



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:09 PM UTC

PDB ID : 2D1G / pdb_00002d1g
Title : Structure of Francisella tularensis Acid Phosphatase A (AcpA) bound to orthovanadate
Authors : Felts, R.L.; Reilly, T.J.; Tanner, J.J.
Deposited on : 2005-08-20
Resolution : 1.75 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

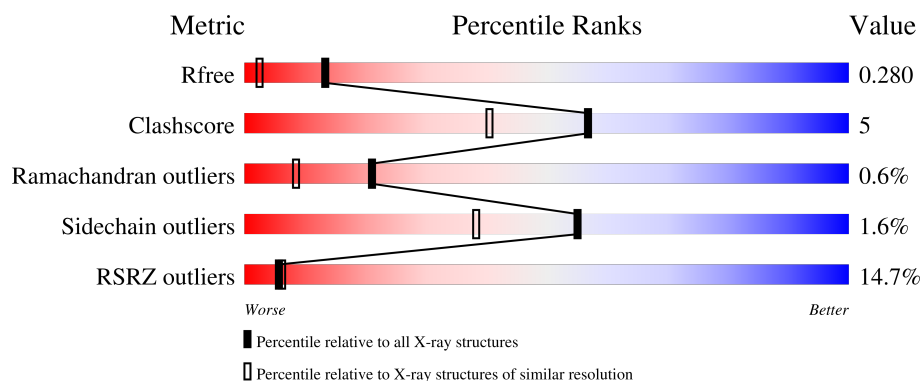
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	498	
1	B	498	

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	VO4	B	901	-	-	X	-
5	ETX	A	1006	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8182 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.

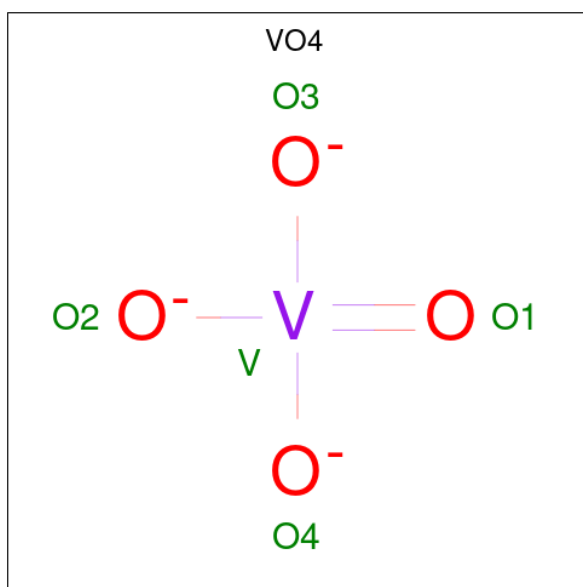
- Molecule 1 is a protein called acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	5	0
			3817	2413	644	746	14			
1	B	472	Total	C	N	O	S	0	1	0
			3725	2352	630	730	13			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q2A5P7
A	375	ASP	ALA	SEE REMARK 999	UNP Q2A5P7
A	376	TRP	GLY	SEE REMARK 999	UNP Q2A5P7
A	377	ASP	ILE	SEE REMARK 999	UNP Q2A5P7
A	378	SER	ALA	SEE REMARK 999	UNP Q2A5P7
A	379	THR	HIS	SEE REMARK 999	UNP Q2A5P7
A	494	HIS	-	expression tag	UNP Q2A5P7
A	495	HIS	-	expression tag	UNP Q2A5P7
A	496	HIS	-	expression tag	UNP Q2A5P7
A	497	HIS	-	expression tag	UNP Q2A5P7
A	498	HIS	-	expression tag	UNP Q2A5P7
B	1	MET	-	initiating methionine	UNP Q2A5P7
B	375	ASP	ALA	SEE REMARK 999	UNP Q2A5P7
B	376	TRP	GLY	SEE REMARK 999	UNP Q2A5P7
B	377	ASP	ILE	SEE REMARK 999	UNP Q2A5P7
B	378	SER	ALA	SEE REMARK 999	UNP Q2A5P7
B	379	THR	HIS	SEE REMARK 999	UNP Q2A5P7
B	494	HIS	-	expression tag	UNP Q2A5P7
B	495	HIS	-	expression tag	UNP Q2A5P7
B	496	HIS	-	expression tag	UNP Q2A5P7
B	497	HIS	-	expression tag	UNP Q2A5P7
B	498	HIS	-	expression tag	UNP Q2A5P7

- Molecule 2 is VANADATE ION (CCD ID: VO4) (formula: O₄V).

