLN:HG3	1:C:777:HIS:ND1	2.35	0.41
1:C:168:LEU:HD11	1:C:388:LEU:HD13	2.00	0.41
1:C:619:PRO:HD2	8:C:1322:HOH:O	2.20	0.41
1:A:336:PHE:HB3	1:A:387:PHE:HB2	2.02	0.41
1:A:520:TYR:HE2	1:A:579:LEU:HD12	1.86	0.41
1:A:791:LEU:O	1:A:810:PRO:HA	2.21	0.41
1:A:678:GLU:H	5:A:1004:EDO:C1	2.34	0.41
1:C:61:ARG:HD3	1:C:81:GLU:OE2	2.21	0.41
1:C:565:MET:HE3	1:C:569:SER:HB3	2.03	0.41
2:D:83:LYS:HD3	2:D:83:LYS:N	2.24	0.41
1:A:53:ILE:HB	1:A:376:ARG:HH22	1.85	0.41
1:A:69:LEU:HD12	1:A:69:LEU:HA	1.82	0.41
1:C:458:LYS:HG2	1:C:525:TRP:HB3	2.03	0.41
1:A:158:LEU:HB2	1:A:170:VAL:HB	2.03	0.40
1:A:534:PHE:HB3	1:A:600:TYR:HB3	2.02	0.40
1:C:881:GLU:HA	1:C:904:HIS:O	2.20	0.40
1:C:58:SER:HB2	1:C:174:GLY:HA2	2.03	0.40
1:C:250:GLU:OE1	1:C:259:LYS:NZ	2.37	0.40
1:A:849:PRO:HB2	1:A:912:GLU:HB3	2.03	0.40
1:A:599:LEU:C	1:A:599:LEU:HD23	2.46	0.40
1:A:910:TRP:CE3	1:A:954:GLY:HA2	2.56	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	851/977 (87%)	828 (97%)	23 (3%)	0	100	100
1	C	858/977 (88%)	831 (97%)	26 (3%)	1 (0%)	48	56
2	B	81/547 (15%)	79 (98%)	2 (2%)	0	100	100
2	D	83/547 (15%)	81 (98%)	2 (2%)	0	100	100
All	All	1873/3048 (62%)	1819 (97%)	53 (3%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	576	VAL

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	742/846 (88%)	728 (98%)	14 (2%)	50	64
1	C	736/846 (87%)	716 (97%)	20 (3%)	39	52
2	B	67/478 (14%)	66 (98%)	1 (2%)	57	71
2	D	67/478 (14%)	64 (96%)	3 (4%)	24	31
All	All	1612/2648 (61%)	1574 (98%)	38 (2%)	43	56

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	37	ASN
1	A	96	LYS
1	A	137	SER
1	A	249	GLU
1	A	349	SER
1	A	370	THR
1	A	424	ASN
1	A	446	ASP
1	A	576	VAL
1	A	902	LYS
1	A	921	LYS
1	A	929	THR
1	A	935	SER
2	B	48	PHE
1	C	65	ASP
1	C	79	ILE
1	C	81	GLU
1	C	96	LYS
1	C	97	ASP
1	C	142	VAL
1	C	163	ASP
1	C	169	SER
1	C	185	ARG
1	C	349	SER
1	C	424	ASN
1	C	446	ASP
1	C	500	ARG
1	C	797	VAL
1	C	802	GLN
1	C	808	HIS
1	C	863	GLN
1	C	902	LYS
1	C	906	GLU
1	C	944	GLU
2	D	48	PHE
2	D	74	SER
2	D	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS

