



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:58 PM GMT

PDB ID : 1RGU  
Title : The crystal structure of human Tyrosyl-DNA Phosphodiesterase complexed with vanadate, octopamine, and tetranucleotide AGTG  
Authors : Davies, D.R.; Interthal, H.; Champoux, J.J.; Hol, W.G.  
Deposited on : 2003-11-13  
Resolution : 2.22 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

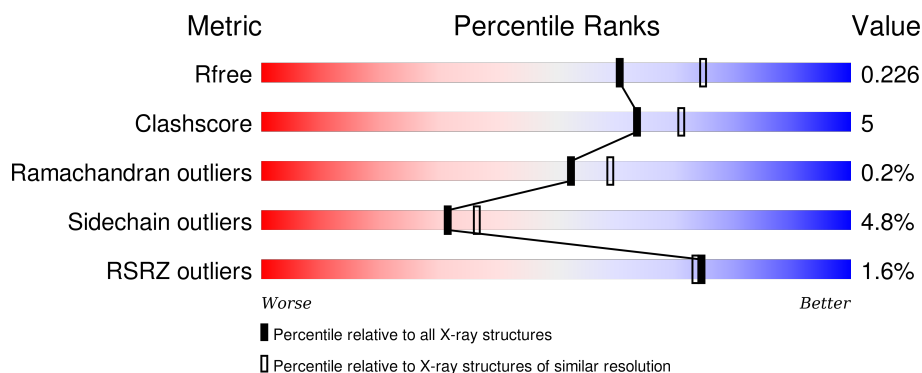
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.22 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))
$R_{free}$	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	D	4	<div> <div></div> <div>75%</div> <div>25%</div> </div>
1	F	4	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>
2	A	485	<div> <div>2%</div> <div>75%</div> <div>12%</div> <div>12%</div> </div>
2	B	485	<div> <div>%</div> <div>74%</div> <div>14%</div> <div>12%</div> </div>

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
3	VO4	A	699	-	-	X	-
3	VO4	B	699	-	-	X	-
4	SPM	A	999	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7141 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 DNA chain called 5'-D(\*AP\*GP\*TP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	3	Total	C	N	O	P	0	0	0
			53	25	7	18	3			
1	F	2	Total	C	N	O	P	0	0	0
			42	20	7	13	2			

- Molecule 2 is a protein called Tyrosyl-DNA phosphodiesterase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	425	Total	C	N	O	S	0	0	0
			3394	2208	573	602	11			
2	B	429	Total	C	N	O	S	0	0	0
			3426	2230	578	607	11			

There are 56 discrepancies between the modelled and reference sequences:

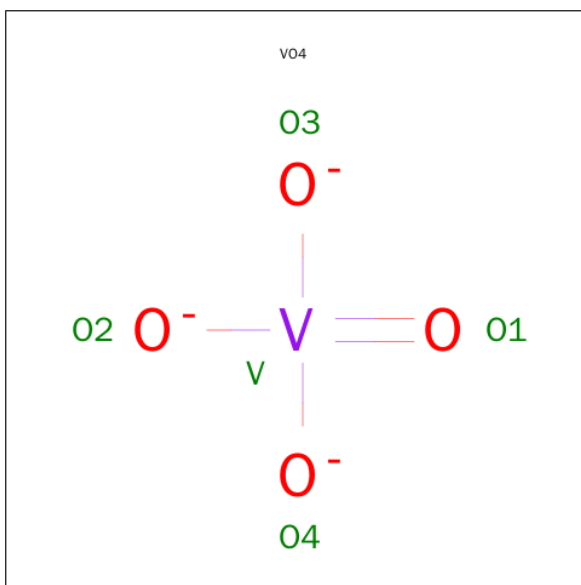
Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	CLONING ARTIFACT	UNP Q9NUW8
A	125	GLY	-	CLONING ARTIFACT	UNP Q9NUW8
A	126	SER	-	CLONING ARTIFACT	UNP Q9NUW8
A	127	SER	-	CLONING ARTIFACT	UNP Q9NUW8
A	128	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
A	129	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
A	130	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
A	131	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
A	132	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
A	133	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
A	134	SER	-	CLONING ARTIFACT	UNP Q9NUW8
A	135	SER	-	CLONING ARTIFACT	UNP Q9NUW8
A	136	GLY	-	CLONING ARTIFACT	UNP Q9NUW8
A	137	LEU	-	CLONING ARTIFACT	UNP Q9NUW8
A	138	VAL	-	CLONING ARTIFACT	UNP Q9NUW8
A	139	PRO	-	CLONING ARTIFACT	UNP Q9NUW8