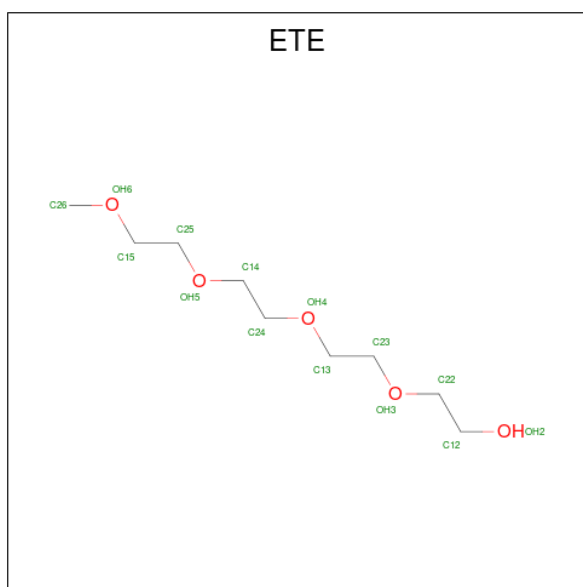


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	V	0	0
			5	4	1		
2	B	1	Total	O	V	0	0
			5	4	1		

- Molecule 3 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

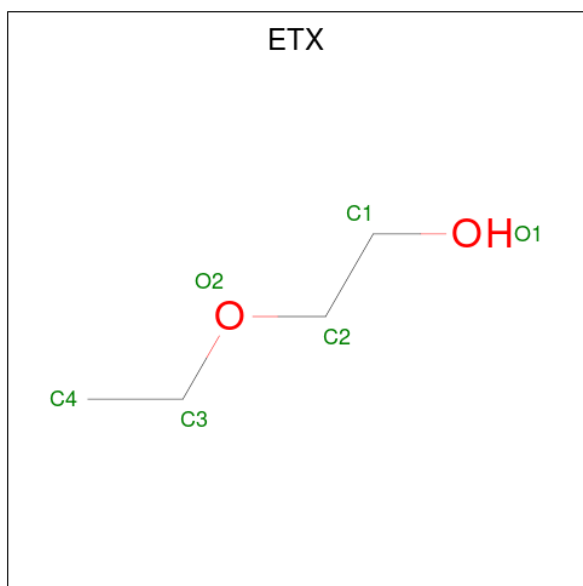
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	X	0	0
			1	1		
3	B	1	Total	X	0	0
			1	1		

- Molecule 4 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



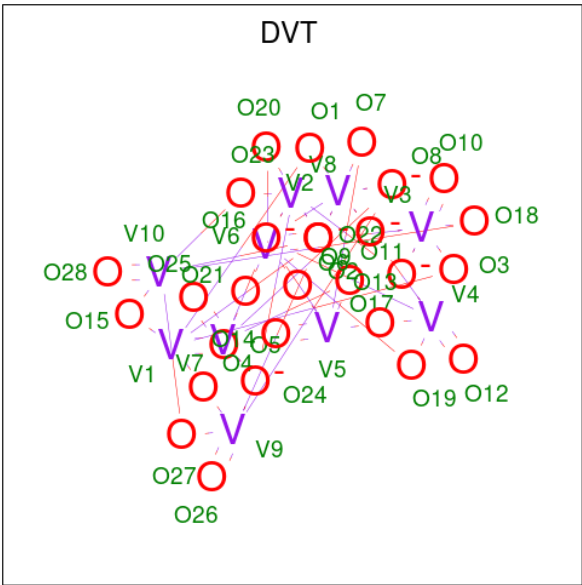
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	9	5		

- Molecule 5 is 2-ETHOXYETHANOL (CCD ID: ETX) (formula: $C_4H_{10}O_2$).