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Mol	Chain	Res	Type
1	A	545	ASN
1	A	808	HIS
2	B	50	GLN
2	B	76	HIS
1	C	37	ASN
1	C	647	HIS
1	C	802	GLN
1	C	808	HIS
1	C	811	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 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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	SO4	C	1004	-	4,4,4	0.22	0	6,6,6	0.26	0
4	SO4	C	1003	-	4,4,4	0.22	0	6,6,6	0.20	0
5	EDO	C	1006	-	3,3,3	0.40	0	2,2,2	0.46	0
5	EDO	C	1005	-	3,3,3	0.44	0	2,2,2	0.42	0
4	SO4	A	1003	-	4,4,4	0.28	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	1104	-	3,3,3	0.42	0	2,2,2	0.48	0
5	EDO	C	1008	-	3,3,3	0.38	0	2,2,2	0.49	0
4	SO4	C	1002	-	4,4,4	0.28	0	6,6,6	0.16	0
5	EDO	C	1007	-	3,3,3	0.45	0	2,2,2	0.44	0
5	EDO	A	1005	-	3,3,3	0.44	0	2,2,2	0.35	0
6	PEG	B	1101	-	6,6,6	0.49	0	5,5,5	0.27	0
4	SO4	A	1002	-	4,4,4	0.28	0	6,6,6	0.27	0
3	VND	C	1001	-	17,17,17	0.98	1 (5%)	21,24,24	1.67	2 (9%)
5	EDO	C	1011	-	3,3,3	0.49	0	2,2,2	0.35	0
5	EDO	C	1009	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	A	1006	-	3,3,3	0.53	0	2,2,2	0.19	0
3	VND	A	1001	-	17,17,17	0.88	1 (5%)	21,24,24	1.08	1 (4%)
5	EDO	C	1010	-	3,3,3	0.39	0	2,2,2	0.73	0
5	EDO	A	1004	-	3,3,3	0.36	0	2,2,2	0.61	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
5	EDO	A	1005	-	-	1/1/1/1	-
5	EDO	C	1011	-	-	1/1/1/1	-
6	PEG	B	1101	-	-	2/4/4/4	-
5	EDO	C	1009	-	-	1/1/1/1	-
5	EDO	B	1104	-	-	1/1/1/1	-
5	EDO	C	1008	-	-	0/1/1/1	-
5	EDO	A	1006	-	-	0/1/1/1	-
3	VND	A	1001	-	-	0/8/31/31	0/1/1/1
5	EDO	C	1010	-	-	1/1/1/1	-
5	EDO	C	1006	-	-	1/1/1/1	-
5	EDO	C	1005	-	-	0/1/1/1	-
5	EDO	C	1007	-	-	0/1/1/1	-
5	EDO	A	1004	-	-	0/1/1/1	-
3	VND	C	1001	-	-	0/8/31/31	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	VND	O1-C6	-2.78	1.39	1.44
3	C	1001	VND	O1-C6	-2.54	1.40	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	VND	C8-N1-C2	-5.34	106.26	114.05
3	C	1001	VND	C1-C2-N1	-3.99	103.23	112.03
3	A	1001	VND	C3-C4-C5	-2.24	107.98	111.18

There are no chirality outliers.

All (8) torsion outliers are listed below:

