wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 09:49 pm BST

PDB ID	:	3ZX2
Title	:	NTPDase1 in complex with Decavanadate
Authors	:	Zebisch, M.; Schaefer, P.; Straeter, N.
Deposited on	:	2011-08-04
Resolution	:	1.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

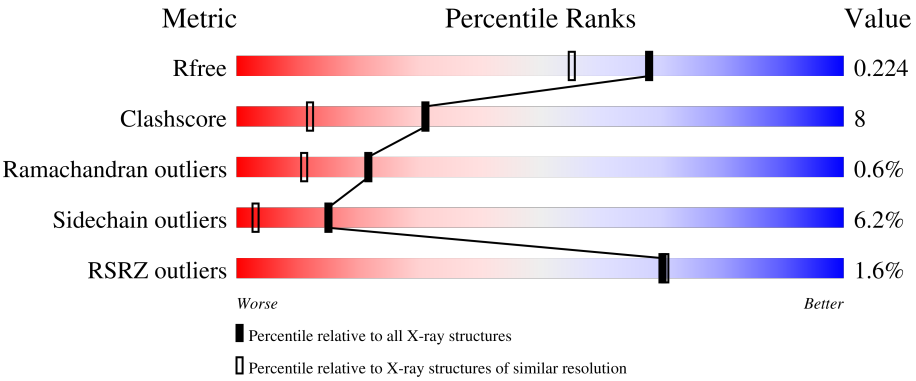
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.81 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}	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82-1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	452	73% 13% • 12%
1	B	452	2% 67% 19% • 12%
1	C	452	70% 15% • 13%
1	D	452	71% 15% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	D	503	-	-	X	-
3	ACY	A	511	-	-	X	-
3	ACY	B	511	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13563 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 ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	9	0
			3178	2051	512	595	20			
1	B	399	Total	C	N	O	S	0	4	0
			3172	2045	513	594	20			
1	C	393	Total	C	N	O	S	0	4	0
			3129	2024	502	583	20			
1	D	396	Total	C	N	O	S	0	7	0
			3166	2044	509	592	21			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP P97687
A	16	ALA	-	expression tag	UNP P97687
A	17	HIS	-	expression tag	UNP P97687
A	18	HIS	-	expression tag	UNP P97687
A	19	HIS	-	expression tag	UNP P97687
A	20	HIS	-	expression tag	UNP P97687
A	21	HIS	-	expression tag	UNP P97687
A	22	HIS	-	expression tag	UNP P97687
A	23	VAL	-	expression tag	UNP P97687
A	24	GLY	-	expression tag	UNP P97687
A	25	THR	-	expression tag	UNP P97687
A	26	GLY	-	expression tag	UNP P97687
A	27	SER	-	expression tag	UNP P97687
A	28	ASN	-	expression tag	UNP P97687
A	29	ASP	-	expression tag	UNP P97687
A	30	ASP	-	expression tag	UNP P97687
A	31	ASP	-	expression tag	UNP P97687
A	32	ASP	-	expression tag	UNP P97687
A	33	LYS	-	expression tag	UNP P97687
A	34	SER	-	expression tag	UNP P97687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	PRO	-	expression tag	UNP P97687
A	36	ASP	-	expression tag	UNP P97687
A	37	PRO	-	expression tag	UNP P97687
A	80	GLN	LEU	SEE REMARK 999	UNP P97687
A	190	LYS	-	linker	UNP P97687
A	191	THR	-	linker	UNP P97687
A	192	PRO	-	linker	UNP P97687
A	204	GLY	-	linker	UNP P97687
A	205	GLY	-	linker	UNP P97687
A	206	SER	-	linker	UNP P97687
A	220	ILE	VAL	SEE REMARK 999	UNP P97687
A	227	SER	GLN	SEE REMARK 999	UNP P97687
A	331	ILE	PHE	conflict	UNP P97687
B	15	MET	-	expression tag	UNP P97687
B	16	ALA	-	expression tag	UNP P97687
B	17	HIS	-	expression tag	UNP P97687
B	18	HIS	-	expression tag	UNP P97687
B	19	HIS	-	expression tag	UNP P97687
B	20	HIS	-	expression tag	UNP P97687
B	21	HIS	-	expression tag	UNP P97687
B	22	HIS	-	expression tag	UNP P97687
B	23	VAL	-	expression tag	UNP P97687
B	24	GLY	-	expression tag	UNP P97687
B	25	THR	-	expression tag	UNP P97687
B	26	GLY	-	expression tag	UNP P97687
B	27	SER	-	expression tag	UNP P97687
B	28	ASN	-	expression tag	UNP P97687
B	29	ASP	-	expression tag	UNP P97687
B	30	ASP	-	expression tag	UNP P97687
B	31	ASP	-	expression tag	UNP P97687
B	32	ASP	-	expression tag	UNP P97687
B	33	LYS	-	expression tag	UNP P97687
B	34	SER	-	expression tag	UNP P97687
B	35	PRO	-	expression tag	UNP P97687
B	36	ASP	-	expression tag	UNP P97687
B	37	PRO	-	expression tag	UNP P97687
B	80	GLN	LEU	SEE REMARK 999	UNP P97687
B	190	LYS	-	linker	UNP P97687
B	191	THR	-	linker	UNP P97687
B	192	PRO	-	linker	UNP P97687
B	204	GLY	-	linker	UNP P97687
B	205	GLY	-	linker	UNP P97687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	SER	-	linker	UNP P97687
B	220	ILE	VAL	SEE REMARK 999	UNP P97687
B	227	SER	GLN	SEE REMARK 999	UNP P97687
B	331	ILE	PHE	conflict	UNP P97687
C	15	MET	-	expression tag	UNP P97687
C	16	ALA	-	expression tag	UNP P97687
C	17	HIS	-	expression tag	UNP P97687
C	18	HIS	-	expression tag	UNP P97687
C	19	HIS	-	expression tag	UNP P97687
C	20	HIS	-	expression tag	UNP P97687
C	21	HIS	-	expression tag	UNP P97687
C	22	HIS	-	expression tag	UNP P97687
C	23	VAL	-	expression tag	UNP P97687
C	24	GLY	-	expression tag	UNP P97687
C	25	THR	-	expression tag	UNP P97687
C	26	GLY	-	expression tag	UNP P97687
C	27	SER	-	expression tag	UNP P97687
C	28	ASN	-	expression tag	UNP P97687
C	29	ASP	-	expression tag	UNP P97687
C	30	ASP	-	expression tag	UNP P97687
C	31	ASP	-	expression tag	UNP P97687
C	32	ASP	-	expression tag	UNP P97687
C	33	LYS	-	expression tag	UNP P97687
C	34	SER	-	expression tag	UNP P97687
C	35	PRO	-	expression tag	UNP P97687
C	36	ASP	-	expression tag	UNP P97687
C	37	PRO	-	expression tag	UNP P97687
C	80	GLN	LEU	SEE REMARK 999	UNP P97687
C	190	LYS	-	linker	UNP P97687
C	191	THR	-	linker	UNP P97687
C	192	PRO	-	linker	UNP P97687
C	204	GLY	-	linker	UNP P97687
C	205	GLY	-	linker	UNP P97687
C	206	SER	-	linker	UNP P97687
C	220	ILE	VAL	SEE REMARK 999	UNP P97687
C	227	SER	GLN	SEE REMARK 999	UNP P97687
C	331	ILE	PHE	conflict	UNP P97687
D	15	MET	-	expression tag	UNP P97687
D	16	ALA	-	expression tag	UNP P97687
D	17	HIS	-	expression tag	UNP P97687
D	18	HIS	-	expression tag	UNP P97687
D	19	HIS	-	expression tag	UNP P97687