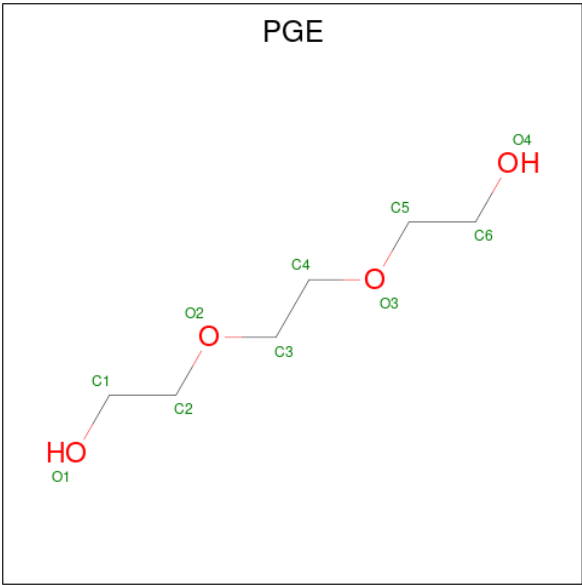
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is DECAVANADATE (CCD ID: DVT) (formula: $O_{28}V_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	V	0	0
			38	28	10		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	345	Total 345	O 345	0	0
8	B	205	Total 205	O 205	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.08Å 144.40Å 123.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 – 1.75 44.28 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.28-1.75) 97.1 (44.28-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 1.75Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.198 , 0.231 0.263 , 0.280	Depositor DCC
R_{free} test set	4923 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8182	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ETE, DVT, PGE, ETX, VO4, UNX

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	0.65	0/3941	0.84	6/5362 (0.1%)
1	B	0.75	7/3836 (0.2%)	0.81	1/5224 (0.0%)
All	All	0.70	7/7777 (0.1%)	0.83	7/10586 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	ASP	CG-OD2	8.63	1.41	1.25
1	B	215	ASP	CG-OD1	8.15	1.40	1.25
1	B	267	ALA	C-O	7.04	1.32	1.23
1	B	263	SER	C-N	6.13	1.42	1.33
1	B	223	SER	CB-OG	5.86	1.53	1.42
1	B	281	SER	C-O	5.85	1.30	1.23
1	B	11	TYR	CG-CD2	5.34	1.50	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	VAL	N-CA-C	14.87	129.99	108.58
1	A	67	VAL	N-CA-CB	-6.45	103.69	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ASN	N-CA-C	6.04	119.43	111.28
1	A	66	PHE	CA-C-N	5.09	128.94	122.37
1	A	66	PHE	C-N-CA	5.09	128.94	122.37
1	A	132	ASP	CA-C-N	5.04	130.77	121.70
1	A	132	ASP	C-N-CA	5.04	130.77	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	ASP	Peptide
1	A	132	ASP	Peptide
1	A	43	GLU	Peptide
1	A	66	PHE	Peptide
1	B	495	HIS	Peptide

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	3817	0	3537	31	0
1	B	3725	0	3413	38	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
4	A	14	0	20	1	0
5	A	6	0	10	4	0
6	B	38	0	0	1	0
7	B	20	0	28	0	0
8	A	345	0	0	3	0
8	B	205	0	0	4	0
All	All	8182	0	7008	68	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 5.