*Continued on next page...*

*Continued from previous page...*

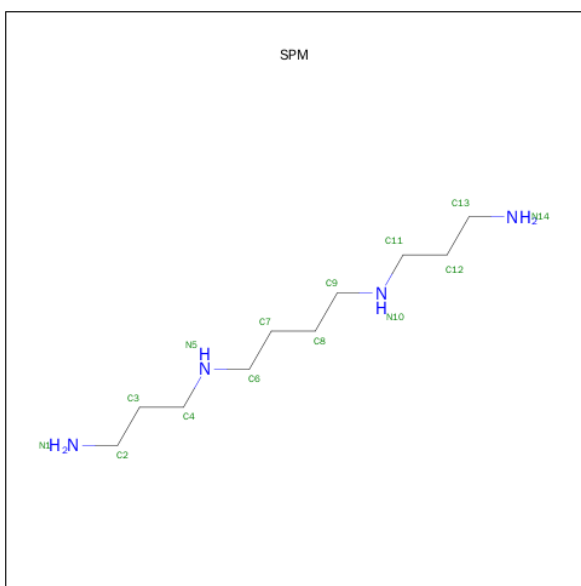
Chain	Residue	Modelled	Actual	Comment	Reference
A	140	ARG	-	CLONING ARTIFACT	UNP Q9NUW8
A	141	GLY	-	CLONING ARTIFACT	UNP Q9NUW8
A	142	SER	-	CLONING ARTIFACT	UNP Q9NUW8
A	143	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
A	144	MET	-	CLONING ARTIFACT	UNP Q9NUW8
A	145	LEU	-	CLONING ARTIFACT	UNP Q9NUW8
A	146	GLU	-	CLONING ARTIFACT	UNP Q9NUW8
A	147	ASP	-	CLONING ARTIFACT	UNP Q9NUW8
A	148	PRO	-	CLONING ARTIFACT	UNP Q9NUW8
A	322	ASN	ASP	ENGINEERED	UNP Q9NUW8
A	328	THR	MET	ENGINEERED	UNP Q9NUW8
A	548	LEU	PHE	ENGINEERED	UNP Q9NUW8
B	124	MET	-	CLONING ARTIFACT	UNP Q9NUW8
B	125	GLY	-	CLONING ARTIFACT	UNP Q9NUW8
B	126	SER	-	CLONING ARTIFACT	UNP Q9NUW8
B	127	SER	-	CLONING ARTIFACT	UNP Q9NUW8
B	128	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
B	129	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
B	130	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
B	131	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
B	132	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
B	133	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
B	134	SER	-	CLONING ARTIFACT	UNP Q9NUW8
B	135	SER	-	CLONING ARTIFACT	UNP Q9NUW8
B	136	GLY	-	CLONING ARTIFACT	UNP Q9NUW8
B	137	LEU	-	CLONING ARTIFACT	UNP Q9NUW8
B	138	VAL	-	CLONING ARTIFACT	UNP Q9NUW8
B	139	PRO	-	CLONING ARTIFACT	UNP Q9NUW8
B	140	ARG	-	CLONING ARTIFACT	UNP Q9NUW8
B	141	GLY	-	CLONING ARTIFACT	UNP Q9NUW8
B	142	SER	-	CLONING ARTIFACT	UNP Q9NUW8
B	143	HIS	-	CLONING ARTIFACT	UNP Q9NUW8
B	144	MET	-	CLONING ARTIFACT	UNP Q9NUW8
B	145	LEU	-	CLONING ARTIFACT	UNP Q9NUW8
B	146	GLU	-	CLONING ARTIFACT	UNP Q9NUW8
B	147	ASP	-	CLONING ARTIFACT	UNP Q9NUW8
B	148	PRO	-	CLONING ARTIFACT	UNP Q9NUW8
B	322	ASN	ASP	ENGINEERED	UNP Q9NUW8
B	328	THR	MET	ENGINEERED	UNP Q9NUW8
B	548	LEU	PHE	ENGINEERED	UNP Q9NUW8

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O<sub>4</sub>V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			3	2	1		
3	B	1	Total	O	V	0	0
			3	2	1		