Continued on next page...

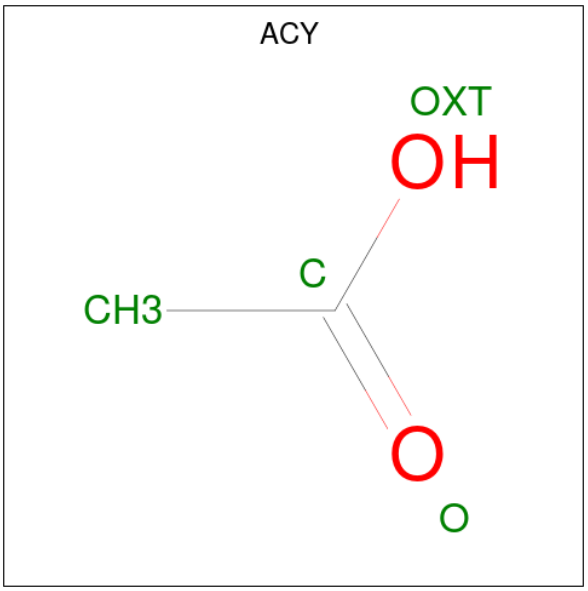
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP P97687
D	21	HIS	-	expression tag	UNP P97687
D	22	HIS	-	expression tag	UNP P97687
D	23	VAL	-	expression tag	UNP P97687
D	24	GLY	-	expression tag	UNP P97687
D	25	THR	-	expression tag	UNP P97687
D	26	GLY	-	expression tag	UNP P97687
D	27	SER	-	expression tag	UNP P97687
D	28	ASN	-	expression tag	UNP P97687
D	29	ASP	-	expression tag	UNP P97687
D	30	ASP	-	expression tag	UNP P97687
D	31	ASP	-	expression tag	UNP P97687
D	32	ASP	-	expression tag	UNP P97687
D	33	LYS	-	expression tag	UNP P97687
D	34	SER	-	expression tag	UNP P97687
D	35	PRO	-	expression tag	UNP P97687
D	36	ASP	-	expression tag	UNP P97687
D	37	PRO	-	expression tag	UNP P97687
D	80	GLN	LEU	SEE REMARK 999	UNP P97687
D	190	LYS	-	linker	UNP P97687
D	191	THR	-	linker	UNP P97687
D	192	PRO	-	linker	UNP P97687
D	204	GLY	-	linker	UNP P97687
D	205	GLY	-	linker	UNP P97687
D	206	SER	-	linker	UNP P97687
D	220	ILE	VAL	SEE REMARK 999	UNP P97687
D	227	SER	GLN	SEE REMARK 999	UNP P97687
D	331	ILE	PHE	conflict	UNP P97687

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

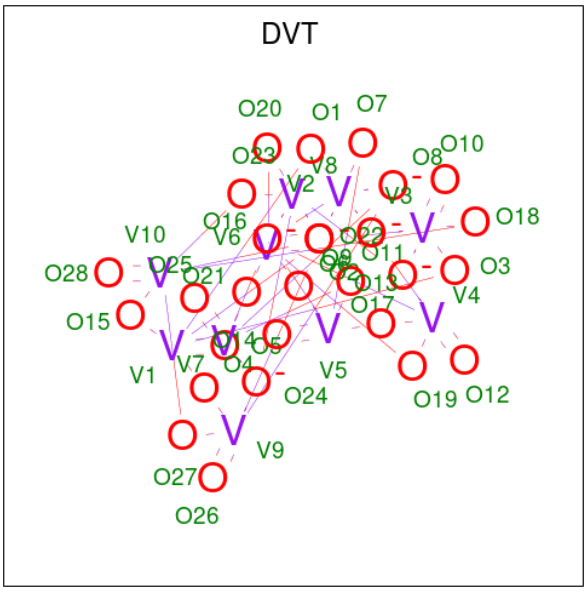
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Cl 5 5	0	0
2	B	5	Total Cl 5 5	0	0
2	C	5	Total Cl 5 5	0	0
2	D	8	Total Cl 8 8	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 4 is DECAVANADATE (three-letter code: DVT) (formula: $O_{28}V_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O V 38 28 10	0	0
4	B	1	Total O V 38 28 10	0	1
4	C	1	Total O V 38 28 10	0	1
4	D	1	Total O V 38 28 10	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0
5	C	2	Total Na 2 2	0	0
5	D	3	Total Na 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	169	Total O 170 170	0	1
6	B	130	Total O 130 130	0	0

Continued on next page...

Continued from previous page...

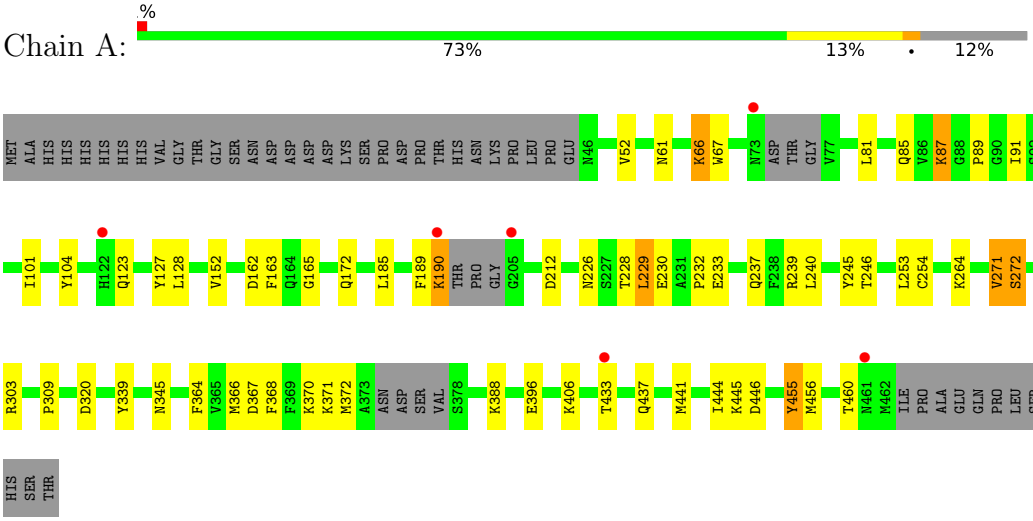
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	191	Total O 191 191	0	0
6	D	218	Total O 218 218	0	0

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.

