Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 05:51 PM EDT

PDB ID	:	7JTY
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 (i) 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 (i)) were used in the production of this report:

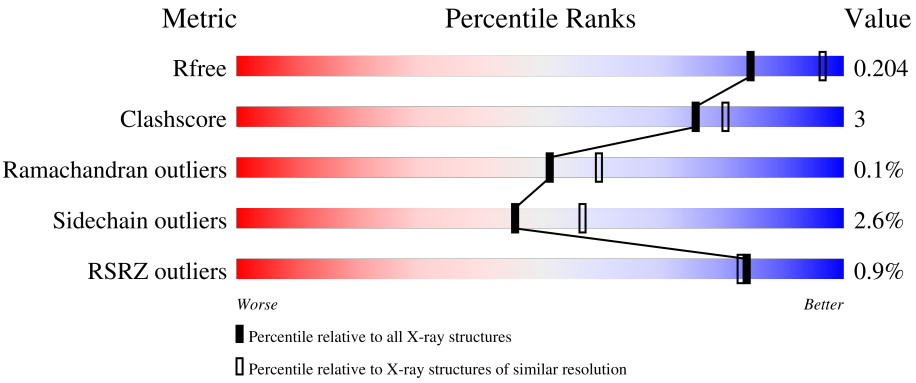
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (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 <=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	% 79% 8% 13%
1	C	977	79% 8% • 12%
2	B	547	15% • 85%
2	D	547	% 15% • 84%

2 Entry composition (i)

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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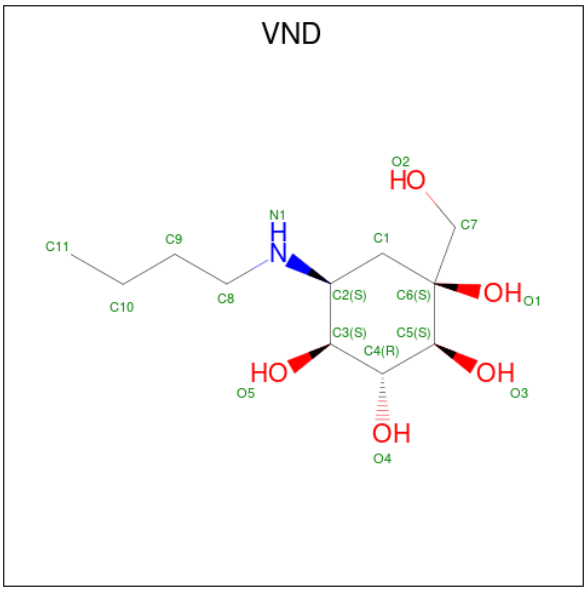
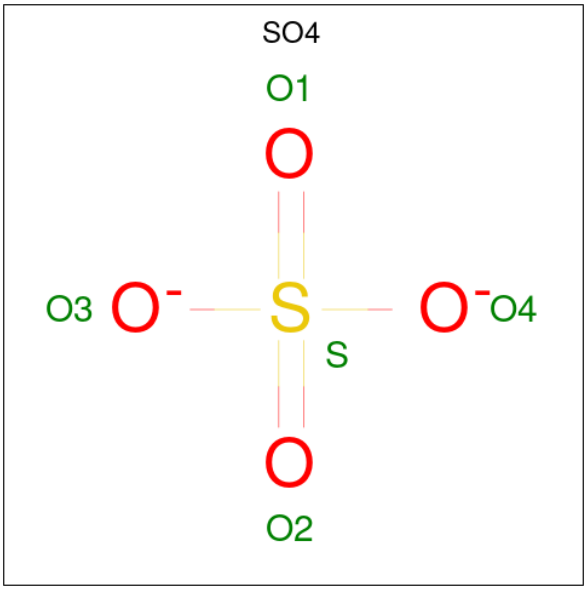
Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP O08795
D	-5	LEU	-	expression tag	UNP O08795
D	-4	LEU	-	expression tag	UNP O08795
D	-3	SER	-	expression tag	UNP O08795
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 (three-letter code: VND) (formula: $C_{11}H_{23}NO_5$) (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 (three-letter code: SO4) (formula: O_4S).