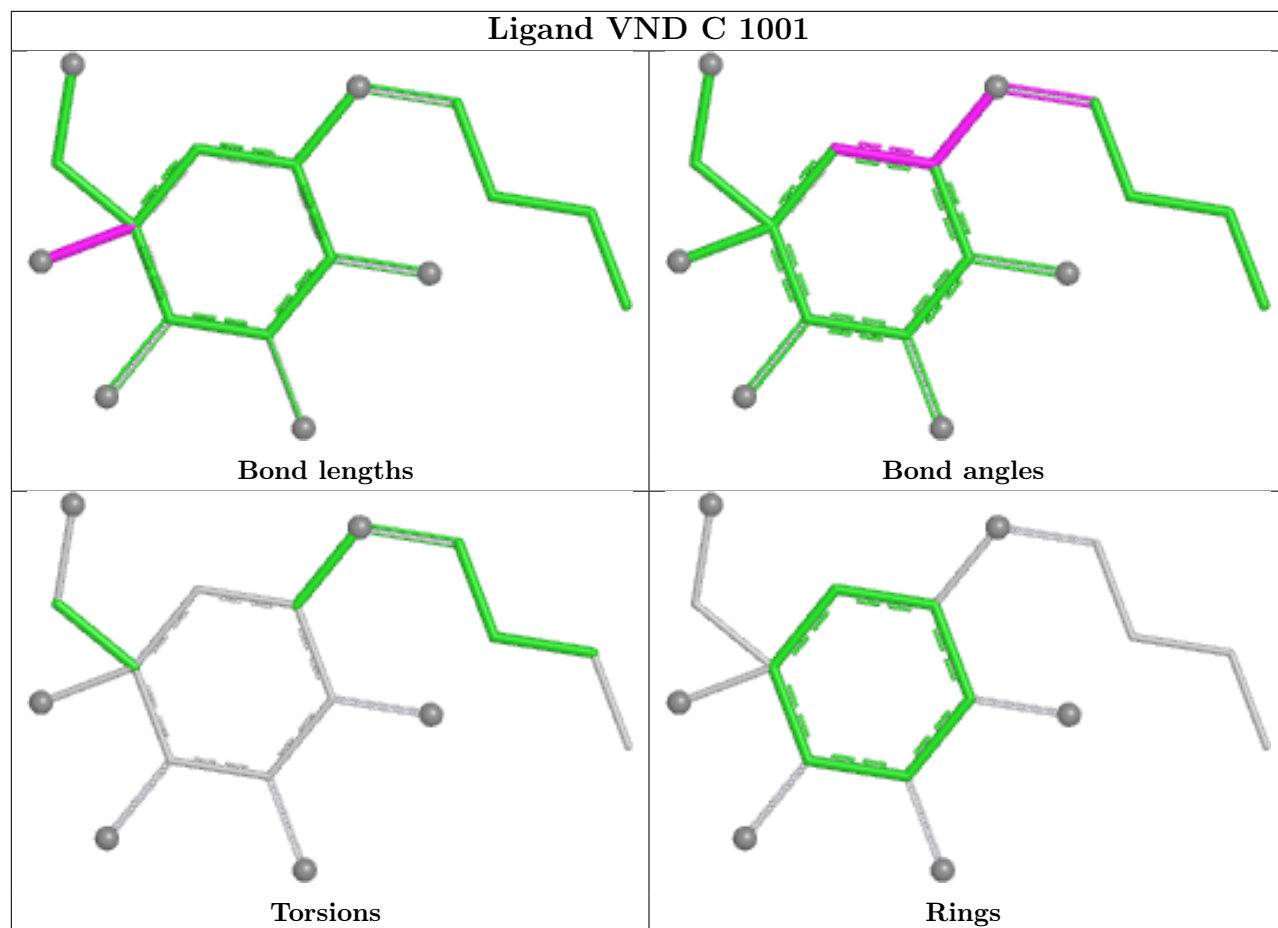
Mol	Chain	Res	Type	Atoms
5	B	1104	EDO	O1-C1-C2-O2
5	C	1011	EDO	O1-C1-C2-O2
5	C	1009	EDO	O1-C1-C2-O2
5	A	1005	EDO	O1-C1-C2-O2
6	B	1101	PEG	O1-C1-C2-O2
5	C	1006	EDO	O1-C1-C2-O2
5	C	1010	EDO	O1-C1-C2-O2
6	B	1101	PEG	C4-C3-O2-C2