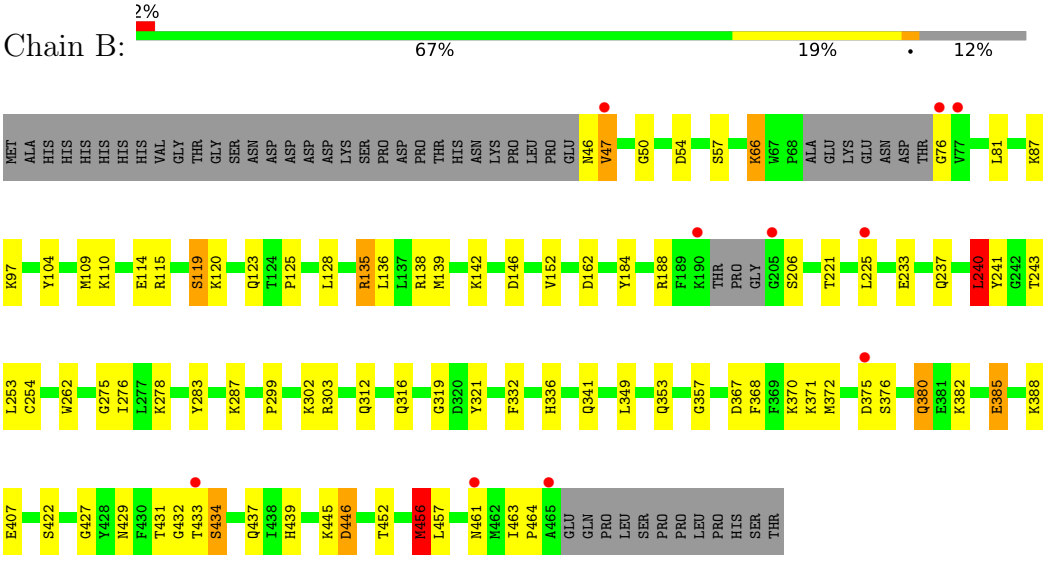
• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

Chain A:



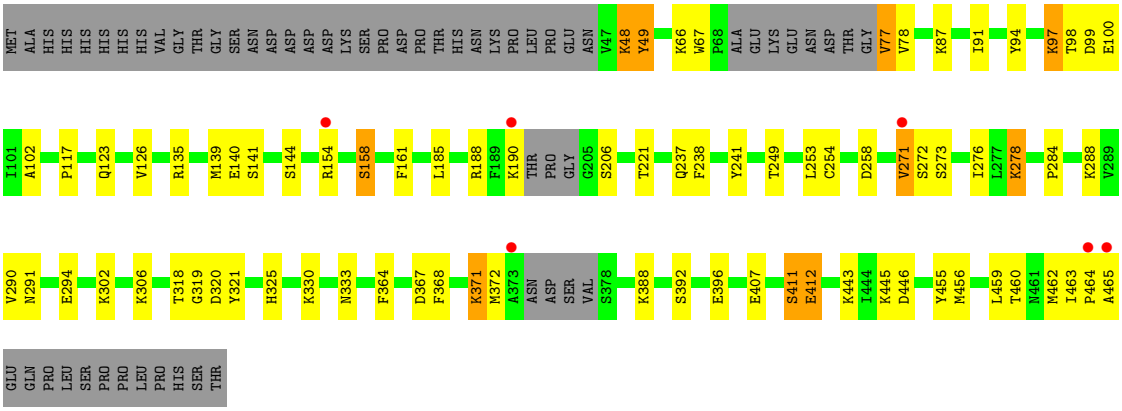
• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

Chain B:



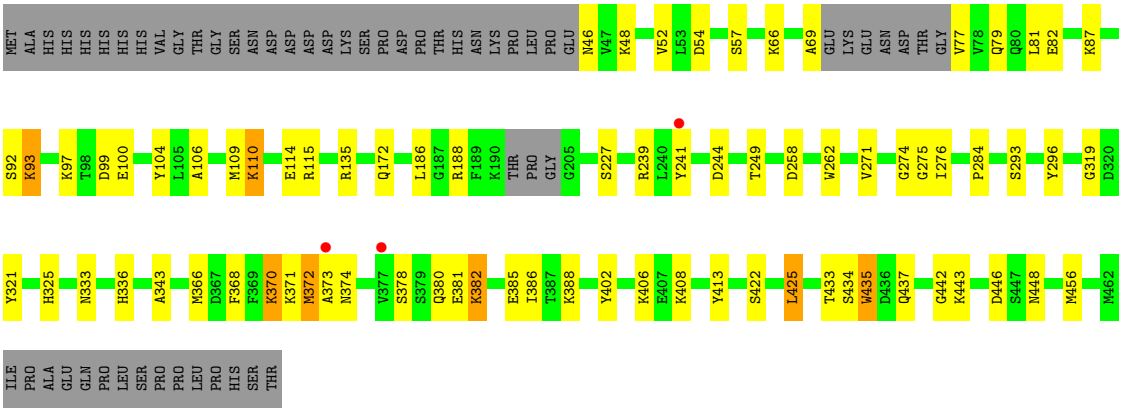
• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

Chain C:



• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.92Å 80.98Å 165.52Å 90.00° 117.49° 90.00°	Depositor
Resolution (Å)	146.83 – 1.81 146.83 – 1.81	Depositor EDS
% Data completeness (in resolution range)	73.1 (146.83-1.81) 73.2 (146.83-1.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.98 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.175 , 0.224 0.175 , 0.224	Depositor DCC
R_{free} test set	1270 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13563	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: CL, DVT, ACY, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.04	4/3285 (0.1%)	1.05	7/4436 (0.2%)
1	B	0.99	1/3262 (0.0%)	1.05	8/4408 (0.2%)
1	C	1.05	2/3221 (0.1%)	1.07	10/4351 (0.2%)
1	D	1.07	5/3267 (0.2%)	1.05	8/4414 (0.2%)
All	All	1.04	12/13035 (0.1%)	1.06	33/17609 (0.2%)

