



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:37 AM GMT

PDB ID : 2B30  
Title : Initial Crystallographic Structural Analysis of a putative HAD/COF-like hydrolase from Plasmodium vivax  
Authors : Robien, M.A.; Bosch, J.; Hol, W.G.J.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)  
Deposited on : 2005-09-19  
Resolution : 2.70 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

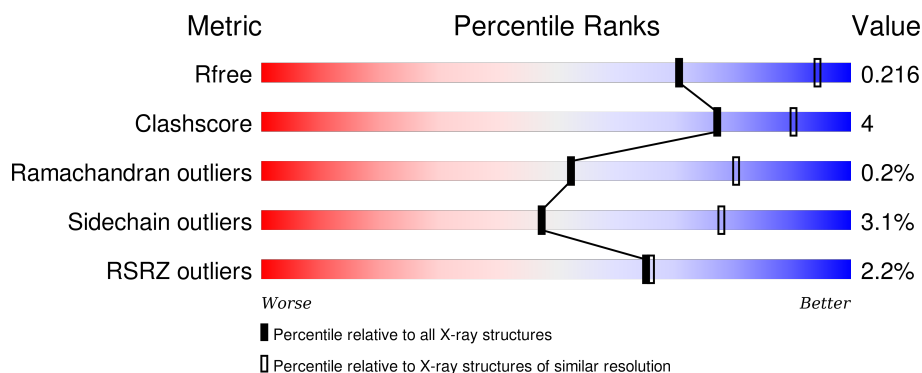
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	A	301	<div> <div>3%</div> <div>79%</div> <div>13%</div> <div>6%</div> </div>
1	B	301	<div> <div>3%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	C	301	<div> <div>%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	D	301	<div> <div>2%</div> <div>78%</div> <div>16%</div> <div>6%</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	CL	A	303	-	-	-	X
3	CL	C	303	-	-	-	X
3	CL	D	303	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9169 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 Pvivax hypothetical protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	75	0	0
			2261	1449	370	432	10			
1	B	284	Total	C	N	O	S	72	0	0
			2261	1449	370	432	10			
1	C	284	Total	C	N	O	S	73	1	0
			2266	1453	370	432	11			
1	D	284	Total	C	N	O	S	78	1	0
			2266	1453	370	432	11			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

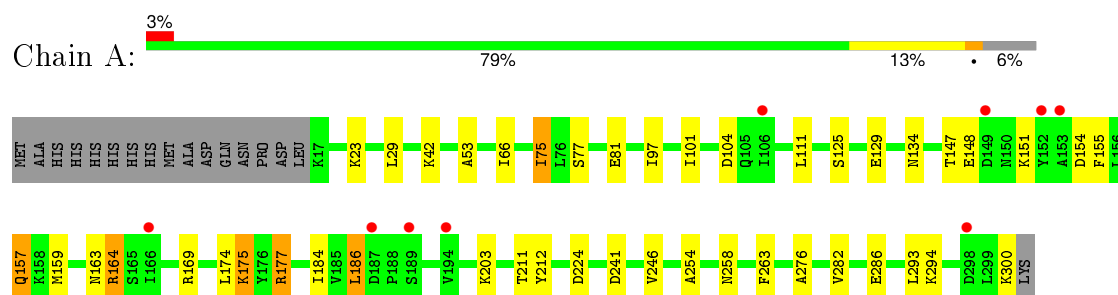
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	23	Total 23	O 23	0	0
4	C	34	Total 34	O 34	0	0
4	D	27	Total 27	O 27	0	0

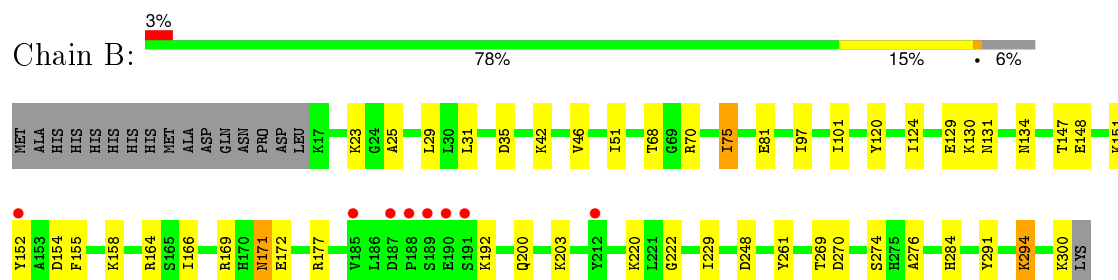
### 3 Residue-property plots [i](#)

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.