All (68) 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:B:175:SER:OG	1:B:386:ASP:OD2	1.61	1.14
1:B:254:GLN:HG2	8:B:2162:HOH:O	1.74	0.85
1:A:401:GLN:HE22	1:B:431:HIS:H	1.27	0.82
1:B:26:ASN:HD21	1:B:36:HIS:HE1	1.30	0.78
1:B:214:ASP:OD1	1:B:302:HIS:HE1	1.71	0.71
1:A:131:ASN:ND2	1:A:133:THR:CB	2.53	0.71
1:A:26:ASN:HD21	1:A:36:HIS:HE1	1.39	0.71
1:B:175:SER:OG	3:B:701:UNX:UNK	1.72	0.70
1:A:257:PHE:O	1:A:302:HIS:HD2	1.75	0.70
1:B:53:MET:HG3	1:B:145:TYR:CE1	2.31	0.66
1:B:153:ALA:H	1:B:360:GLN:HE21	1.44	0.65
1:B:25:ALA:HA	1:B:28:LEU:HD22	1.79	0.65
1:A:365:ASN:HD22	5:A:1006:ETX:H12	1.61	0.64
1:A:131:ASN:HD22	1:A:133:THR:CB	2.11	0.63
1:A:372:GLN:HE22	1:A:480:ILE:HD12	1.63	0.63
1:B:175:SER:HB2	2:B:901:VO4:O1	2.02	0.59
1:A:214:ASP:OD1	1:A:302:HIS:HE1	1.86	0.58
1:B:372:GLN:HE21	1:B:372:GLN:HA	1.69	0.57
1:B:257:PHE:O	1:B:302:HIS:HD2	1.87	0.56
1:B:284:TYR:HD1	8:B:2162:HOH:O	1.88	0.55
1:B:26:ASN:ND2	1:B:36:HIS:HE1	2.01	0.54
1:B:478:LYS:HG3	8:B:2165:HOH:O	2.07	0.54
1:A:100:GLN:NE2	1:A:275:ASN:HD21	2.05	0.54
1:B:175:SER:CB	1:B:386:ASP:OD2	2.55	0.54
1:A:401:GLN:NE2	1:B:431:HIS:H	2.01	0.53
1:B:26:ASN:HD21	1:B:36:HIS:CE1	2.19	0.53
1:A:53:MET:HE1	1:A:83:LEU:HD11	1.91	0.53
1:A:153:ALA:H	1:A:360:GLN:NE2	2.07	0.53
1:B:153:ALA:H	1:B:360:GLN:NE2	2.05	0.52
1:A:365:ASN:HD22	5:A:1006:ETX:C1	2.22	0.52
1:B:26:ASN:ND2	1:B:36:HIS:CE1	2.78	0.51
1:A:174:PRO:HB2	2:A:801:VO4:O3	2.10	0.51
1:A:445:TYR:HD1	4:A:1001:ETE:H222	1.75	0.51
1:B:495:HIS:ND1	6:B:2001:DVT:O18	2.44	0.51
1:B:215:ASP:OD2	1:B:301:HIS:HA	2.11	0.51
1:A:55:PRO:HB2	1:A:68:ALA:HB2	1.93	0.50
1:B:495:HIS:HB3	1:B:497:HIS:O	2.12	0.49
1:A:459:LYS:HD2	8:A:1065:HOH:O	2.13	0.49
1:A:26:ASN:ND2	1:A:36:HIS:HE1	2.09	0.48
1:A:97:ARG:NH1	8:A:1279:HOH:O	2.35	0.48
1:A:239:ILE:HB	1:A:440:LEU:CD1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PHE:HB3	1:A:322:ASP:HA	1.94	0.48
1:B:97:ARG:HB3	1:B:150:THR:OG1	2.13	0.48
1:B:264:GLY:C	1:B:266:THR:H	2.21	0.47
1:B:257:PHE:HB3	1:B:322:ASP:HA	1.95	0.47
1:A:131:ASN:HD22	1:A:134:TYR:H	1.62	0.46
1:B:198:GLU:HA	1:B:198:GLU:OE2	2.15	0.46
1:A:26:ASN:HD21	1:A:36:HIS:CE1	2.28	0.46
1:B:214:ASP:OD1	1:B:302:HIS:CE1	2.61	0.46
1:B:403:SER:HB2	1:B:409:GLN:OE1	2.15	0.45
1:A:100:GLN:HE22	1:A:275:ASN:HD21	1.63	0.45
5:A:1006:ETX:C2	8:A:1307:HOH:O	2.65	0.45
1:B:55:PRO:HB2	1:B:68:ALA:HB2	1.99	0.44
1:B:44:ASN:ND2	2:B:901:VO4:O2	2.43	0.44
1:B:257:PHE:N	8:B:2162:HOH:O	2.50	0.44
1:B:53:MET:HG3	1:B:145:TYR:CD1	2.54	0.43
1:A:372:GLN:HE22	1:A:480:ILE:CD1	2.29	0.43
1:B:355:ASN:HB2	1:B:356:PRO:HD2	2.00	0.43
1:A:26:ASN:ND2	1:A:36:HIS:CE1	2.87	0.42
1:A:239:ILE:HB	1:A:440:LEU:HD11	2.02	0.42
1:A:365:ASN:HB3	5:A:1006:ETX:H31	2.02	0.42
1:B:100:GLN:NE2	1:B:275:ASN:HD21	2.17	0.42
1:A:132:ASP:N	1:A:133:THR:CB	2.82	0.42
1:B:239:ILE:HB	1:B:440:LEU:CD1	2.51	0.41
1:B:257:PHE:O	1:B:302:HIS:CD2	2.73	0.40
1:B:344:PRO:O	1:B:345:GLY:C	2.63	0.40
1:A:250:TRP:HA	1:A:338:VAL:O	2.22	0.40
1:A:153:ALA:H	1:A:360:GLN:HE21	1.68	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	482/498 (97%)	468 (97%)	12 (2%)	2 (0%)	30	15
1	B	465/498 (93%)	449 (97%)	12 (3%)	4 (1%)	14	4
All	All	947/996 (95%)	917 (97%)	24 (2%)	6 (1%)	21	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	THR
1	B	264	GLY
1	B	496	HIS
1	A	174	PRO
1	B	265	LYS
1	B	174	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/436 (94%)	405 (98%)	6 (2%)	57	41
1	B	399/436 (92%)	392 (98%)	7 (2%)	51	33
All	All	810/872 (93%)	797 (98%)	13 (2%)	55	38