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	1
1	D	0	1
All	All	0	2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	GLU	CG-CD	6.60	1.61	1.51
1	D	413	TYR	CE2-CZ	-6.29	1.30	1.38
1	A	455	TYR	CE2-CZ	6.11	1.46	1.38
1	D	99	ASP	CB-CG	6.09	1.64	1.51
1	D	435	TRP	CD2-CE2	5.97	1.48	1.41

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	ASP	CB-CG-OD2	-8.97	110.23	118.30
1	C	320	ASP	CB-CG-OD1	8.64	126.07	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	456	MET	CA-CB-CG	-8.45	98.93	113.30
1	D	99	ASP	CB-CG-OD1	8.28	125.75	118.30
1	B	240	LEU	CA-CB-CG	7.95	133.58	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	SER	Peptide
1	D	274	GLY	Peptide

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	3178	0	3094	63	0
1	B	3172	0	3093	70	0
1	C	3129	0	3064	42	0
1	D	3166	0	3102	43	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	8	0	0	4	0
3	A	4	0	3	8	0
3	B	8	0	6	4	0
3	C	8	0	6	0	0
3	D	8	0	6	0	0
4	A	38	0	0	2	0
4	B	38	0	0	0	0
4	C	38	0	0	1	0
4	D	38	0	0	5	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
6	A	170	0	0	6	0
6	B	130	0	0	4	0
6	C	191	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	218	0	0	3	0
All	All	13563	0	12374	204	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 8.

The worst 5 of 204 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:MET:CE	3:A:511:ACY:H1	1.39	1.48
1:A:366:MET:HE2	3:A:511:ACY:CH3	1.60	1.30
1:A:229:LEU:HD22	1:B:139:MET:SD	1.76	1.24
1:A:437[A]:GLN:OE1	6:A:2133:HOH:O	1.61	1.15
1:D:52:VAL:HG23	1:D:456:MET:CE	1.85	1.07

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	397/452 (88%)	376 (95%)	21 (5%)	0	100 100
1	B	397/452 (88%)	375 (94%)	17 (4%)	5 (1%)	10 2
1	C	389/452 (86%)	370 (95%)	17 (4%)	2 (0%)	25 14
1	D	397/452 (88%)	377 (95%)	17 (4%)	3 (1%)	16 6
All	All	1580/1808 (87%)	1498 (95%)	72 (5%)	10 (1%)	22 11

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	461	ASN
1	C	99	ASP
1	D	435	TRP
1	B	319	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	344/390 (88%)	328 (95%)	16 (5%)	22 7
1	B	344/390 (88%)	320 (93%)	24 (7%)	12 2
1	C	340/390 (87%)	313 (92%)	27 (8%)	10 1
1	D	346/390 (89%)	325 (94%)	21 (6%)	15 3
All	All	1374/1560 (88%)	1286 (94%)	88 (6%)	15 3

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	302	LYS
1	D	93	LYS
1	C	364	PHE
1	C	456	MET
1	D	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	314	GLN
1	C	389	ASN
1	D	380	GLN
1	C	333	ASN
1	C	458	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 40 ligands modelled in this entry, 29 are monoatomic - leaving 11 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	DVT	D	531	-	60,60,60	0.84	1 (1%)	-		
3	ACY	B	512	-	3,3,3	1.23	0	3,3,3	0.59	0
4	DVT	B	531[A]	-	60,60,60	0.72	1 (1%)	-		
3	ACY	C	512	-	3,3,3	0.82	0	3,3,3	1.09	0
4	DVT	C	531[B]	-	60,60,60	0.75	1 (1%)	-		
3	ACY	C	511	-	3,3,3	0.77	0	3,3,3	1.32	0
4	DVT	A	531	-	60,60,60	0.70	0	-		
3	ACY	D	512	-	3,3,3	1.12	0	3,3,3	0.79	0
3	ACY	B	511	-	3,3,3	0.82	0	3,3,3	1.70	1 (33%)
3	ACY	D	511	-	3,3,3	0.75	0	3,3,3	1.43	0
3	ACY	A	511	-	3,3,3	1.16	0	3,3,3	1.89	2 (66%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	531	DVT	O12-V4	-3.32	1.56	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	531[A]	DVT	O10-V3	2.79	1.64	1.60
4	C	531[B]	DVT	O2-V3	-2.28	2.18	2.26

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	511	ACY	OXT-C-O	-2.47	112.97	122.05
3	B	511	ACY	OXT-C-CH3	2.31	124.74	115.18
3	A	511	ACY	OXT-C-CH3	2.16	124.10	115.18

There are no chirality outliers.

There are no torsion outliers.

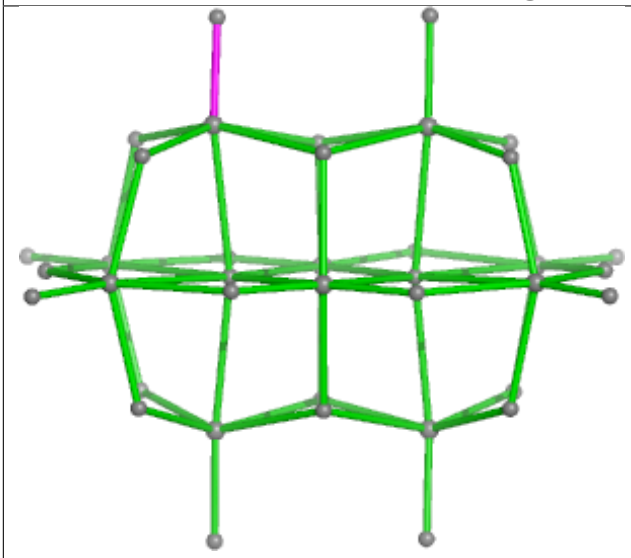
There are no ring outliers.

5 monomers are involved in 20 short contacts:

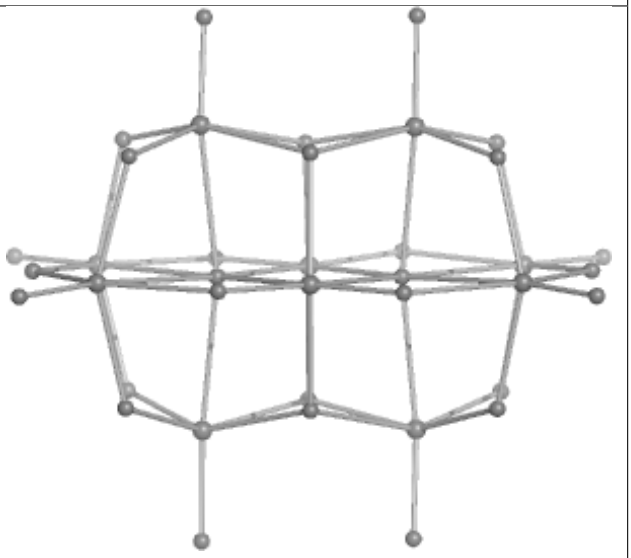
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	531	DVT	5	0
4	C	531[B]	DVT	1	0
4	A	531	DVT	2	0
3	B	511	ACY	4	0
3	A	511	ACY	8	0

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.