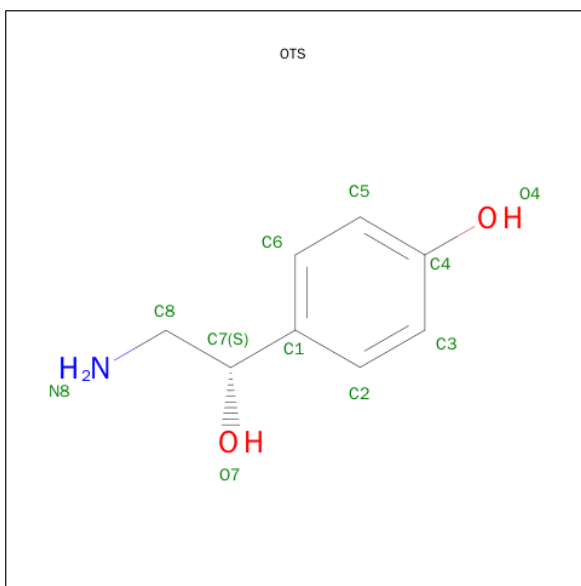
- Molecule 4 is SPERMINE (three-letter code: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			14	10	4		

- Molecule 5 is 4-(2S-AMINO-1-HYDROXYETHYL)PHENOL (three-letter code: OTS)

(formula: C<sub>8</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	8	1	2		
5	B	1	Total	C	N	O	0	0
			11	8	1	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	82	Total	O	0	0
			82	82		
6	B	96	Total	O	0	0
			96	96		
6	D	2	Total	O	0	0
			2	2		
6	F	4	Total	O	0	0
			4	4		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5'-D(\*AP\*GP\*TP\*G)-3'

Chain D: 




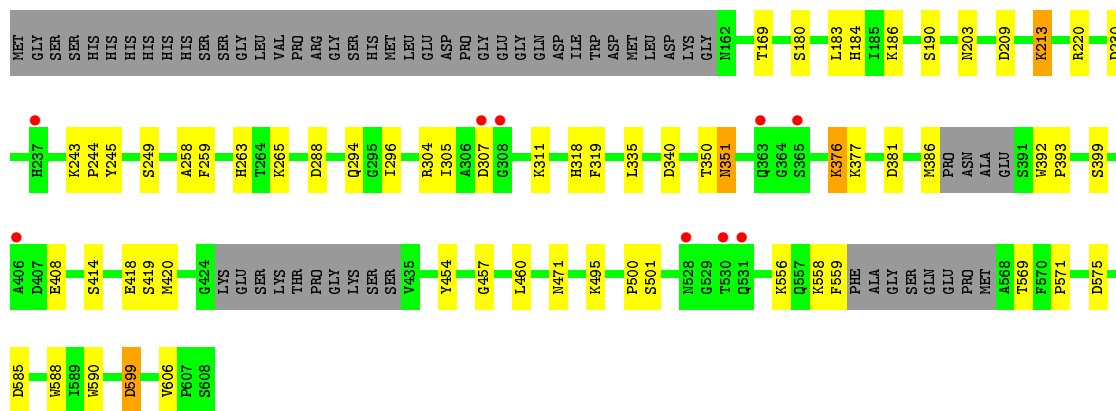
- Molecule 1: 5'-D(\*AP\*GP\*TP\*G)-3'

Chain F: 




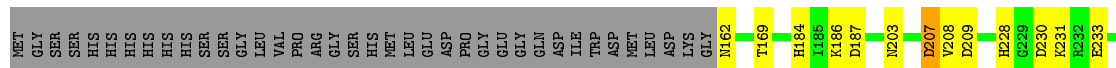
- Molecule 2: Tyrosyl-DNA phosphodiesterase 1

Chain A: 