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	67	VAL
1	A	289	GLU
1	A	341	LEU
1	A	372	GLN
1	A	377	ASP
1	B	21	LEU
1	B	28	LEU
1	B	106	HIS
1	B	289	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	341	LEU
1	B	475	LYS
1	B	495	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	26	ASN
1	A	36	HIS
1	A	71	ASN
1	A	100	GLN
1	A	131	ASN
1	A	302	HIS
1	A	316	GLN
1	A	320	GLN
1	A	347	GLN
1	A	360	GLN
1	A	365	ASN
1	A	372	GLN
1	A	401	GLN
1	A	457	ASN
1	B	9	ASN
1	B	19	GLN
1	B	23	ASN
1	B	26	ASN
1	B	36	HIS
1	B	98	ASN
1	B	100	GLN
1	B	110	GLN
1	B	181	ASN
1	B	241	HIS
1	B	302	HIS
1	B	316	GLN
1	B	320	GLN
1	B	360	GLN
1	B	372	GLN
1	B	457	ASN
1	B	474	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are unknown - leaving 7 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	$\# Z > 2$
7	PGE	B	1002	-	9,9,9	0.42	0	8,8,8	0.28	0
4	ETE	A	1001	-	13,13,13	0.53	0	12,12,12	0.20	0
7	PGE	B	1004	-	9,9,9	0.48	0	8,8,8	0.40	0
6	DVT	B	2001	-	60,60,60	0.92	3 (5%)	-		
2	VO4	A	801	-	0,4,4	-	-	-		
5	ETX	A	1006	-	5,5,5	0.45	0	4,4,4	0.44	0
2	VO4	B	901	-	0,4,4	-	-	-		

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
7	PGE	B	1002	-	-	1/7/7/7	-
4	ETE	A	1001	-	-	1/11/11/11	-
5	ETX	A	1006	-	-	1/3/3/3	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	B	1004	-	-	0/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2001	DVT	O12-V4	2.54	1.63	1.60
6	B	2001	DVT	O2-V10	-2.36	2.26	2.33
6	B	2001	DVT	O16-V5	-2.23	2.26	2.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

