

# Full wwPDB X-ray Structure Validation Report (i)

#### Jun 12, 2024 – 11:23 am BST

PDB ID	:	8RPI
Title	:	JanthE from Janthinobacterium sp. HH01, lactyl-ThDP
Authors	:	Lanza, L.; Leogrande, C.; Rabe von Pappenheim, F.; Tittmann, K.; Mueller,
		М.
Deposited on	:	2024-01-16
Resolution	:	2.71  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity		4 09b 467
Mon robity	•	4.020-407
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.71 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622(2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 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	А	619	93%	5%•
1	В	619	2% 92%	6% ••
1	С	619	3% 93%	5%•
1	D	619	2% 92%	7% •
1	Е	619	% 93%	5% •



Mol	Chain	Length	Quality of chain	
1	F	619	5%	E 9/



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 56761 atoms, of which 27989 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.

Mol	Chain	Residues			Atom	s			ZeroOcc	AltConf	Trace
1	Δ	605	Total	С	Η	Ν	0	$\mathbf{S}$	0	4	0
	A	005	9296	2959	4629	814	862	32	0	4	0
1	В	608	Total	С	Η	Ν	0	S	0	6	0
1	D	008	9349	2974	4653	822	869	31	0	0	0
1	С	605	Total	С	Η	Ν	0	S	0	4	0
1	U	005	9296	2959	4629	814	862	32	0	4	0
1	а	608	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	6	0
1	D	000	9351	2974	4655	822	869	31	0	0	0
1	E	605	Total	$\mathbf{C}$	Η	Ν	Ο	$\mathbf{S}$	0	6	0
1		000	9321	2965	4643	818	863	32	0	0	0
1	F	508	Total	$\mathbf{C}$	Η	N	0	$\mathbf{S}$	0	4	0
	T,	090	9177	2924	4563	805	854	31			

• Molecule 1 is a protein called Thiamine pyrophosphate-binding protein.

• Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\rm C_{27}H_{33}N_9O_{15}P_2).$ 





Mol	Chain	Residues		A	Aton	ıs			ZeroOcc	AltConf
2	Λ	1	Total	С	Η	Ν	Ο	Р	0	0
	A	1	84	27	31	9	15	2	0	0
2	В	1	Total	С	Η	Ν	Ο	Р	0	0
2	D	1	84	27	31	9	15	2	0	0
2	С	1	Total	С	Η	Ν	Ο	Р	0	0
2	U	1	84	27	31	9	15	2	0	0
2	л	1	Total	С	Η	Ν	Ο	Р	0	0
2	D	1	84	27	31	9	15	2	0	0
2	E	1	Total	С	Η	Ν	Ο	Р	0	Ο
2	Ľ	1	84	27	31	9	15	2	0	0
2	F	1	Total	С	Η	Ν	Ō	Р	0	0
	T,	1	84	27	31	9	15	2	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0
3	С	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	Ε	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

• Molecule 4 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-CARBOXY-1-H YDROXYETHYL)-5-(2-{[HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHY L)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDL) (formula:  $C_{15}H_{23}N_4O_{10}P_2S$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		A	ton	ıs			ZeroOcc	AltConf		
4	Δ	1	Total	С	Ν	Ο	Р	S	0	0		
4	A	1	32	15	4	10	2	1	0	0		
4	В	1	Total	С	Ν	Ο	Р	S	0	0		
4	D	1	32	15	4	10	2	1	0	0		
4	С	1	Total	С	Ν	Ο	Р	$\mathbf{S}$	0	0		
4	U	U	U	1	32	15	4	10	2	1	0	0
4	Л	1	Total	С	Ν	Ο	Р	$\mathbf{S}$	0	0		
4	D	1	32	15	4	10	2	1	0	0		
4	F	1	Total	С	Ν	Ο	Р	S	0	0		
4	Ľ	1	32	15	4	10	2	1	0	0		
4	F	1	Total	С	Ν	Ο	Р	S	0	0		
4	T,		32	15	4	10	2	1	0	0		