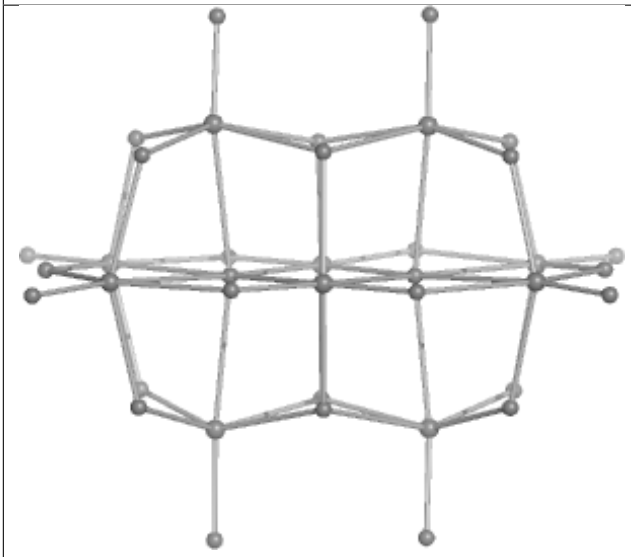
Ligand DVT D 531



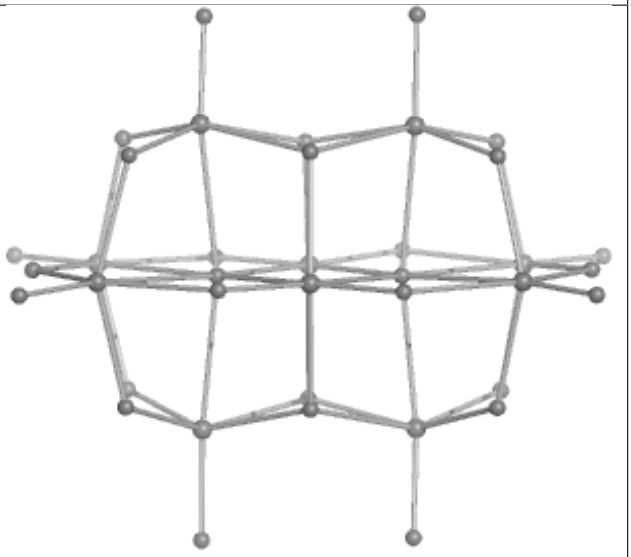
Bond lengths



Bond angles

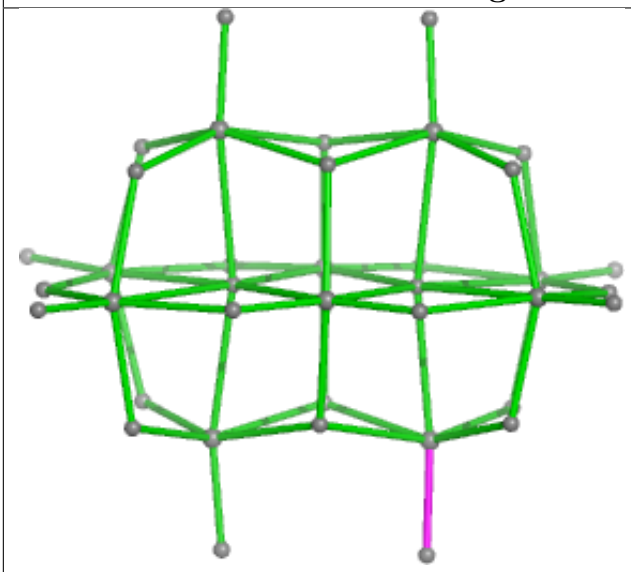


Torsions

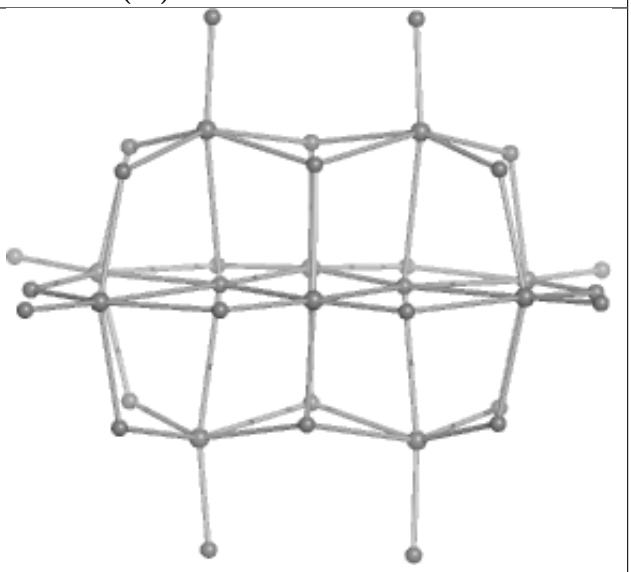


Rings

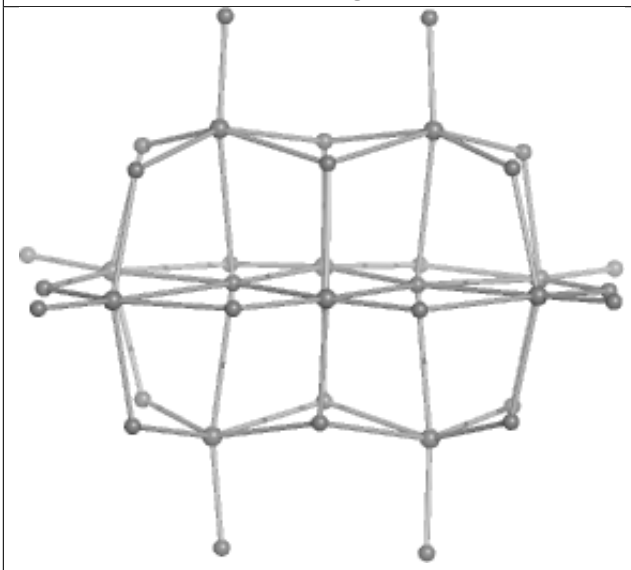
Ligand DVT B 531 (A)