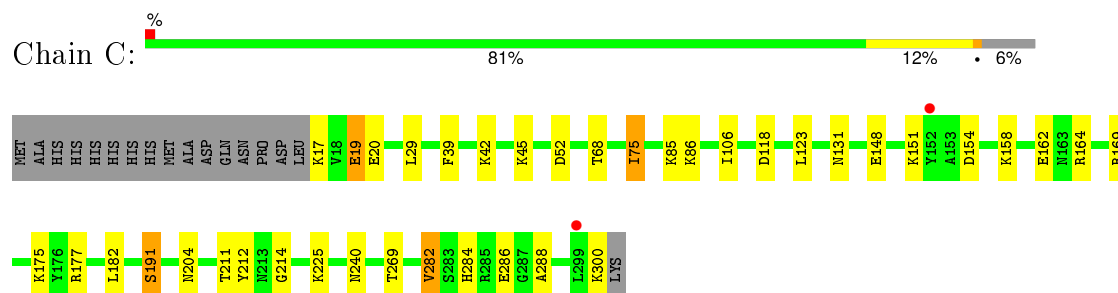
#### • Molecule 1: Pvivax hypothetical protein



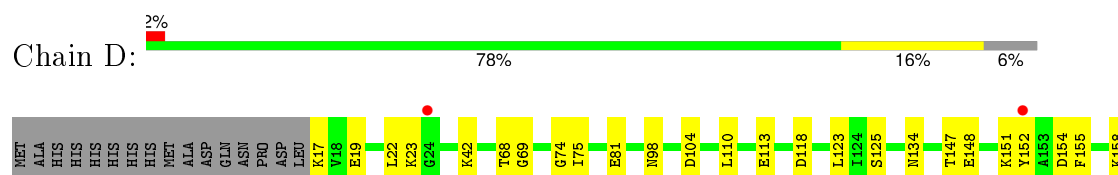
#### • Molecule 1: Pvivax hypothetical protein

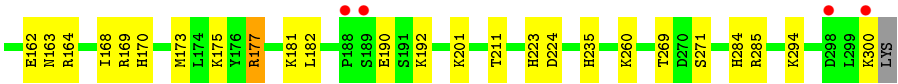


#### • Molecule 1: Pvivax hypothetical protein



#### • Molecule 1: Pvivax hypothetical protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.10 Å 101.79 Å 97.34 Å 90.00° 93.93° 90.00°	Depositor
Resolution (Å)	37.24 – 2.70 37.24 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.24-2.70) 99.5 (37.24-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.68 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.197 , 0.260 0.210 , 0.216	Depositor DCC
$R_{free}$ test set	1704 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.4	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	2 of 34203 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9169	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CL