• Molecule 5 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula:  $C_{18}H_{38}O_{10}$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
Б	В	1	Total	С	Η	0	0	0
0	D	1	59	18	31	10	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	48	Total         O           48         48	0	0
6	В	36	$\begin{array}{cc} \text{Total} & \text{O} \\ 36 & 36 \end{array}$	0	0
6	С	32	$\begin{array}{cc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$	0	0
6	D	43	Total O 43 43	0	0
6	Ε	37	$\begin{array}{cc} \text{Total} & \text{O} \\ 37 & 37 \end{array}$	0	0
6	F	14	Total O 14 14	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.

- Chain A: 93% 5% • LEU GLU HIS HIS HIS HIS HIS HIS • Molecule 1: Thiamine pyrophosphate-binding protein Chain B: 92% 6% •• • Molecule 1: Thiamine pyrophosphate-binding protein Chain C: 5%• 93% • Molecule 1: Thiamine pyrophosphate-binding protein Chain D: 92% 7%
- Molecule 1: Thiamine pyrophosphate-binding protein



# 

# N393 V401 V401 V401 M434 P434 P433 P444 P443 P444 P444 P444 P444 P444 P444 P453 P454 P451 P452 P553 </t

 $\bullet$  Molecule 1: Thiamine pyrophosphate-binding protein





• Molecule 1: Thiamine pyrophosphate-binding protein





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	174.15Å 118.54Å 202.05Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $96.72^{\circ}$ $90.00^{\circ}$	Depositor
Resolution(A)	85.69 - 2.71	Depositor
Resolution (A)	85.69 - 2.71	EDS
% Data completeness	95.5 (85.69-2.71)	Depositor
(in resolution range)	95.5 (85.69 - 2.71)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.09 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.195 , $0.234$	Depositor
$n, n_{free}$	0.195 , $0.234$	DCC
$R_{free}$ test set	5315 reflections $(5.02\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	61.4	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 27.0	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	56761	wwPDB-VP
Average B, all atoms $(Å^2)$	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: TDL, MG, FAD, 2PE

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).

Mal	Chain	Bond lengths		Bond angles		
1VIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.32	0/4779	0.51	0/6483	
1	В	0.36	0/4814	0.53	1/6531~(0.0%)	
1	С	0.28	0/4779	0.50	0/6483	
1	D	0.27	0/4814	0.50	0/6531	
1	Е	0.28	0/4797	0.50	0/6507	
1	F	0.28	0/4727	0.50	0/6412	
All	All	0.30	0/28710	0.51	1/38947~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	179	ASP	CB-CG-OD1	5.19	122.97	118.30