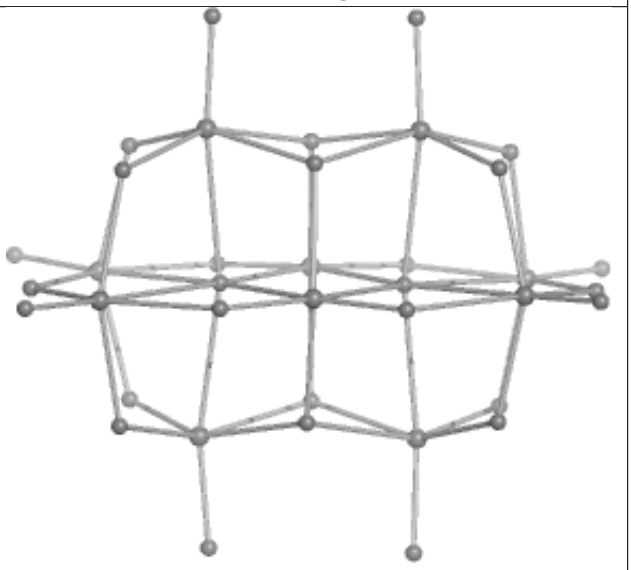
Bond lengths



Bond angles

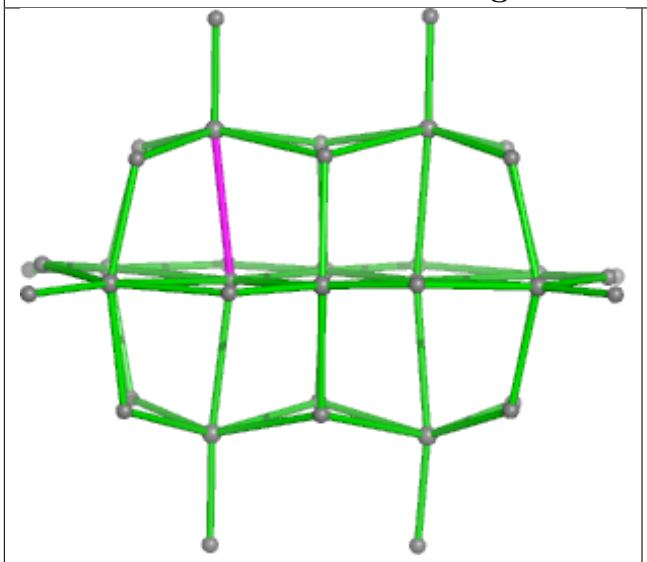


Torsions

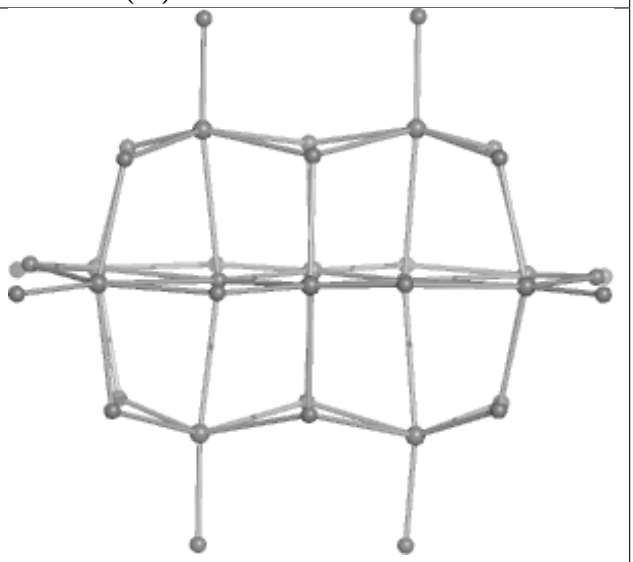


Rings

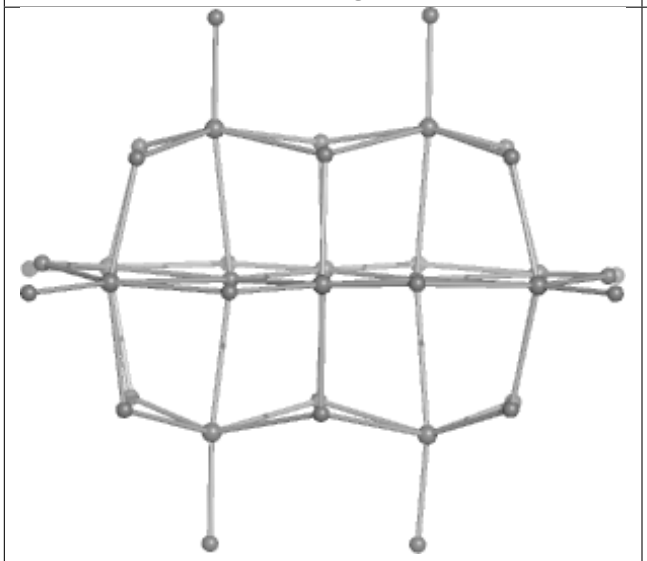
Ligand DVT C 531 (B)



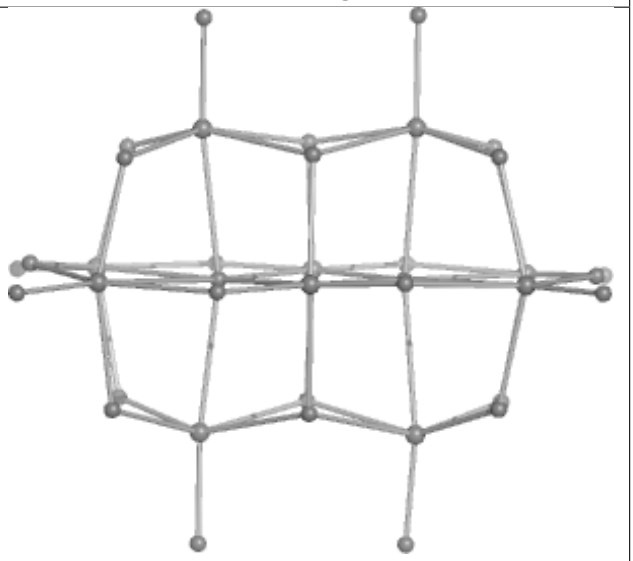
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	396/452 (87%)	-0.19	6 (1%)	71	72	21, 43, 79, 126	9 (2%)
1	B	399/452 (88%)	-0.09	10 (2%)	58	58	23, 47, 80, 106	4 (1%)
1	C	393/452 (86%)	-0.15	6 (1%)	71	72	24, 46, 82, 100	4 (1%)
1	D	396/452 (87%)	-0.40	3 (0%)	82	83	19, 40, 72, 95	7 (1%)
All	All	1584/1808 (87%)	-0.21	25 (1%)	70	70	19, 44, 80, 126	24 (1%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	465	ALA	4.4
1	B	433	THR	3.5
1	B	190	LYS	3.4
1	B	76	GLY	3.3
1	A	433	THR	3.2

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

There are no monosaccharides in this entry.