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	1.59	13/2299 (0.6%)	1.00	19/3099 (0.6%)
1	B	1.28	13/2299 (0.6%)	1.09	16/3099 (0.5%)
1	C	1.60	11/2307 (0.5%)	0.91	13/3109 (0.4%)
1	D	1.49	14/2307 (0.6%)	1.05	16/3109 (0.5%)
All	All	1.49	51/9212 (0.6%)	1.02	64/12416 (0.5%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	ASP	CB-CG	-41.68	0.64	1.51
1	B	164	ARG	CB-CG	-38.27	0.49	1.52
1	A	23	LYS	CA-CB	36.51	2.34	1.53
1	D	148	GLU	CB-CG	-36.39	0.83	1.52
1	C	164	ARG	CB-CG	-34.41	0.59	1.52
1	C	20	GLU	CB-CG	33.38	2.15	1.52
1	A	294	LYS	CB-CG	-28.98	0.74	1.52
1	D	294	LYS	CB-CG	-26.81	0.80	1.52
1	A	148	GLU	CB-CG	-26.48	1.01	1.52
1	A	164	ARG	CB-CG	-25.23	0.84	1.52
1	A	42	LYS	CB-CG	-23.74	0.88	1.52
1	D	300	LYS	CB-CG	-23.63	0.88	1.52
1	D	42	LYS	CB-CG	-23.20	0.90	1.52
1	B	177	ARG	CG-CD	-22.38	0.96	1.51
1	C	148	GLU	CB-CG	-22.30	1.09	1.52
1	D	177	ARG	CG-CD	-21.96	0.97	1.51
1	A	154	ASP	CB-CG	-20.74	1.08	1.51
1	B	129	GLU	CB-CG	-18.80	1.16	1.52
1	C	118	ASP	CB-CG	-18.49	1.12	1.51
1	A	177	ARG	CG-CD	-18.43	1.05	1.51
1	D	285	ARG	CB-CG	-16.33	1.08	1.52
1	B	148	GLU	CB-CG	-16.02	1.21	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	151	LYS	CB-CG	14.61	1.92	1.52
1	D	118	ASP	CB-CG	-14.47	1.21	1.51
1	A	129	GLU	CG-CD	-13.62	1.31	1.51
1	A	81	GLU	CB-CG	-13.18	1.27	1.52
1	B	81	GLU	CB-CG	-12.63	1.28	1.52
1	B	23	LYS	CB-CG	-11.83	1.20	1.52
1	D	151	LYS	CB-CG	-11.21	1.22	1.52
1	B	169	ARG	CB-CG	-10.77	1.23	1.52
1	C	19	GLU	CB-CG	-10.52	1.32	1.52
1	D	201	LYS	CB-CG	-10.36	1.24	1.52
1	D	192	LYS	CB-CG	-9.48	1.26	1.52
1	B	300	LYS	CB-CG	-9.46	1.27	1.52
1	C	42	LYS	CB-CG	-9.05	1.28	1.52
1	D	81	GLU	CA-CB	-7.79	1.36	1.53
1	D	169	ARG	CB-CG	-7.60	1.32	1.52
1	D	164	ARG	CB-CG	7.28	1.72	1.52
1	A	175	LYS	CG-CD	-7.04	1.28	1.52
1	B	154	ASP	CB-CG	-6.93	1.37	1.51
1	C	300	LYS	CB-CG	6.78	1.70	1.52
1	A	157	GLN	CB-CG	-6.60	1.34	1.52
1	B	130	LYS	CB-CG	-6.59	1.34	1.52
1	B	158	LYS	CB-CG	-6.41	1.35	1.52
1	A	300	LYS	CB-CG	-6.37	1.35	1.52
1	C	169	ARG	CB-CG	-5.82	1.36	1.52
1	D	23	LYS	CA-CB	-5.73	1.41	1.53
1	B	192	LYS	CG-CD	5.55	1.71	1.52
1	C	158	LYS	CB-CG	-5.51	1.37	1.52
1	A	151	LYS	CA-CB	-5.19	1.42	1.53
1	B	42	LYS	CB-CG	-5.14	1.38	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ASP	CB-CG-OD2	23.06	139.05	118.30
1	B	23	LYS	CA-CB-CG	22.47	162.83	113.40
1	D	151	LYS	CA-CB-CG	-21.69	65.69	113.40
1	A	294	LYS	CA-CB-CG	21.02	159.64	113.40
1	B	151	LYS	CA-CB-CG	-20.74	67.77	113.40
1	D	294	LYS	CA-CB-CG	18.69	154.51	113.40
1	A	23	LYS	N-CA-CB	-17.92	78.35	110.60
1	B	154	ASP	CB-CG-OD1	-17.66	102.40	118.30
1	D	23	LYS	CB-CG-CD	16.39	154.20	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	GLU	CA-CB-CG	-16.25	77.64	113.40