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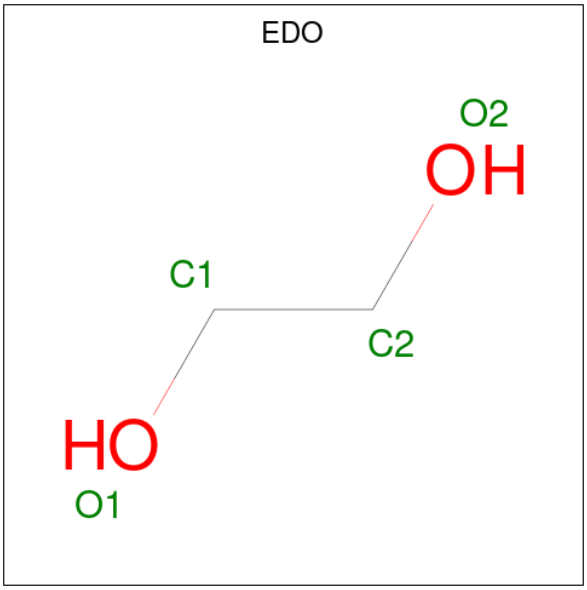
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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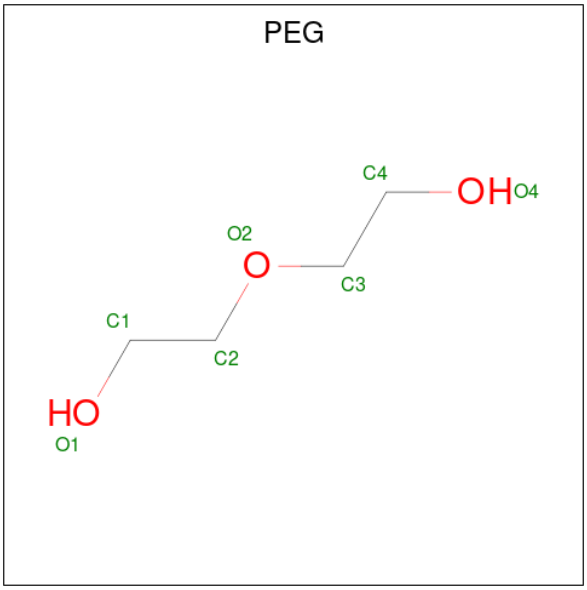
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is water.

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

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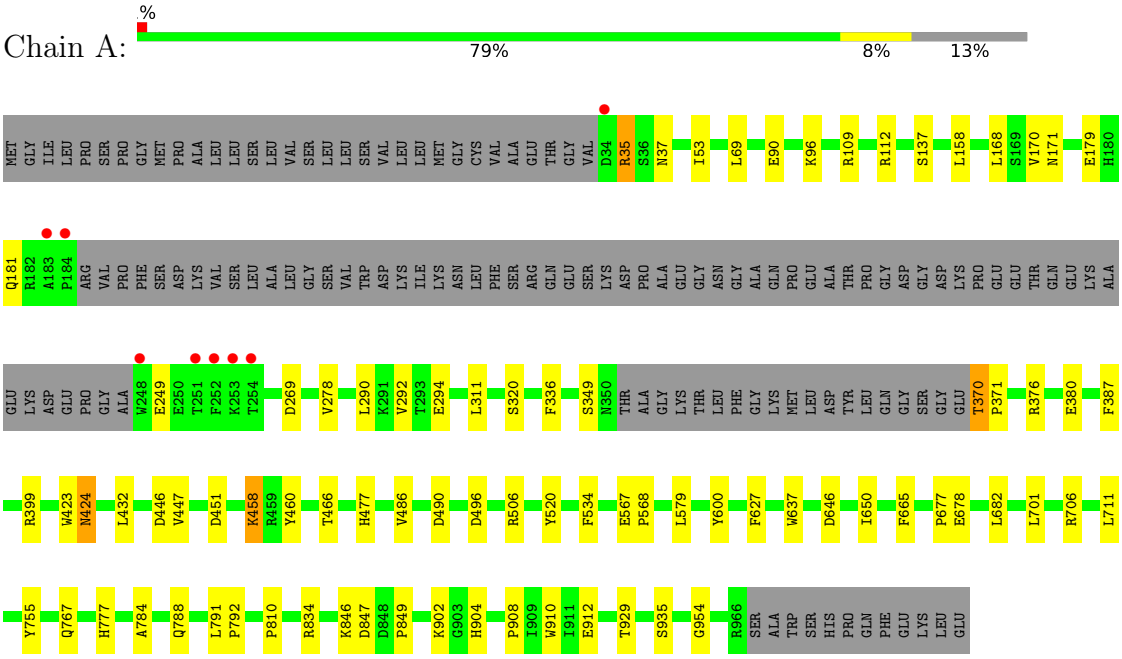
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	30	Total O 30 30	0	0
8	C	369	Total O 369 369	0	0
8	D	21	Total O 21 21	0	0

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.