6.4 Ligands

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.

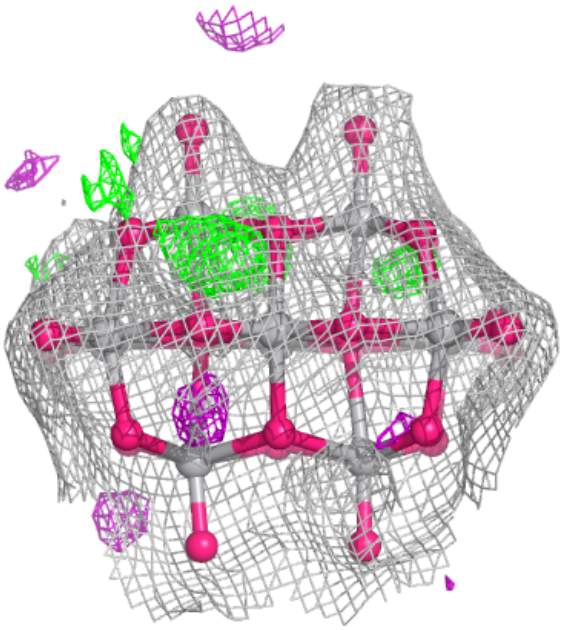
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACY	B	511	4/4	0.79	0.14	56,59,68,69	0
3	ACY	A	511	4/4	0.82	0.11	36,47,50,56	0
2	CL	D	501	1/1	0.88	0.13	47,47,47,47	0
5	NA	B	521	1/1	0.89	0.10	59,59,59,59	0
5	NA	D	523	1/1	0.89	0.11	63,63,63,63	0
2	CL	B	501	1/1	0.93	0.11	48,48,48,48	0
2	CL	B	505	1/1	0.94	0.09	47,47,47,47	0
3	ACY	B	512	4/4	0.95	0.09	41,44,50,51	0
4	DVT	C	531[B]	38/38	0.95	0.09	34,45,50,58	38
2	CL	A	506	1/1	0.95	0.12	60,60,60,60	0
2	CL	A	501	1/1	0.95	0.12	45,45,45,45	0
3	ACY	D	512	4/4	0.96	0.08	40,41,42,43	0
4	DVT	B	531[A]	38/38	0.96	0.08	40,49,58,62	38
2	CL	D	509	1/1	0.96	0.06	41,41,41,41	1
2	CL	C	501	1/1	0.96	0.06	44,44,44,44	0
5	NA	D	522	1/1	0.96	0.05	60,60,60,60	0
3	ACY	C	511	4/4	0.96	0.10	32,35,38,38	0
2	CL	C	503	1/1	0.97	0.09	48,48,48,48	0
2	CL	B	506	1/1	0.97	0.15	58,58,58,58	0
2	CL	D	507	1/1	0.97	0.07	41,41,41,41	0
5	NA	C	521	1/1	0.97	0.05	53,53,53,53	0
2	CL	D	508	1/1	0.97	0.08	56,56,56,56	0
2	CL	C	502	1/1	0.97	0.11	48,48,48,48	0
2	CL	B	503	1/1	0.98	0.06	49,49,49,49	0
2	CL	A	503	1/1	0.98	0.08	41,41,41,41	0
4	DVT	D	531	38/38	0.98	0.07	30,37,41,43	38
3	ACY	C	512	4/4	0.98	0.05	31,34,36,37	0
3	ACY	D	511	4/4	0.98	0.06	36,37,40,43	0
5	NA	C	522	1/1	0.98	0.03	32,32,32,32	0
5	NA	D	521	1/1	0.98	0.04	38,38,38,38	0
2	CL	C	506	1/1	0.98	0.04	38,38,38,38	0
4	DVT	A	531	38/38	0.98	0.06	34,42,47,49	38
2	CL	D	506	1/1	0.99	0.08	46,46,46,46	0
2	CL	B	502	1/1	0.99	0.03	43,43,43,43	0
2	CL	C	505	1/1	0.99	0.09	45,45,45,45	0
2	CL	A	502	1/1	0.99	0.06	44,44,44,44	0
2	CL	A	505	1/1	0.99	0.05	45,45,45,45	0
2	CL	D	502	1/1	0.99	0.09	43,43,43,43	0
2	CL	D	505	1/1	0.99	0.06	43,43,43,43	0
2	CL	D	503	1/1	1.00	0.04	38,38,38,38	0

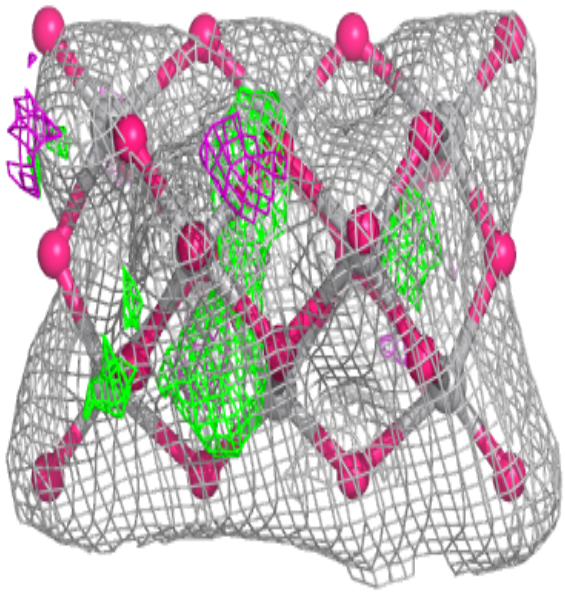
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

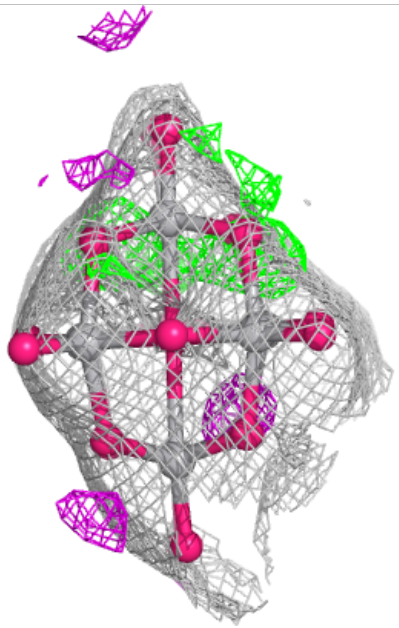
orientation to approximate a three-dimensional view.