1	B	177	ARG	CB-CG-CD	16.25	153.84	111.60
1	C	154	ASP	CB-CG-OD1	16.07	132.77	118.30
1	D	151	LYS	CB-CG-CD	-15.79	70.53	111.60
1	C	151	LYS	CA-CB-CG	-15.58	79.13	113.40
1	A	42	LYS	CA-CB-CG	14.26	144.78	113.40
1	A	177	ARG	CB-CG-CD	14.05	148.13	111.60
1	A	23	LYS	CB-CA-C	-13.49	83.41	110.40
1	D	177	ARG	CB-CG-CD	13.36	146.32	111.60
1	C	17	LYS	CA-CB-CG	13.23	142.50	113.40
1	C	154	ASP	CB-CG-OD2	-11.01	108.39	118.30
1	D	158	LYS	CA-CB-CG	-10.31	90.71	113.40
1	A	164	ARG	CA-CB-CG	10.28	136.02	113.40
1	D	285	ARG	CA-CB-CG	10.16	135.75	113.40
1	B	177	ARG	CG-CD-NE	10.14	133.09	111.80
1	B	23	LYS	CB-CG-CD	10.09	137.84	111.60
1	D	192	LYS	CA-CB-CG	9.90	135.17	113.40
1	D	42	LYS	CA-CB-CG	9.81	134.99	113.40
1	C	164	ARG	CA-CB-CG	9.26	133.78	113.40
1	B	154	ASP	CA-CB-CG	8.99	133.18	113.40
1	D	148	GLU	CB-CG-CD	-8.98	89.96	114.20
1	A	154	ASP	CB-CG-OD2	8.94	126.35	118.30
1	D	154	ASP	CB-CG-OD2	8.82	126.24	118.30
1	C	148	GLU	CB-CG-CD	-8.51	91.24	114.20
1	D	164	ARG	CA-CB-CG	-8.00	95.80	113.40
1	B	192	LYS	CB-CG-CD	7.80	131.89	111.60
1	A	177	ARG	CG-CD-NE	7.74	128.05	111.80
1	A	129	GLU	CG-CD-OE2	7.72	133.74	118.30
1	C	151	LYS	CB-CG-CD	-7.69	91.59	111.60
1	A	129	GLU	CG-CD-OE1	-7.61	103.08	118.30
1	A	294	LYS	CB-CG-CD	7.44	130.94	111.60
1	B	294	LYS	CB-CG-CD	-7.33	92.53	111.60
1	B	42	LYS	CA-CB-CG	6.93	128.66	113.40
1	A	169	ARG	CB-CG-CD	6.79	129.26	111.60
1	B	130	LYS	CB-CG-CD	6.24	127.83	111.60
1	C	42	LYS	CA-CB-CG	6.22	127.09	113.40
1	C	19	GLU	CA-CB-CG	6.21	127.05	113.40
1	A	148	GLU	CA-CB-CG	6.18	127.00	113.40
1	C	20	GLU	CB-CG-CD	-6.12	97.69	114.20
1	D	294	LYS	CB-CG-CD	6.08	127.42	111.60
1	D	192	LYS	CB-CG-CD	6.01	127.22	111.60
1	B	164	ARG	CA-CB-CG	5.95	126.50	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	LYS	CA-CB-CG	5.93	126.45	113.40
1	B	148	GLU	CB-CG-CD	-5.90	98.27	114.20
1	A	164	ARG	CB-CG-CD	5.81	126.71	111.60
1	D	177	ARG	CG-CD-NE	5.73	123.84	111.80
1	A	175	LYS	CB-CG-CD	5.69	126.40	111.60
1	C	118	ASP	CB-CG-OD1	5.66	123.40	118.30
1	B	151	LYS	CB-CG-CD	-5.41	97.53	111.60
1	A	154	ASP	CA-CB-CG	5.33	125.13	113.40
1	A	169	ARG	CA-CB-CG	-5.30	101.74	113.40
1	B	192	LYS	CG-CD-CE	5.29	127.77	111.90
1	A	104	ASP	CB-CG-OD1	5.13	122.91	118.30
1	A	129	GLU	CB-CG-CD	5.06	127.87	114.20
1	D	23	LYS	N-CA-CB	5.04	119.67	110.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2261	0	2287	17	1
1	B	2261	0	2287	20	0
1	C	2266	0	2296	18	1
1	D	2266	0	2296	17	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	23	0	0	0	0
4	B	23	0	0	1	0
4	C	34	0	0	3	0
4	D	27	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9169	0	9166	65	2