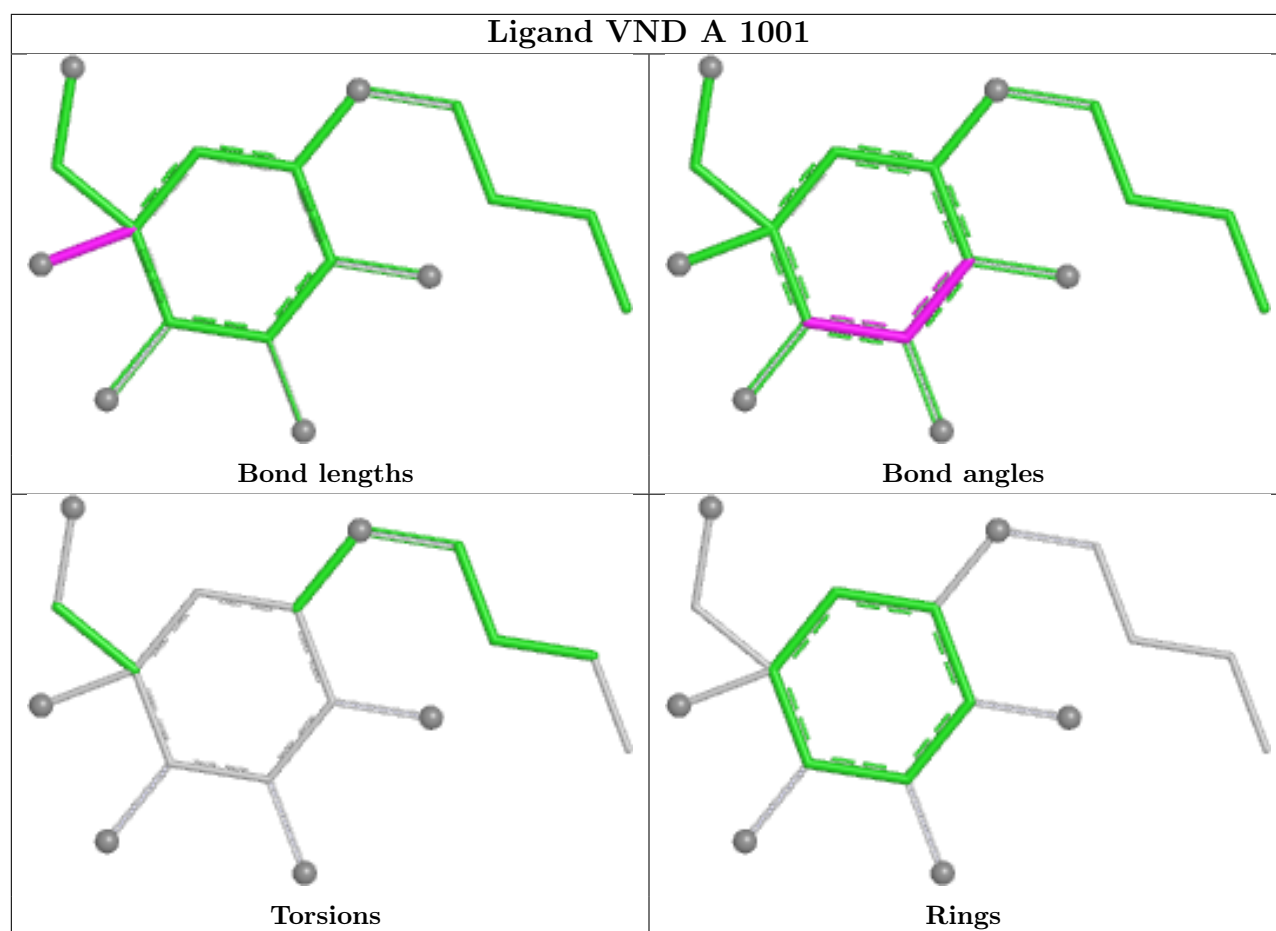
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	SO4	1	0
4	C	1002	SO4	1	0
5	C	1007	EDO	1	0
5	A	1005	EDO	1	0
5	A	1006	EDO	1	0
5	A	1004	EDO	2	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	851/977 (87%)	-0.35	17 (1%) 65 63	20, 35, 57, 102	6 (0%)
1	C	857/977 (87%)	0.02	44 (5%) 33 30	18, 40, 76, 102	7 (0%)
2	B	83/547 (15%)	0.32	7 (8%) 17 15	33, 49, 81, 91	0
2	D	85/547 (15%)	0.71	13 (15%) 5 4	33, 51, 89, 100	0
All	All	1876/3048 (61%)	-0.10	81 (4%) 40 37	18, 38, 74, 102	13 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PRO	5.5
1	A	248	TRP	4.8
2	D	117	ARG	4.7
2	D	80	THR	4.6
1	C	370	THR	4.6
1	A	183	ALA	4.5
1	A	350	ASN	4.3
2	D	34	SER	4.1
1	A	370	THR	3.9
1	A	71	PRO	3.9
2	D	33	GLU	3.9
2	D	81	GLY	3.9
1	C	76	VAL	3.9
1	A	251	THR	3.8
1	C	185	ARG	3.7
1	C	57	LEU	3.7
1	C	71	PRO	3.6
1	C	130	VAL	3.4
1	A	70	GLY	3.3
2	D	78	THR	3.3
1	A	252	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	43	THR	3.3
1	C	126	ALA	3.2
1	C	244	GLU	3.2
1	C	138	VAL	3.1
1	C	802	GLN	3.1
1	C	795	GLU	3.1
2	D	82	TYR	3.0
2	B	78	THR	3.0
1	C	329	PHE	3.0
1	A	133[A]	ARG	3.0
1	A	255	HIS	2.9
2	B	82	TYR	2.9
1	A	34	ASP	2.9
1	A	253	LYS	2.9
1	A	256	SER	2.8
1	A	254	THR	2.8
1	C	143	ALA	2.8
1	C	131	SER	2.7
1	C	56	GLY	2.7
1	C	78	LEU	2.7
1	C	170	VAL	2.7
1	C	350	ASN	2.7
1	C	129	SER	2.7
1	C	808	HIS	2.6
2	B	48	PHE	2.6
1	C	132	GLY	2.6
2	D	77	CYS	2.6
1	C	54	ARG	2.5
2	D	83	LYS	2.5
1	C	906	GLU	2.5
1	C	86	LEU	2.5
1	A	329	PHE	2.4
1	C	82	VAL	2.4
1	C	165	SER	2.4
2	B	35	LYS	2.4
1	C	75	THR	2.4
1	A	69	LEU	2.4
2	D	85	LEU	2.4
1	C	794	GLN	2.3
2	B	43	THR	2.3
2	D	40	LEU	2.3
1	C	174	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	58	SER	2.3
1	C	63	LEU	2.2
1	C	60	TYR	2.2
2	B	38	THR	2.2
2	B	117	ARG	2.2
1	C	184	PRO	2.2
1	C	107	GLU	2.2
1	C	330	HIS	2.2
1	C	64	LEU	2.1
1	C	156	PHE	2.1
1	C	442	ASN	2.1
1	C	88	VAL	2.1
1	C	65	ASP	2.1
1	C	59	PRO	2.1
1	C	172	ALA	2.0
2	D	44	ALA	2.0
1	C	34	ASP	2.0
1	C	371	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	SO4	A	1003	5/5	0.74	0.14	64,64,76,90	0
4	SO4	C	1002	5/5	0.75	0.12	70,75,87,96	0
5	EDO	C	1008	4/4	0.80	0.17	67,67,75,75	0
5	EDO	C	1007	4/4	0.82	0.17	47,56,62,62	0
5	EDO	B	1104	4/4	0.84	0.15	49,50,52,56	0