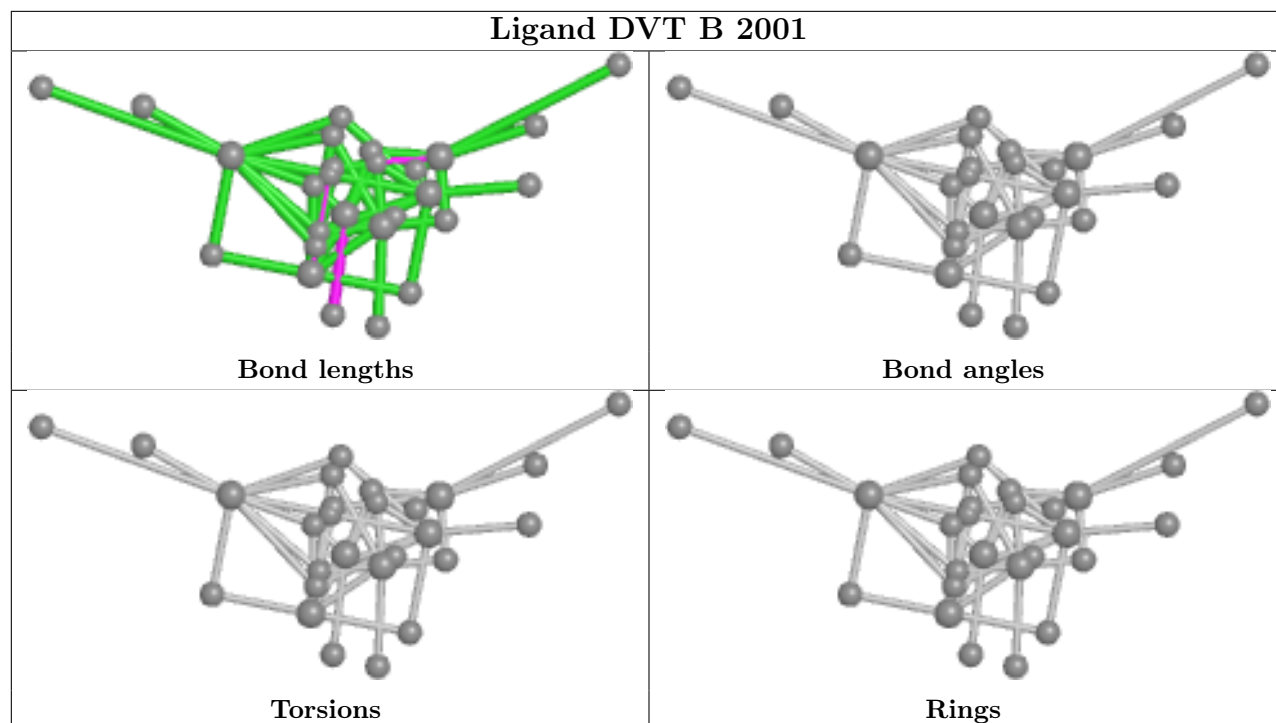
Mol	Chain	Res	Type	Atoms
5	A	1006	ETX	O1-C1-C2-O2
7	B	1002	PGE	C3-C4-O3-C5
4	A	1001	ETE	OH4-C13-C23-OH3