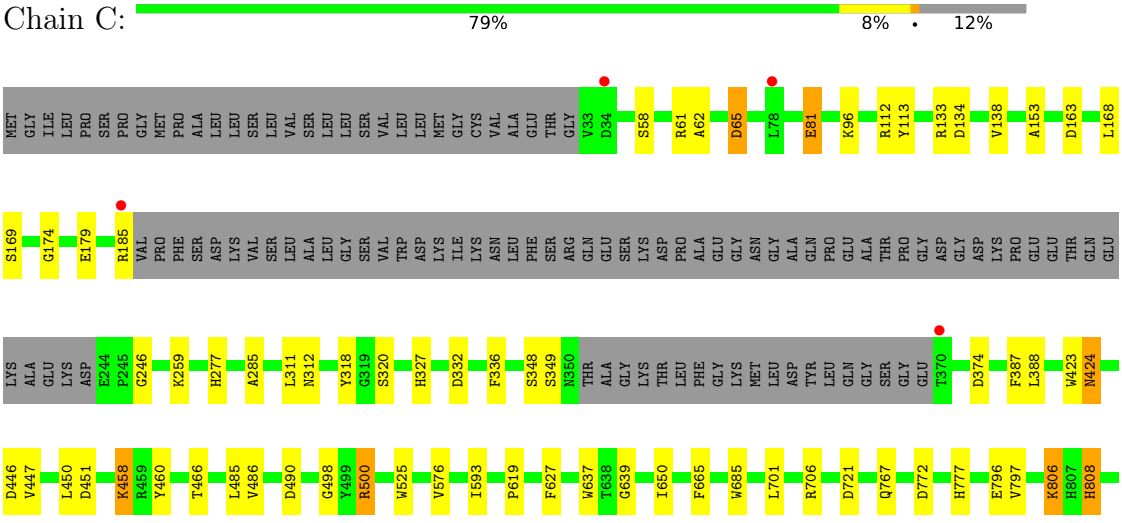
• Molecule 1: Alpha glucosidase 2 alpha neutral subunit

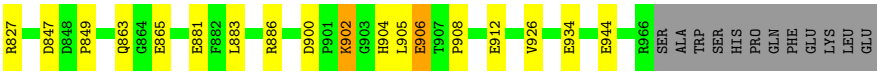
Chain A:



• Molecule 1: Alpha glucosidase 2 alpha neutral subunit

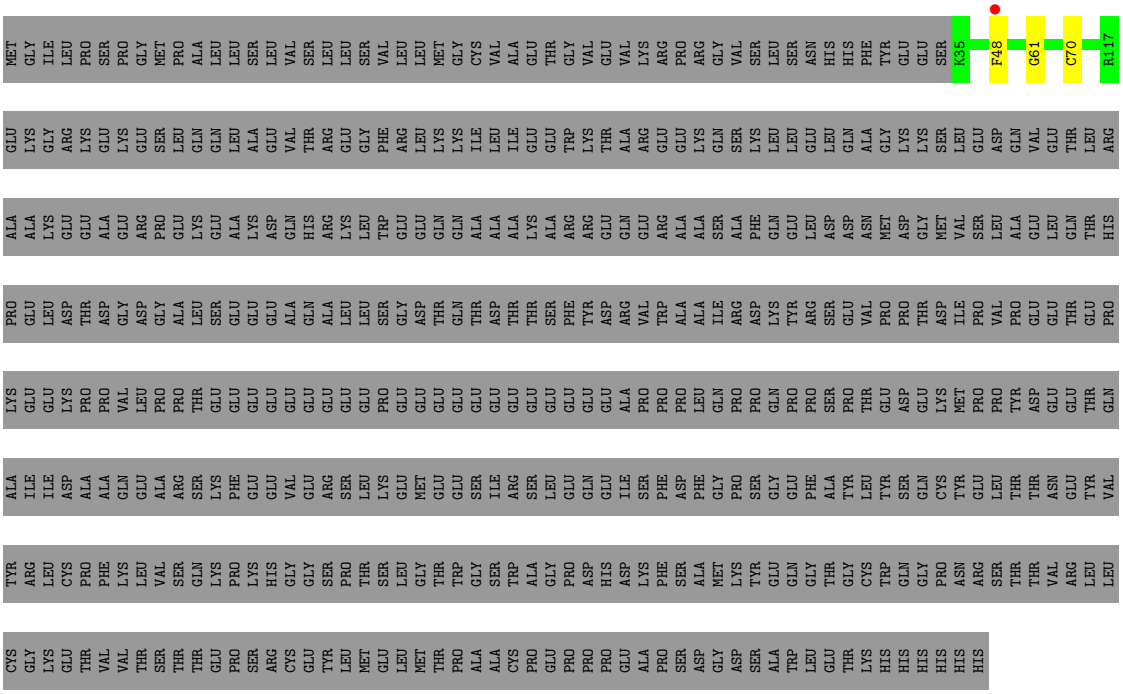
Chain C:





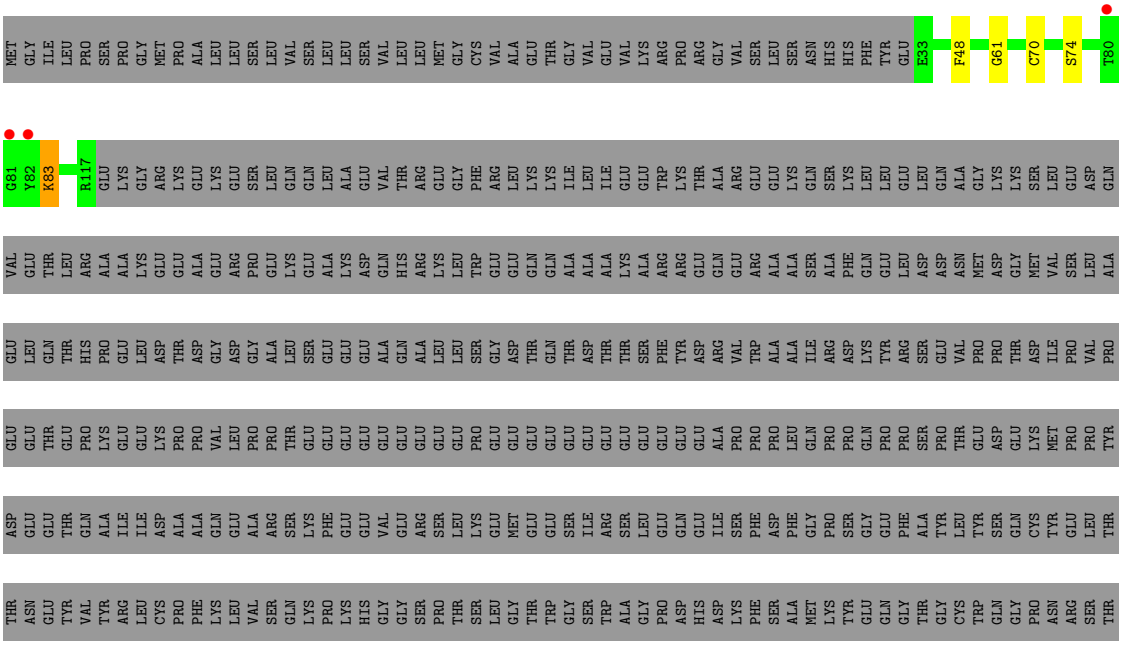
• Molecule 2: Glucosidase 2 subunit beta

Chain B:



• Molecule 2: Glucosidase 2 subunit beta

Chain D:



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

4 Data and refinement statistics (i)

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 43.15 – 2.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.17-2.21) 96.5 (43.15-2.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.170 , 0.203 0.170 , 0.204	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)	0.34 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	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	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, EDO, CA, VND, PEG

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	0.35	0/7096	0.56	1/9664 (0.0%)
1	C	0.34	0/7112	0.56	0/9687
2	B	0.36	0/603	0.61	0/826
2	D	0.34	0/618	0.60	0/846
All	All	0.35	0/15429	0.56	1/21023 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	LEU	CA-CB-CG	5.44	127.82	115.30

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	6868	0	6601	45	0
1	C	6881	0	6587	44	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	0	1	0
4	C	15	0	0	1	0
5	A	12	0	18	3	0
5	B	4	0	6	0	0
5	C	28	0	42	0	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	11	0
8	B	30	0	0	0	0
8	C	369	0	0	8	0
8	D	21	0	0	0	0
All	All	15943	0	14243	91	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 (91) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:849:PRO:HB2	1:A:912:GLU:HB3	2.03	0.40
1:A:846:LYS:NZ	8:A:1124:HOH:O	2.45	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 (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	851/977 (87%)	828 (97%)	23 (3%)	0	100 100
1	C	858/977 (88%)	831 (97%)	26 (3%)	1 (0%)	51 60
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%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	576	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	742/846 (88%)	726 (98%)	16 (2%)	52 64
1	C	736/846 (87%)	714 (97%)	22 (3%)	41 51
2	B	67/478 (14%)	66 (98%)	1 (2%)	65 76
2	D	67/478 (14%)	64 (96%)	3 (4%)	27 33
All	All	1612/2648 (61%)	1570 (97%)	42 (3%)	46 57

All (42) 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	458	LYS

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Mol	Chain	Res	Type
1	A	637	TRP
1	A	665	PHE
1	A	706	ARG
1	A	902	LYS
1	A	929	THR
1	A	935	SER
2	B	48	PHE
1	C	65	ASP
1	C	81	GLU
1	C	96	LYS
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	458	LYS
1	C	500	ARG
1	C	637	TRP
1	C	665	PHE
1	C	685	TRP
1	C	706	ARG
1	C	797	VAL
1	C	806	LYS
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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	808	HIS
1	C	811	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
5	EDO	C	1009	-	3,3,3	0.50	0	2,2,2	0.24	0
5	EDO	C	1007	-	3,3,3	0.48	0	2,2,2	0.40	0
3	VND	C	1001	-	17,17,17	1.00	1 (5%)	21,24,24	1.75	2 (9%)
5	EDO	A	1006	-	3,3,3	0.56	0	2,2,2	0.15	0
4	SO4	A	1002	-	4,4,4	0.17	0	6,6,6	0.25	0
4	SO4	A	1003	-	4,4,4	0.19	0	6,6,6	0.38	0
5	EDO	A	1004	-	3,3,3	0.38	0	2,2,2	0.58	0
3	VND	A	1001	-	17,17,17	0.90	1 (5%)	21,24,24	1.15	2 (9%)
5	EDO	C	1011	-	3,3,3	0.52	0	2,2,2	0.31	0
6	PEG	B	1101	-	6,6,6	0.48	0	5,5,5	0.27	0
4	SO4	C	1002	-	4,4,4	0.16	0	6,6,6	0.15	0
5	EDO	C	1005	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	C	1006	-	3,3,3	0.43	0	2,2,2	0.42	0
4	SO4	C	1003	-	4,4,4	0.12	0	6,6,6	0.18	0
5	EDO	A	1005	-	3,3,3	0.47	0	2,2,2	0.31	0
5	EDO	C	1008	-	3,3,3	0.41	0	2,2,2	0.45	0
5	EDO	B	1104	-	3,3,3	0.45	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	C	1004	-	4,4,4	0.12	0	6,6,6	0.31	0
5	EDO	C	1010	-	3,3,3	0.42	0	2,2,2	0.71	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	C	1009	-	-	1/1/1/1	-
5	EDO	C	1007	-	-	0/1/1/1	-
5	EDO	C	1011	-	-	1/1/1/1	-
6	PEG	B	1101	-	-	2/4/4/4	-
5	EDO	A	1006	-	-	0/1/1/1	-
5	EDO	B	1104	-	-	1/1/1/1	-
5	EDO	C	1005	-	-	0/1/1/1	-
5	EDO	C	1006	-	-	1/1/1/1	-
3	VND	C	1001	-	-	0/8/31/31	0/1/1/1
5	EDO	A	1005	-	-	1/1/1/1	-
5	EDO	A	1004	-	-	0/1/1/1	-
5	EDO	C	1010	-	-	1/1/1/1	-
3	VND	A	1001	-	-	0/8/31/31	0/1/1/1
5	EDO	C	1008	-	-	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	-2.73	1.39	1.44
3	C	1001	VND	O1-C6	-2.49	1.40	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1001	VND	C8-N1-C2	-5.61	106.26	114.20
3	C	1001	VND	C1-C2-N1	-4.01	103.23	112.11
3	A	1001	VND	C3-C4-C5	-2.41	107.98	111.30
3	A	1001	VND	C8-N1-C2	-2.07	111.28	114.20