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 4.

All (65) 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:134:ASN:OD1	1:B:147:THR:HG21	1.88	0.74
1:B:68:THR:HG21	1:B:75:ILE:HD12	1.72	0.71
1:D:68:THR:HG21	1:D:75:ILE:HD11	1.78	0.65
1:A:134:ASN:OD1	1:A:147:THR:HG21	1.97	0.64
1:D:68:THR:HG21	1:D:75:ILE:CD1	2.28	0.64
1:A:184:ILE:HG22	1:A:186:LEU:HD13	1.80	0.62
1:B:97:ILE:HD12	1:B:101:ILE:HD12	1.81	0.61
1:C:282:VAL:HG22	1:C:286:GLU:HB2	1.83	0.60
1:B:68:THR:HG21	1:B:75:ILE:CD1	2.31	0.59
1:A:97:ILE:HD12	1:A:101:ILE:HD12	1.83	0.59
1:C:52:ASP:OD1	1:C:86:LYS:NZ	2.38	0.57
1:C:68:THR:HG21	1:C:75:ILE:CD1	2.34	0.57
1:C:123:LEU:HD21	1:C:182:LEU:HD12	1.88	0.56
1:D:74:GLY:HA2	1:D:162:GLU:HG3	1.87	0.56
1:C:68:THR:HG21	1:C:75:ILE:HD12	1.86	0.56
1:A:203:LYS:NZ	1:B:274:SER:O	2.32	0.56
1:D:134:ASN:OD1	1:D:147:THR:HG21	2.05	0.56
1:B:31:LEU:HD13	1:B:229:ILE:HD13	1.88	0.55
1:A:276:ALA:O	1:B:203:LYS:NZ	2.40	0.54
1:A:282:VAL:HG22	1:A:286:GLU:HB2	1.90	0.54
1:B:166:ILE:HG21	1:C:106:ILE:HG23	1.91	0.53
1:A:258:ASN:HD22	1:B:222:GLY:HA2	1.73	0.52
1:A:101:ILE:HA	1:A:111:LEU:O	2.10	0.52
1:C:191:SER:OG	1:C:214:GLY:O	2.29	0.51
1:B:152:TYR:HB3	1:B:155:PHE:HB2	1.94	0.51
1:A:66:ILE:HG21	1:A:75:ILE:HD13	1.94	0.50
1:D:113:GLU:HG3	1:D:223:HIS:CE1	2.48	0.49
1:A:246:VAL:HA	1:A:263:PHE:O	2.15	0.47
1:B:269:THR:HG22	1:B:270:ASP:N	2.29	0.47
1:D:69:GLY:O	1:D:181:LYS:HE2	2.15	0.47
1:B:166:ILE:HG21	1:C:106:ILE:CG2	2.45	0.47
1:D:104:ASP:HB3	1:D:110:LEU:HD11	1.97	0.46
1:C:211:THR:HG22	1:C:212:TYR:H	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:HD21	1:D:182:LEU:HD12	1.96	0.46
1:D:269:THR:HG22	1:D:271:SER:H	1.81	0.45
1:D:170:HIS:O	1:D:173[B]:MET:HG3	2.17	0.44
1:B:35:ASP:OD2	1:B:70:ARG:HD2	2.17	0.44
1:A:77:SER:OG	1:A:163:ASN:ND2	2.50	0.44
1:C:282:VAL:CG1	1:C:288:ALA:HA	2.48	0.44
1:A:53:ALA:HB1	1:A:293:LEU:HD12	2.00	0.44
1:C:225:LYS:HG3	4:C:310:HOH:O	2.18	0.43
1:B:291:TYR:O	1:B:294:LYS:HG2	2.18	0.43
1:B:171:ASN:HD22	1:B:172:GLU:N	2.17	0.43
1:D:168:ILE:HD11	1:D:173[A]:MET:SD	2.59	0.43
1:A:66:ILE:HG21	1:A:75:ILE:CD1	2.48	0.43
1:C:204:ASN:HB3	1:D:260:LYS:HA	2.01	0.42
1:D:98:ASN:O	1:D:224:ASP:HA	2.19	0.42
1:A:224:ASP:OD2	1:A:254:ALA:HB3	2.20	0.42
1:C:131:ASN:HB3	4:C:325:HOH:O	2.18	0.41
1:C:211:THR:HG22	1:C:212:TYR:N	2.35	0.41
1:A:155:PHE:O	1:A:159:MET:HB2	2.20	0.41
1:A:211:THR:HG22	1:A:212:TYR:N	2.35	0.41
1:A:203:LYS:NZ	1:B:276:ALA:O	2.50	0.41
1:B:220:LYS:NZ	4:B:319:HOH:O	2.53	0.41
1:B:25:ALA:HB2	1:B:261:TYR:CZ	2.55	0.41
1:C:39:PHE:CE1	1:C:45:LYS:HA	2.55	0.41
1:C:282:VAL:HG22	1:C:286:GLU:CB	2.50	0.41
1:D:134:ASN:OD1	1:D:147:THR:CG2	2.68	0.41
1:D:152:TYR:HB3	1:D:155:PHE:HB2	2.02	0.41
1:D:163:ASN:N	4:D:317:HOH:O	2.41	0.41
1:C:240:ASN:HB2	4:C:309:HOH:O	2.21	0.41
1:B:46:VAL:HG12	1:B:51:ILE:HD12	2.01	0.41
1:D:68:THR:HG21	1:D:75:ILE:HD12	2.01	0.40
1:C:106:ILE:O	1:C:106:ILE:HG22	2.22	0.40
1:B:120:TYR:CZ	1:B:124:ILE:HD11	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:NZ	1:D:235:HIS:O[1_655]	1.74	0.46
1:C:177:ARG:NH2	1:D:177:ARG:NE[1_655]	2.08	0.12