Electron density around DVT C 531 (B):

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

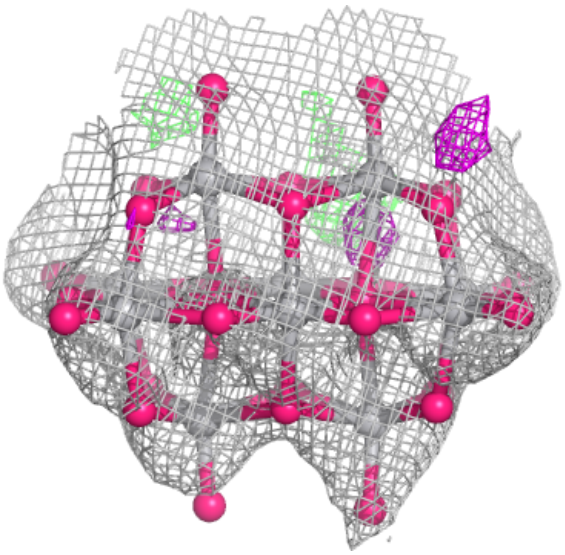


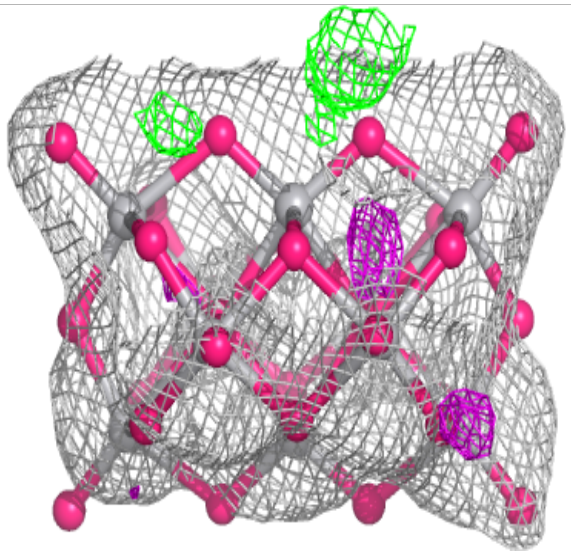


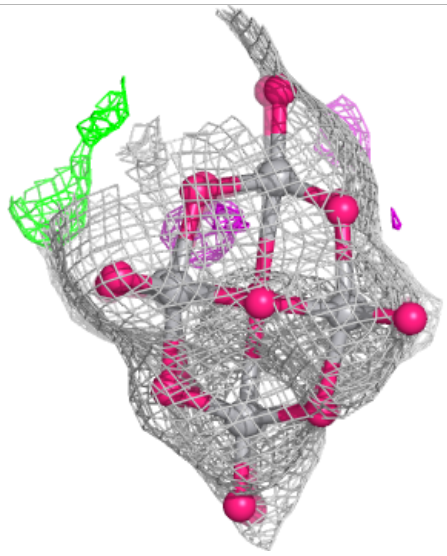


Electron density around DVT B 531 (A):

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

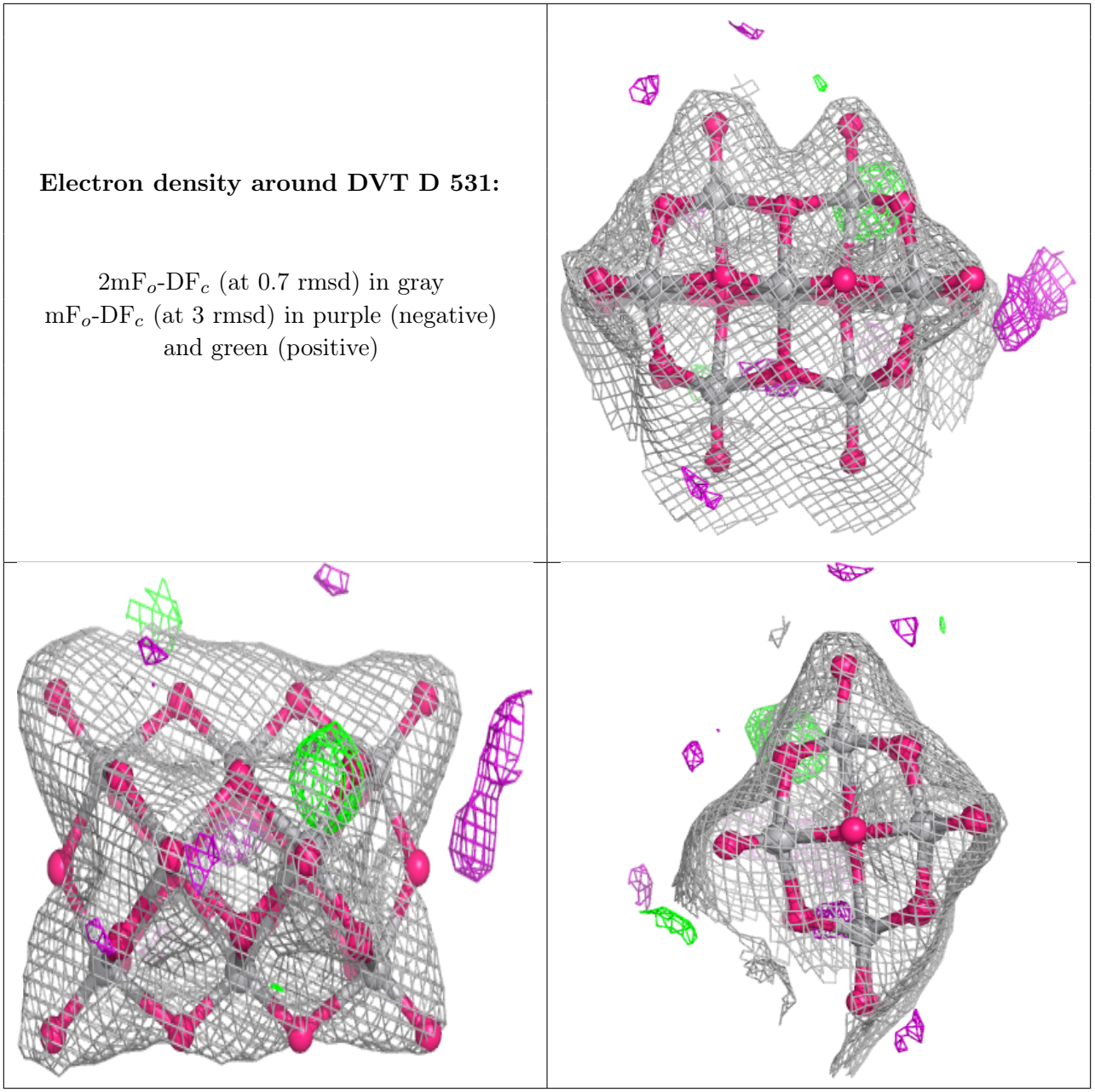






Electron density around DVT D 531:

$2mF_o$-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.