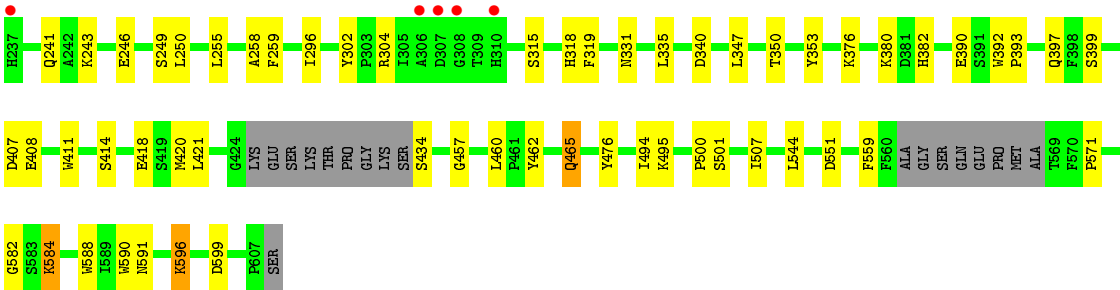


- Molecule 2: Tyrosyl-DNA phosphodiesterase 1

Chain B: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.72Å 104.56Å 193.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.22 48.30 – 2.22	Depositor EDS
% Data completeness (in resolution range)	92.9 (50.00-2.22) 92.9 (48.30-2.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.187 , 0.231 0.185 , 0.226	Depositor DCC
$R_{free}$ test set	2398 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 47192 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, OTS, SPM

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	D	0.92	0/58	1.38	0/87
1	F	0.86	0/46	1.77	3/69 (4.3%)
2	A	0.47	0/3505	0.69	6/4765 (0.1%)
2	B	0.51	0/3540	0.70	7/4816 (0.1%)
All	All	0.50	0/7149	0.72	16/9737 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	209	ASP	CB-CG-OD2	7.43	124.99	118.30
2	B	599	ASP	CB-CG-OD2	7.00	124.60	118.30
2	A	340	ASP	CB-CG-OD2	6.97	124.57	118.30
2	B	407	ASP	CB-CG-OD2	6.56	124.21	118.30
2	B	551	ASP	CB-CG-OD2	6.01	123.71	118.30
2	B	209	ASP	CB-CG-OD2	5.98	123.68	118.30
2	B	207	ASP	CB-CG-OD2	5.86	123.58	118.30
1	F	805	DT	C5-C4-O4	-5.86	120.80	124.90
2	A	599	ASP	CB-CG-OD2	5.77	123.49	118.30
2	A	585	ASP	CB-CG-OD2	5.68	123.41	118.30
2	B	187	ASP	CB-CG-OD2	5.65	123.39	118.30
2	A	230	ASP	CB-CG-OD2	5.54	123.29	118.30
2	B	340	ASP	CB-CG-OD2	5.36	123.12	118.30
1	F	805	DT	N3-C4-O4	5.18	123.01	119.90
1	F	805	DT	O4'-C1'-N1	-5.17	104.38	108.00
2	A	575	ASP	CB-CG-OD2	5.06	122.86	118.30