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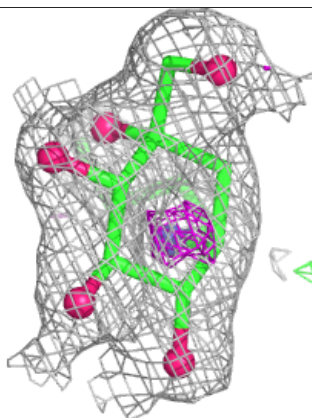
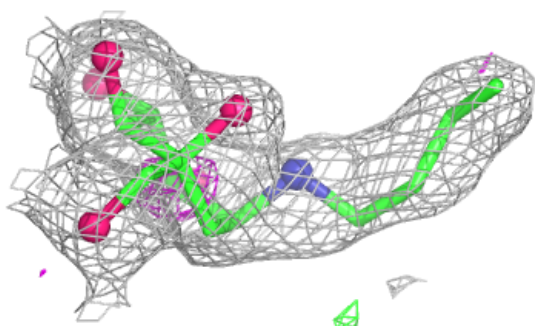
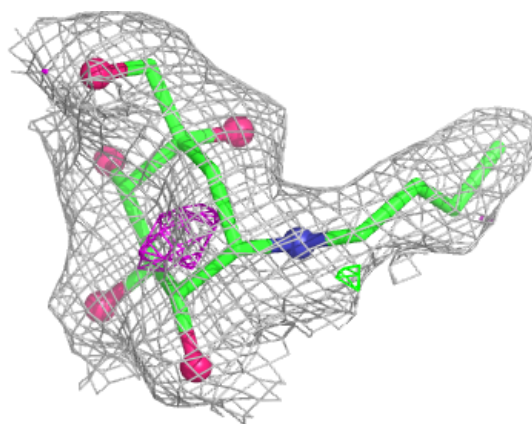
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1002	5/5	0.84	0.17	61,62,77,98	0
4	SO4	C	1004	5/5	0.84	0.16	67,67,77,92	0
5	EDO	C	1009	4/4	0.84	0.19	48,49,52,57	0
5	EDO	A	1005	4/4	0.85	0.16	59,62,67,72	0
5	EDO	A	1006	4/4	0.85	0.20	46,47,47,51	0
5	EDO	C	1005	4/4	0.88	0.19	48,66,70,70	0
5	EDO	C	1011	4/4	0.88	0.16	50,51,54,55	0
6	PEG	B	1101	7/7	0.90	0.12	48,53,59,59	0
5	EDO	A	1004	4/4	0.91	0.11	47,50,51,62	0
4	SO4	C	1003	5/5	0.91	0.10	62,65,80,81	0
5	EDO	C	1010	4/4	0.93	0.11	44,45,48,50	0
3	VND	C	1001	17/17	0.94	0.10	31,39,52,54	0
3	VND	A	1001	17/17	0.95	0.09	32,39,46,53	0
5	EDO	C	1006	4/4	0.97	0.08	41,42,43,50	0
7	CA	D	601	1/1	0.99	0.03	40,40,40,40	0
7	CA	D	602	1/1	0.99	0.02	33,33,33,33	0
7	CA	B	1102	1/1	1.00	0.01	39,39,39,39	0
7	CA	B	1103	1/1	1.00	0.02	35,35,35,35	0