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	ETE	1	0
6	B	2001	DVT	1	0
2	A	801	VO4	1	0
5	A	1006	ETX	4	0
2	B	901	VO4	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	481/498 (96%)	0.83	24 (4%) 34 39	13, 24, 30, 41	7 (1%)
1	B	472/498 (94%)	1.49	116 (24%) 2 2	15, 25, 32, 46	2 (0%)
All	All	953/996 (95%)	1.16	140 (14%) 6 6	13, 25, 31, 46	9 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	HIS	6.9
1	B	498	HIS	5.0
1	B	497	HIS	4.4
1	B	193	PRO	4.1
1	B	139	ASP	4.1
1	B	496	HIS	4.0
1	A	133	THR	4.0
1	B	99	PHE	3.7
1	B	11	TYR	3.7
1	B	140	GLY	3.7
1	B	217	SER	3.4
1	B	264	GLY	3.4
1	A	14	LEU	3.4
1	B	429	VAL	3.4
1	B	344	PRO	3.3
1	B	219	GLY	3.2
1	B	6	SER	3.2
1	B	75	VAL	3.2
1	B	128	GLY	3.1
1	B	216	CYS	3.1
1	B	268	ILE	3.1
1	A	98	ASN	3.0
1	A	132	ASP	3.0
1	A	334	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	191	MET	2.9
1	B	226	THR	2.9
1	B	138	CYS	2.9
1	A	67	VAL	2.9
1	B	22	PHE	2.9
1	B	249	THR	2.8
1	B	281	SER	2.8
1	B	241	HIS	2.8
1	B	229	ALA	2.8
1	B	55	PRO	2.8
1	B	175	SER	2.8
1	B	221	SER	2.8
1	A	262	TYR	2.7
1	B	82	LEU	2.7
1	B	218	TYR	2.7
1	B	234	THR	2.7
1	A	131	ASN	2.7
1	B	227	ASN	2.7
1	B	212	TYR	2.7
1	B	68	ALA	2.7
1	B	101	PRO	2.6
1	B	428	TYR	2.6
1	B	266	THR	2.6
1	B	176	THR	2.6
1	A	130	ASP	2.5
1	A	277	PHE	2.5
1	B	237	TYR	2.5
1	B	57	ALA	2.5
1	B	277	PHE	2.5
1	B	242	TYR	2.5
1	B	349	GLY	2.5
1	B	213	TYR	2.5
1	B	231	ALA	2.5
1	B	188	GLY	2.5
1	B	195	GLY	2.5
1	B	477	LEU	2.4
1	B	302	HIS	2.4
1	B	8	PRO	2.4
1	B	262	TYR	2.4
1	B	72	THR	2.4
1	B	148	GLY	2.4
1	B	155	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	327	TRP	2.4
1	A	470	PHE	2.4
1	B	51	PHE	2.4
1	B	310	TYR	2.4
1	A	268	ILE	2.4
1	B	367	ILE	2.4
1	B	433	LEU	2.4
1	B	282	ARG	2.4
1	B	263	SER	2.3
1	B	73	PRO	2.3
1	B	295	LYS	2.3
1	B	470	PHE	2.3
1	B	279	VAL	2.3
1	B	299	ASN	2.3
1	A	377	ASP	2.3
1	A	13	THR	2.3
1	B	228	THR	2.3
1	B	304	ALA	2.3
1	B	487	LEU	2.3
1	B	20	LYS	2.3
1	B	162	ALA	2.3
1	B	303	LEU	2.3
1	B	445	TYR	2.3
1	B	67	VAL	2.3
1	B	317	ALA	2.2
1	A	119	LEU	2.2
1	B	479	LEU	2.2
1	B	236	GLY	2.2
1	B	230	VAL	2.2
1	B	267	ALA	2.2
1	A	197	LEU	2.2
1	B	256	GLY	2.2
1	B	473	GLU	2.2
1	B	346	TYR	2.2
1	B	449	ILE	2.2
1	B	223	SER	2.2
1	B	158	ALA	2.2
1	B	250	TRP	2.2
1	B	294	TRP	2.2
1	A	296	GLU	2.2
1	B	21	LEU	2.2
1	B	481	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	129	HIS	2.2
1	B	402	PHE	2.2
1	B	79	THR	2.2
1	B	488	VAL	2.1
1	B	255	GLY	2.1
1	A	137	ASN	2.1
1	B	194	SER	2.1
1	B	215	ASP	2.1
1	B	257	PHE	2.1
1	B	300	PRO	2.1
1	B	305	PRO	2.1
1	B	93	TYR	2.1
1	B	423	TYR	2.1
1	B	452	VAL	2.1
1	B	315	ASP	2.1
1	B	476	THR	2.1
1	A	134	TYR	2.1
1	B	145	TYR	2.1
1	B	271	ALA	2.1
1	B	403	SER	2.1
1	B	465	LEU	2.1
1	B	31	THR	2.1
1	B	209	PRO	2.1
1	B	34	ILE	2.1
1	B	450	GLY	2.0
1	B	225	ASP	2.0
1	B	270	ASP	2.0
1	B	395	VAL	2.0
1	B	489	MET	2.0
1	A	22	PHE	2.0
1	A	108	TYR	2.0
1	A	329	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