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	D	53	0	29	0	0
1	F	42	0	23	0	0
2	A	3394	0	3330	30	0
2	B	3426	0	3354	41	0
3	A	3	0	0	3	0
3	B	3	0	0	2	0
4	A	14	0	26	2	0
5	A	11	0	10	0	0
5	B	11	0	10	0	0
6	A	82	0	0	1	0
6	B	96	0	0	1	0
6	D	2	0	0	0	0
6	F	4	0	0	0	0
All	All	7141	0	6782	72	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 (72) 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)
2:B:228:HIS:HD2	2:B:230:ASP:H	1.21	0.89
2:B:465:GLN:HE22	2:B:591:ASN:HD21	1.34	0.76
2:B:408:GLU:OE2	2:B:476:TYR:OH	2.04	0.72
2:B:250:LEU:HD12	2:B:250:LEU:N	2.05	0.71
2:A:213:LYS:N	2:A:213:LYS:HD3	2.06	0.71
3:B:699:VO4:O3	3:B:699:VO4:V	1.51	0.68
3:B:699:VO4:V	3:B:699:VO4:O1	1.50	0.67
3:A:699:VO4:O1	3:A:699:VO4:V	1.49	0.67
3:A:699:VO4:O3	3:A:699:VO4:V	1.52	0.66
2:A:606:VAL:H	4:A:999:SPM:H42	1.59	0.66
2:A:305:ILE:O	6:A:758:HOH:O	2.14	0.66
2:B:228:HIS:CD2	2:B:230:ASP:H	2.09	0.65
2:B:228:HIS:HD2	2:B:230:ASP:N	1.94	0.65
2:A:318:HIS:HE1	2:B:318:HIS:HE1	1.44	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:VAL:H	2:B:241:GLN:NE2	1.96	0.64
2:A:318:HIS:CE1	2:B:318:HIS:HE1	2.20	0.59
2:A:376:LYS:HD3	2:A:419:SER:HA	1.85	0.59
2:A:556:LYS:HB2	2:A:569:THR:HG22	1.85	0.57
2:A:457:GLY:HA3	2:A:588:TRP:CZ2	2.42	0.55
2:B:500:PRO:HA	2:B:507:ILE:HG22	1.90	0.54
2:B:319:PHE:CG	2:B:350:THR:HG21	2.42	0.53
2:B:584:LYS:NZ	2:B:584:LYS:H	2.06	0.53
2:B:414:SER:O	2:B:418:GLU:HB2	2.08	0.53
2:B:584:LYS:HZ2	2:B:584:LYS:H	1.57	0.53
2:A:351:ASN:HD22	2:A:351:ASN:C	2.15	0.50
2:B:376:LYS:HE3	6:B:897:HOH:O	2.12	0.49
2:A:243:LYS:HB3	2:A:244:PRO:HD3	1.94	0.48
2:B:249:SER:C	2:B:250:LEU:HD12	2.33	0.48
2:B:559:PHE:CE1	2:B:571:PRO:HB2	2.48	0.48
2:A:318:HIS:CE1	2:B:318:HIS:CE1	3.00	0.47
2:B:582:GLY:HA3	2:B:584:LYS:HZ1	1.79	0.47
2:B:382:HIS:HB2	2:B:544:LEU:HD13	1.97	0.47
2:A:169:THR:HA	2:A:183:LEU:O	2.15	0.47
2:A:559:PHE:CE1	2:A:571:PRO:HB2	2.50	0.46
2:A:377:LYS:HE2	2:A:381:ASP:OD2	2.14	0.46
2:B:393:PRO:O	2:B:500:PRO:HD2	2.14	0.46
2:A:454:TYR:CD2	2:A:599:ASP:HB3	2.51	0.46
2:B:596:LYS:HD2	2:B:596:LYS:HA	1.57	0.45
2:B:169:THR:HG22	2:B:296:ILE:HD11	1.98	0.45
2:B:465:GLN:HE22	2:B:591:ASN:ND2	2.09	0.45
2:B:390:GLU:H	2:B:390:GLU:CD	2.19	0.45
2:B:397:GLN:HE22	2:B:494:ILE:HG23	1.82	0.45
2:A:606:VAL:N	4:A:999:SPM:H42	2.31	0.44
2:A:399:SER:HB2	2:A:460:LEU:HD23	2.00	0.44
2:B:353:TYR:CE1	2:B:544:LEU:HD12	2.52	0.43
2:A:169:THR:HG22	2:A:296:ILE:HD11	2.00	0.43
2:B:302:TYR:CD1	2:B:347:LEU:HA	2.54	0.43
2:A:184:HIS:CD2	2:A:186:LYS:H	2.36	0.43
2:B:250:LEU:CD1	2:B:250:LEU:N	2.77	0.43
2:A:263:HIS:NE2	3:A:699:VO4:O1	2.52	0.43
2:B:457:GLY:HA3	2:B:588:TRP:CZ2	2.53	0.43
2:B:184:HIS:CD2	2:B:186:LYS:H	2.37	0.42
2:B:399:SER:HB2	2:B:460:LEU:HD23	2.00	0.42
2:B:231:LYS:NZ	2:B:255:LEU:O	2.51	0.42
2:A:414:SER:O	2:A:418:GLU:HB2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:258:ALA:O	2:A:259:PHE:HB2	2.19	0.42
2:A:393:PRO:HD2	2:A:500:PRO:O	2.20	0.42
2:B:421:LEU:C	2:B:421:LEU:HD12	2.40	0.42
2:A:319:PHE:CG	2:A:350:THR:HG21	2.55	0.41
2:A:184:HIS:HD2	2:A:186:LYS:HB2	1.85	0.41
2:A:213:LYS:NZ	2:A:245:TYR:OH	2.54	0.41
2:B:184:HIS:HD2	2:B:186:LYS:H	1.69	0.41
2:B:228:HIS:CD2	2:B:230:ASP:HB2	2.55	0.41
2:B:207:ASP:HA	2:B:241:GLN:HE22	1.85	0.41
2:B:258:ALA:O	2:B:259:PHE:HB2	2.20	0.41
2:B:335:LEU:HA	2:B:335:LEU:HD23	1.73	0.41
2:B:392:TRP:CD2	2:B:501:SER:HA	2.56	0.40
2:A:558:LYS:O	2:A:559:PHE:C	2.60	0.40
2:A:169:THR:CG2	2:A:294:GLN:HB2	2.52	0.40
2:A:335:LEU:HA	2:A:335:LEU:HD23	1.81	0.40
2:B:582:GLY:HA3	2:B:584:LYS:NZ	2.35	0.40
2:A:392:TRP:CD2	2:A:501:SER:HA	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	417/485 (86%)	400 (96%)	16 (4%)	1 (0%)	52	59
2	B	423/485 (87%)	413 (98%)	9 (2%)	1 (0%)	52	59
All	All	840/970 (87%)	813 (97%)	25 (3%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	307	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	411	TRP