## 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	282/301 (94%)	267 (95%)	14 (5%)	1 (0%)	39	69
1	B	282/301 (94%)	270 (96%)	12 (4%)	0	100	100
1	C	283/301 (94%)	271 (96%)	12 (4%)	0	100	100
1	D	283/301 (94%)	266 (94%)	16 (6%)	1 (0%)	39	69
All	All	1130/1204 (94%)	1074 (95%)	54 (5%)	2 (0%)	52	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	190	GLU
1	A	241	ASP

### 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	250/265 (94%)	242 (97%)	8 (3%)	46	77
1	B	250/265 (94%)	243 (97%)	7 (3%)	51	81
1	C	251/265 (95%)	242 (96%)	9 (4%)	42	73
1	D	251/265 (95%)	244 (97%)	7 (3%)	51	81
All	All	1002/1060 (94%)	971 (97%)	31 (3%)	47	78

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	75	ILE
1	A	125	SER
1	A	157	GLN
1	A	164	ARG
1	A	174	LEU
1	A	177	ARG
1	A	186	LEU
1	B	29	LEU
1	B	75	ILE
1	B	131	ASN
1	B	171	ASN
1	B	200	GLN
1	B	248	ASP
1	B	284	HIS
1	C	19	GLU
1	C	29	LEU
1	C	75	ILE
1	C	162	GLU
1	C	175	LYS
1	C	191	SER
1	C	269	THR
1	C	282	VAL
1	C	284	HIS
1	D	17	LYS
1	D	19	GLU
1	D	22	LEU
1	D	125	SER
1	D	175	LYS
1	D	211	THR
1	D	284	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	200	GLN
1	A	258	ASN
1	B	171	ASN
1	B	197	ASN
1	C	163	ASN
1	C	197	ASN
1	D	131	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	163	ASN
1	D	197	ASN
1	D	242	GLN
1	D	275	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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<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	A	284/301 (94%)	0.28	9 (3%) 51 51	26, 42, 57, 68	18 (6%)
1	B	284/301 (94%)	0.11	8 (2%) 56 57	24, 37, 55, 66	18 (6%)
1	C	284/301 (94%)	0.09	2 (0%) 89 90	25, 38, 51, 62	18 (6%)
1	D	284/301 (94%)	0.08	6 (2%) 67 68	25, 37, 51, 61	18 (6%)
All	All	1136/1204 (94%)	0.14	25 (2%) 65 66	24, 39, 54, 68	72 (6%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	TYR	4.6
1	C	152	TYR	4.4
1	A	153	ALA	4.4
1	B	152	TYR	4.4
1	A	152	TYR	4.0
1	A	189	SER	3.5
1	A	187	ASP	3.5
1	D	298	ASP	3.4
1	A	298	ASP	3.4
1	A	149	ASP	3.1
1	D	189	SER	3.0
1	D	152	TYR	2.9
1	B	188	PRO	2.9
1	B	190	GLU	2.8
1	A	194	VAL	2.6
1	D	300	LYS	2.6
1	D	188	PRO	2.5
1	B	189	SER	2.5
1	B	187	ASP	2.4
1	D	24	GLY	2.3
1	A	106	ILE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	299	LEU	2.1
1	B	185	VAL	2.1
1	A	166	ILE	2.0
1	B	191	SER	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(Å <sup>2</sup> )	Q<0.9
3	CL	C	303	1/1	0.99	0.35	8.57	26,26,26,26	0
3	CL	D	303	1/1	0.97	0.27	4.52	30,30,30,30	0
3	CL	A	303	1/1	0.96	0.29	4.21	31,31,31,31	0
2	CA	A	302	1/1	0.95	0.19	0.66	42,42,42,42	0
3	CL	B	303	1/1	0.97	0.17	0.36	33,33,33,33	0
2	CA	D	302	1/1	0.94	0.15	-0.30	37,37,37,37	0
2	CA	C	302	1/1	0.94	0.15	-0.70	34,34,34,34	0
2	CA	B	302	1/1	0.96	0.14	-1.21	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.