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	1010	EDO	O1-C1-C2-O2
5	C	1006	EDO	O1-C1-C2-O2
6	B	1101	PEG	C4-C3-O2-C2

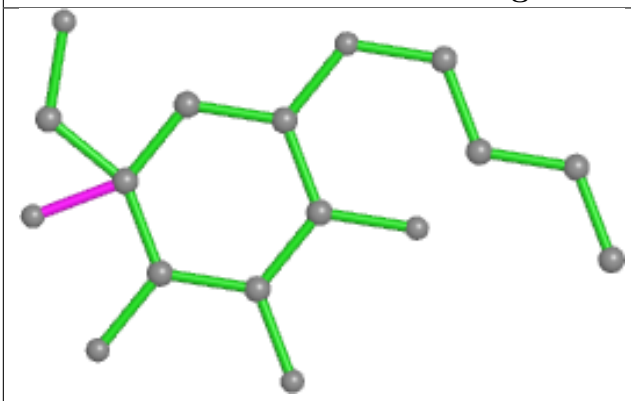
There are no ring outliers.

4 monomers are involved in 5 short contacts:

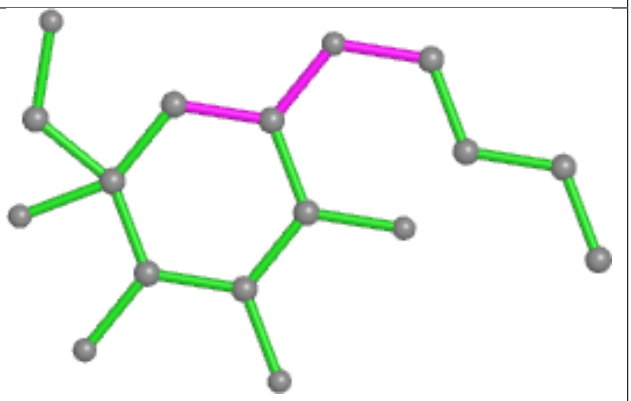
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	SO4	1	0
5	A	1004	EDO	2	0
4	C	1002	SO4	1	0
5	A	1005	EDO	1	0

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 then 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.