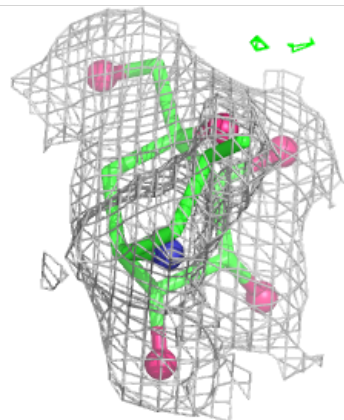
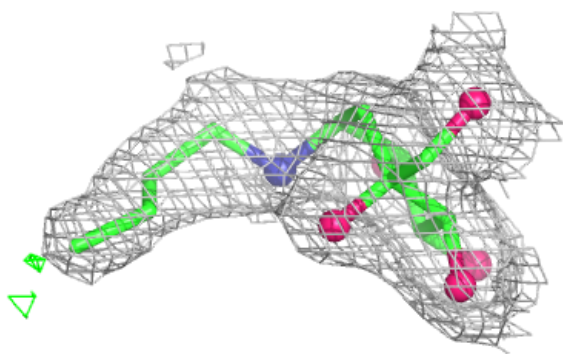
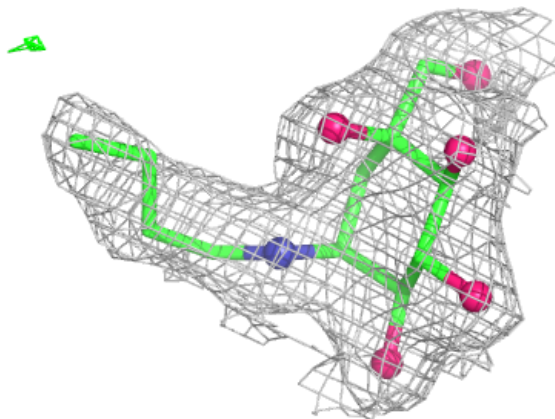
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VND C 1001:

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

**Electron density around VND A 1001:**

$2mF_o-DF_c$ (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.