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	А	4667	4629	4629	15	0
1	В	4696	4653	4649	21	0
1	С	4667	4629	4629	16	0
1	D	4696	4655	4649	18	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ε	4678	4643	4633	15	0
1	F	4614	4563	4561	21	0
2	А	53	31	31	0	0
2	В	53	31	31	1	0
2	С	53	31	31	0	0
2	D	53	31	31	0	0
2	Ε	53	31	31	0	0
2	F	53	31	31	3	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	Ε	1	0	0	0	0
3	F	1	0	0	0	0
4	А	32	0	19	3	0
4	В	32	0	19	4	0
4	С	32	0	19	4	0
4	D	32	0	19	4	0
4	Ε	32	0	19	4	0
4	F	32	0	19	4	0
5	В	28	31	38	2	0
6	А	48	0	0	1	0
6	В	36	0	0	3	0
6	С	32	0	0	0	0
6	D	43	0	0	1	0
6	Е	37	0	0	0	0
6	F	14	0	0	1	0
All	All	28772	27989	28088	122	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 2.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:37:GLU:OE2	1:B:41:ARG:NH1	2.07	0.87
1:B:537:GLU:N	1:B:537:GLU:OE1	2.18	0.77
1:A:174:GLN:OE1	6:A:802:HOH:O	2.10	0.69
1:C:434:MET:SD	4:C:703:TDL:HM43	2.34	0.68
1:D:434:MET:SD	4:D:703:TDL:HM43	2.34	0.67
1:B:177:ARG:NH2	6:B:802:HOH:O	2.28	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:434:MET:SD	4:B:704:TDL:HM43	2.37	0.65
4:D:703:TDL:N4'	4:D:703:TDL:OL1	2.26	0.64
4:A:703:TDL:OL1	4:A:703:TDL:N4'	2.30	0.62
1:C:210:LEU:O	1:C:355:LYS:NZ	2.31	0.62
1:A:434:MET:SD	4:A:703:TDL:HM43	2.40	0.61
4:E:703:TDL:OL1	4:E:703:TDL:N4'	2.28	0.61
1:B:570:VAL:HG11	1:B:578:LEU:HD12	1.83	0.61
1:B:46:GLU:OE2	1:B:450[B]:ARG:NH2	2.31	0.60
1:D:401:VAL:HG11	1:D:444:VAL:HG11	1.85	0.58
1:B:573:ARG:HH22	5:B:703:2PE:H232	1.69	0.57
1:E:434:MET:SD	4:E:703:TDL:HM43	2.44	0.57
4:C:703:TDL:OL1	4:C:703:TDL:N4'	2.31	0.57
1:F:434:MET:SD	4:F:703:TDL:HM43	2.45	0.57
4:F:703:TDL:OL1	4:F:703:TDL:N4'	2.33	0.56
1:A:438:LEU:HB2	1:A:439:PRO:HD3	1.87	0.56
1:F:401:VAL:HG11	1:F:444:VAL:HG11	1.88	0.55
1:E:401:VAL:HG11	1:E:444:VAL:HG11	1.89	0.55
1:C:401:VAL:HG11	1:C:444:VAL:HG11	1.89	0.54
1:E:239:LYS:HE3	1:E:345:ASN:OD1	2.08	0.53
1:C:438:LEU:HB2	1:C:439:PRO:HD3	1.91	0.52
1:A:404:THR:HG22	1:A:456:LEU:HB2	1.92	0.52
1:A:401:VAL:HG11	1:A:444:VAL:HG11	1.92	0.51
1:A:522:ALA:HB2	1:A:553:ILE:HD12	1.92	0.51
1:D:438:LEU:HB2	1:D:439:PRO:HD3	1.92	0.51
4:B:704:TDL:OL1	4:B:704:TDL:N4'	2.37	0.50
1:E:108:LYS:HE3	1:E:109:PHE:CZ	2.47	0.49
4:F:703:TDL:C6'	4:F:703:TDL:HM41	2.42	0.49
2:F:701:FAD:O1A	6:F:802:HOH:O	2.20	0.48
1:C:604:HIS:O	1:C:607:SER:HB2	2.13	0.48
1:B:383:ILE:HD11	1:B:534:GLY:HA2	1.96	0.48
1:A:7:LYS:NZ	1:A:34:HIS:HD2	2.12	0.47
1:B:401:VAL:HG11	1:B:444:VAL:HG11	1.94	0.47