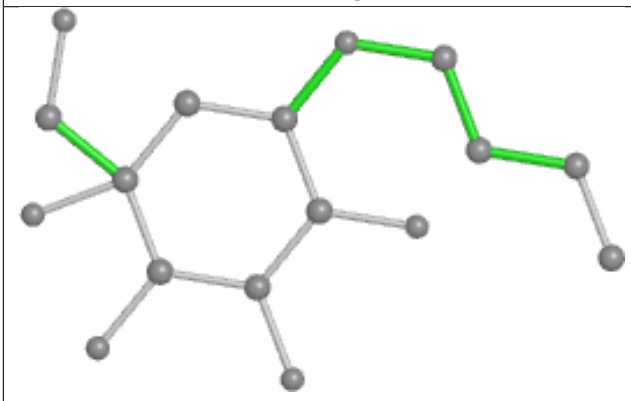
Ligand VND C 1001



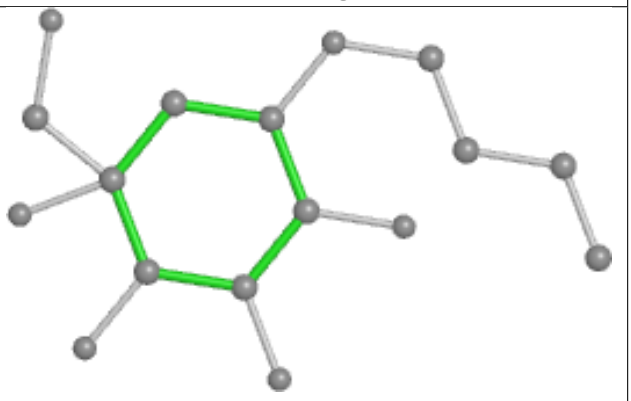
Bond lengths



Bond angles

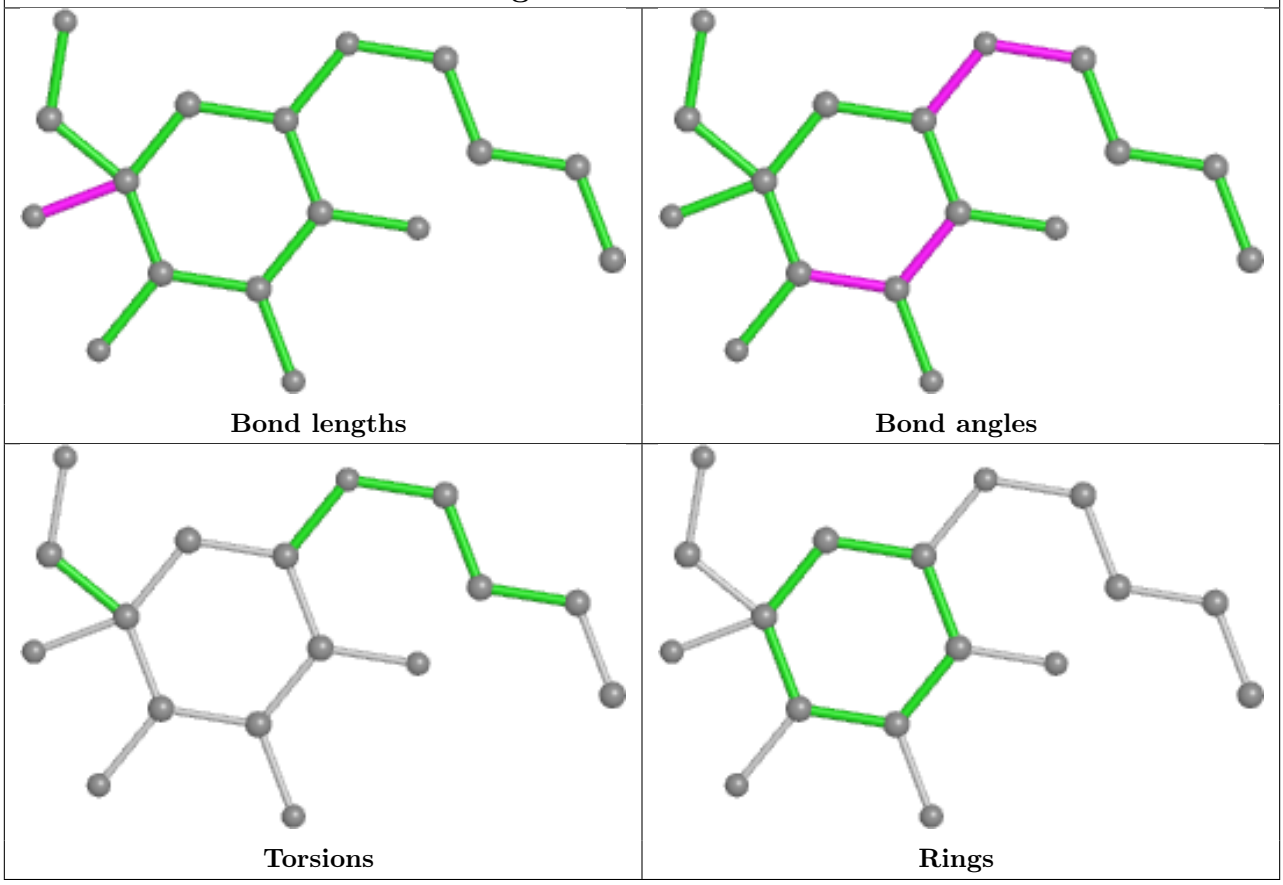


Torsions



Rings

Ligand VND A 1001



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, 95^{th} 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%)	-0.57	8 (0%)	84	83	26, 35, 57, 102	0
1	C	857/977 (87%)	-0.47	4 (0%)	91	90	27, 40, 76, 102	0
2	B	83/547 (15%)	-0.39	1 (1%)	79	77	33, 49, 81, 91	0
2	D	85/547 (15%)	-0.21	3 (3%)	44	41	33, 51, 89, 100	0
All	All	1876/3048 (61%)	-0.50	16 (0%)	84	83	26, 38, 74, 102	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	81	GLY	7.5
1	A	184	PRO	7.4
1	C	185	ARG	4.7
1	A	251	THR	4.7
1	A	254	THR	3.4
1	A	253	LYS	3.2
1	C	78	LEU	3.1
1	A	248	TRP	2.9
1	C	370	THR	2.7
2	D	82	TYR	2.7
2	B	48	PHE	2.6
2	D	80	THR	2.5
1	A	183	ALA	2.5
1	A	34	ASP	2.3
1	A	252	PHE	2.2
1	C	34	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