### 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	
2	A	366/421 (87%)	348 (95%)	18 (5%)	31	35
2	B	369/421 (88%)	352 (95%)	17 (5%)	33	39
All	All	735/842 (87%)	700 (95%)	35 (5%)	31	36

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	180	SER
2	A	190	SER
2	A	203	ASN
2	A	213	LYS
2	A	220	ARG
2	A	249	SER
2	A	265	LYS
2	A	288	ASP
2	A	304	ARG
2	A	311	LYS
2	A	351	ASN
2	A	376	LYS
2	A	386	MET
2	A	408	GLU
2	A	420	MET
2	A	471	ASN
2	A	495	LYS
2	A	590	TRP
2	B	162	ASN
2	B	203	ASN
2	B	233	GLU
2	B	243	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	246	GLU
2	B	304	ARG
2	B	315	SER
2	B	331	ASN
2	B	380	LYS
2	B	420	MET
2	B	434	SER
2	B	462	TYR
2	B	465	GLN
2	B	495	LYS
2	B	584	LYS
2	B	590	TRP
2	B	596	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	184	HIS
2	A	318	HIS
2	A	351	ASN
2	A	363	GLN
2	A	369	ASN
2	A	397	GLN
2	A	531	GLN
2	B	165	GLN
2	B	184	HIS
2	B	228	HIS
2	B	241	GLN
2	B	318	HIS
2	B	331	ASN
2	B	388	ASN
2	B	397	GLN
2	B	465	GLN
2	B	528	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	VO4	A	699	1,2,5	0,2,4	0.00	-	0,1,6	0.00	-
5	OTS	A	995	3	11,11,11	0.91	1 (9%)	13,14,14	0.73	0
4	SPM	A	999	-	13,13,13	0.39	0	12,12,12	1.04	1 (8%)
3	VO4	B	699	1,2,5	0,2,4	0.00	-	0,1,6	0.00	-
5	OTS	B	996	3	11,11,11	0.71	0	13,14,14	0.55	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
3	VO4	A	699	1,2,5	-	0/0/0/0	0/0/0/0
5	OTS	A	995	3	-	0/6/6/6	0/1/1/1
4	SPM	A	999	-	-	0/11/11/11	0/0/0/0
3	VO4	B	699	1,2,5	-	0/0/0/0	0/0/0/0
5	OTS	B	996	3	-	0/6/6/6	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	995	OTS	C1-C7	2.29	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	SPM	C11-N10-C9	2.31	121.52	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	699	VO4	3	0
4	A	999	SPM	2	0
3	B	699	VO4	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	D	3/4 (75%)	-0.65	0 100 100	29, 29, 38, 55	0
1	F	2/4 (50%)	-0.91	0 100 100	27, 27, 27, 34	0
2	A	425/485 (87%)	-0.25	9 (2%) 67 65	17, 30, 51, 66	0
2	B	429/485 (88%)	-0.32	5 (1%) 81 80	13, 25, 45, 60	0
All	All	859/978 (87%)	-0.29	14 (1%) 74 73	13, 28, 49, 66	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	528	ASN	4.4
2	B	307	ASP	3.3
2	B	308	GLY	3.1
2	A	531	GLN	2.6
2	A	308	GLY	2.6
2	A	530	THR	2.5
2	A	365	SER	2.3
2	A	237	HIS	2.3
2	B	310	HIS	2.2
2	A	307	ASP	2.2
2	A	363	GLN	2.2
2	B	237	HIS	2.2
2	A	406	ALA	2.0
2	B	306	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SPM	A	999	14/14	0.87	0.21	2.39	33,44,54,54	0
5	OTS	A	995	11/11	0.97	0.10	0.12	18,28,40,44	0
5	OTS	B	996	11/11	0.97	0.11	-0.00	27,30,43,45	0
3	VO4	A	699	3/5	1.00	0.08	-1.59	15,15,20,20	0
3	VO4	B	699	3/5	1.00	0.09	-1.90	17,17,21,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.