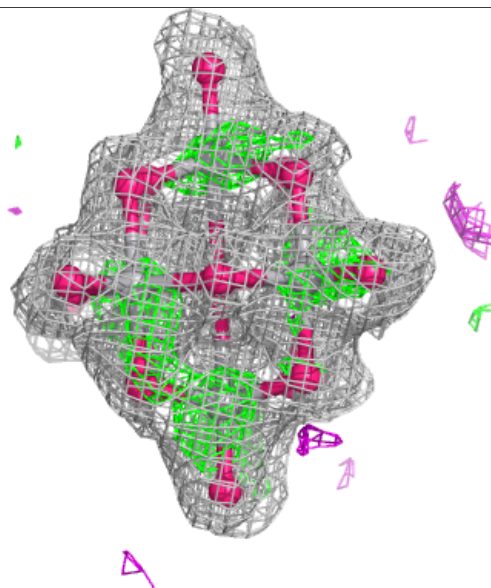
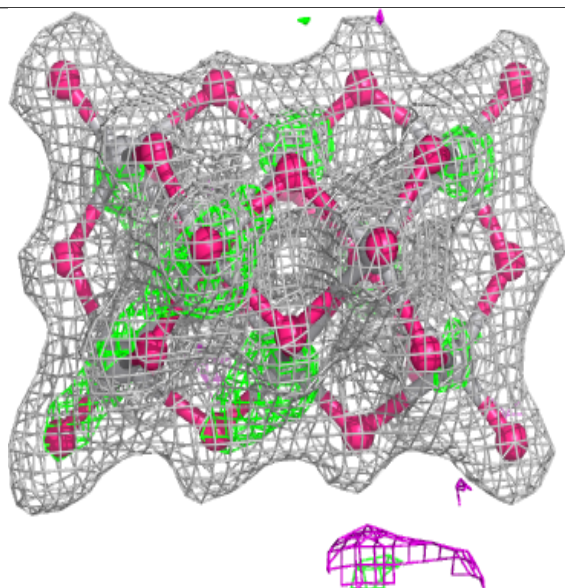
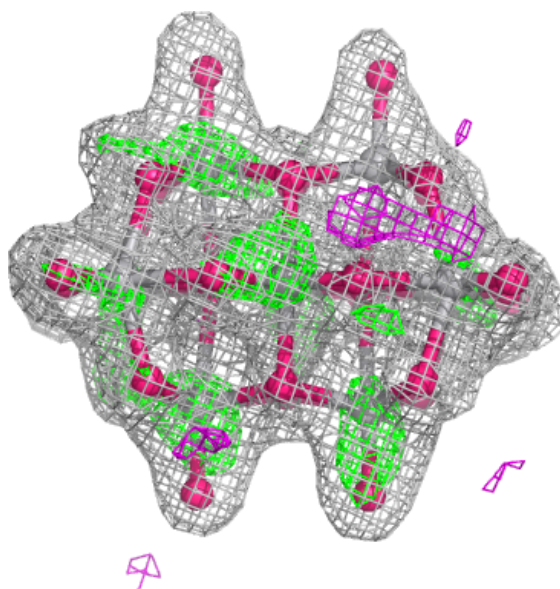
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ETE	A	1001	14/14	0.82	0.17	28,30,39,39	0
7	PGE	B	1004	10/10	0.85	0.15	30,32,34,34	0
7	PGE	B	1002	10/10	0.87	0.14	36,37,38,40	0
2	VO4	B	901	5/5	0.87	0.20	35,35,35,37	0
5	ETX	A	1006	6/6	0.88	0.23	19,27,28,30	0
2	VO4	A	801	5/5	0.97	0.15	15,16,16,20	0
6	DVT	B	2001	38/38	0.97	0.12	21,24,25,26	38
3	UNX	B	701	1/1	0.98	0.17	13,13,13,13	0
3	UNX	A	601	1/1	0.99	0.23	2,2,2,2	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 B 2001:

$2mF_o-DF_c$ (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.