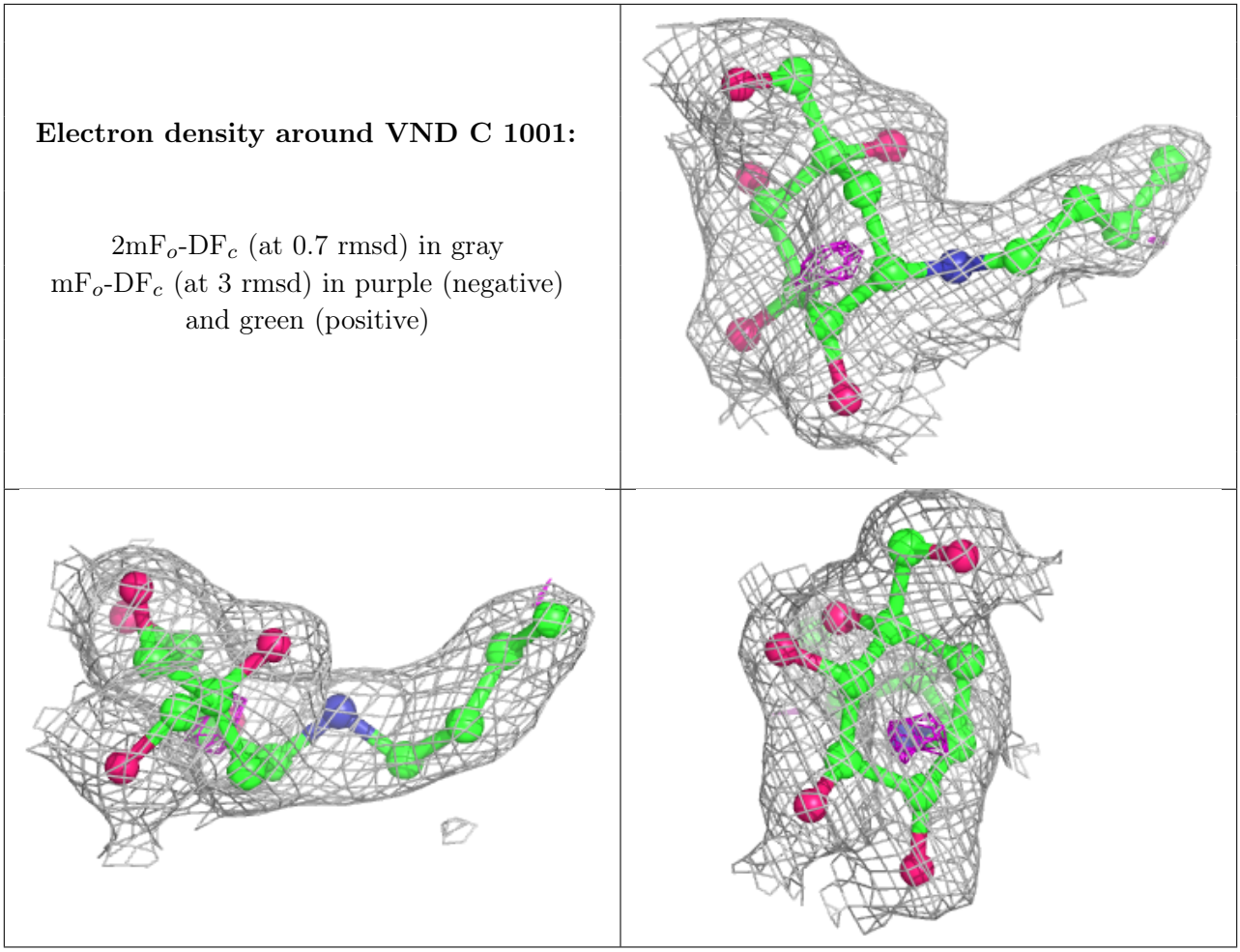
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	EDO	A	1005	4/4	0.84	0.15	59,62,67,72	0
5	EDO	A	1006	4/4	0.85	0.21	46,47,47,51	0
4	SO4	A	1002	5/5	0.87	0.20	61,62,77,98	0
5	EDO	C	1009	4/4	0.87	0.17	48,49,52,57	0
5	EDO	C	1007	4/4	0.88	0.21	47,56,62,62	0
5	EDO	B	1104	4/4	0.88	0.09	49,50,52,56	0
5	EDO	C	1008	4/4	0.89	0.12	67,67,75,75	0
4	SO4	C	1002	5/5	0.90	0.18	70,75,87,96	0
4	SO4	A	1003	5/5	0.91	0.26	64,64,76,90	0
6	PEG	B	1101	7/7	0.93	0.15	48,53,59,59	0
5	EDO	C	1005	4/4	0.94	0.13	48,66,70,70	0
5	EDO	C	1011	4/4	0.95	0.14	50,51,54,55	0
4	SO4	C	1003	5/5	0.96	0.25	62,65,80,81	0
4	SO4	C	1004	5/5	0.96	0.38	67,67,77,92	0
5	EDO	A	1004	4/4	0.96	0.14	47,50,51,62	0
5	EDO	C	1010	4/4	0.97	0.12	44,45,48,50	0
3	VND	C	1001	17/17	0.97	0.15	31,39,52,54	0
3	VND	A	1001	17/17	0.97	0.11	32,39,46,53	0
5	EDO	C	1006	4/4	0.98	0.12	41,42,43,50	0
7	CA	B	1102	1/1	0.99	0.12	39,39,39,39	0
7	CA	D	601	1/1	0.99	0.10	40,40,40,40	0
7	CA	B	1103	1/1	1.00	0.14	35,35,35,35	0
7	CA	D	602	1/1	1.00	0.11	33,33,33,33	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.

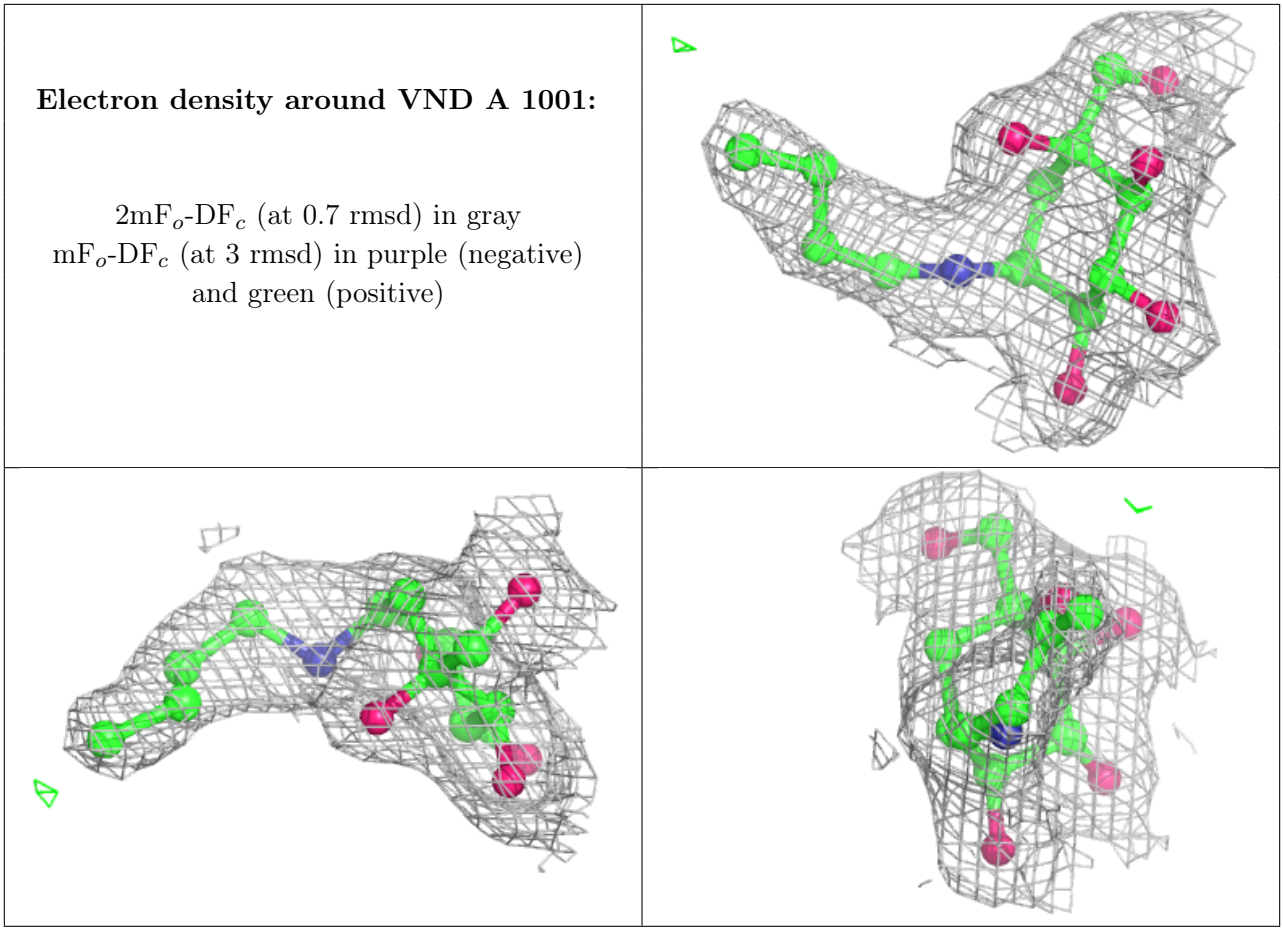
Electron density around VND C 1001:

$2mF_o$-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

There are no such residues in this entry.