4:C:703:TDL:H4'1	4:C:703:TDL:CLA	2.27	0.47
1:E:438:LEU:HB2	1:E:439:PRO:HD3	1.96	0.47
1:F:104:ASN:O	1:F:171:MET:HG3	2.14	0.47
1:B:497:LYS:NZ	6:B:808:HOH:O	2.47	0.47
1:F:237:LEU:O	1:F:241:GLY:N	2.46	0.47
4:E:703:TDL:C6'	4:E:703:TDL:HM41	2.45	0.47
1:D:239:LYS:NZ	1:D:345:ASN:OD1	2.47	0.47
1:F:234:LYS:NZ	1:F:234:LYS:HB2	2.30	0.47
1:A:571:VAL:HG11	1:A:610:LEU:HD13	1.98	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:24:ALA:HB1	1:C:74:LEU:CD2	2.44	0.46
1:D:234:LYS:NZ	1:D:238:GLU:OE2	2.47	0.46
1:D:317:GLU:OE1	6:D:801:HOH:O	2.20	0.46
1:B:438:LEU:HB2	1:B:439:PRO:HD3	1.97	0.46
1:F:220:LEU:HD13	1:F:233:LEU:HD13	1.98	0.46
1:E:383:ILE:HG23	1:E:535:TRP:CZ2	2.51	0.46
1:A:378:ASP:OD1	1:A:387:ARG:HD3	2.16	0.46
4:A:703:TDL:C6'	4:A:703:TDL:HM41	2.46	0.45
1:A:323:LYS:HE2	1:C:316:ASP:OD1	2.16	0.45
1:B:571:VAL:HG21	1:B:610:LEU:HD22	1.99	0.45
1:F:211:ALA:HB2	1:F:352:ILE:HD13	1.98	0.45
1:B:408:THR:N	4:B:704:TDL:O3B	2.48	0.45
5:B:703:2PE:H142	5:B:703:2PE:O10	2.17	0.45
1:D:62:THR:HG21	1:D:440:ALA:HB1	1.99	0.45
1:D:385:SER:OG	1:D:562:GLN:NE2	2.44	0.45
1:B:278:GLN:HG3	1:B:584:GLU:HB3	1.99	0.45
1:F:313:ILE:HB	2:F:701:FAD:C2A	2.46	0.45
1:C:459:ASP:N	1:C:459:ASP:OD1	2.50	0.44
1:D:110:THR:HA	1:D:119:TRP:CE3	2.52	0.44
1:D:571:VAL:HG13	1:D:610:LEU:HD22	1.99	0.44
1:F:12:VAL:HG13	1:F:150:LEU:CD1	2.48	0.44
1:E:215:ARG:HA	1:E:358:TRP:CD1	2.53	0.44
1:B:246:VAL:O	1:B:264:ARG:HG3	2.18	0.44
1:F:110:THR:HA	1:F:119:TRP:CE3	2.52	0.44
1:B:240:LEU:HD21	1:B:344:LEU:HD11	2.00	0.44
4:D:703:TDL:H4'1	4:D:703:TDL:CLA	2.29	0.44
1:C:492:ILE:O	1:C:496:GLN:HG2	2.18	0.43
1:F:312:ASP:OD2	2:F:701:FAD:O3B	2.36	0.43
1:A:405:ASP:OD1	1:A:406:MET:N	2.46	0.43
1:D:17:GLU:OE1	1:D:42:ARG:NE	2.50	0.43
1:D:224:ILE:HD13	1:D:233:LEU:HD21	2.00	0.43
1:D:295:ILE:HB	1:D:302:LEU:HD22	2.00	0.43
1:B:224:ILE:HD13	1:B:233:LEU:HD21	1.99	0.43
1:E:581:PRO:HB2	1:E:585:ASP:HB3	2.01	0.43
1:F:408:THR:N	4:F:703:TDL:O3B	2.51	0.43
1:C:172:ASP:N	1:C:172:ASP:OD1	2.52	0.43
1:E:303:ALA:O	1:E:324:ARG:NH2	2.52	0.43
1:A:363:ARG:O	1:A:367:GLU:HG2	2.19	0.42
1:C:62:THR:HG21	1:C:440:ALA:HB1	1.99	0.42
1:E:110:THR:HA	1:E:119:TRP:CE3	2.55	0.42
1:F:452:GLU:HA	1:F:478:PRO:HG2	2.01	0.42



	1.0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:198:ALA:HB1	1:C:326:GLN:NE2	2.34	0.42
4:B:704:TDL:H4'1	4:B:704:TDL:CLA	2.33	0.42
1:C:278:GLN:HG3	1:C:584:GLU:HB3	2.01	0.42
2:B:701:FAD:H9	2:B:701:FAD:H1'1	1.88	0.42
1:C:200:ALA:HB1	1:C:343:ARG:NH2	2.34	0.42
1:A:383:ILE:HG23	1:A:535:TRP:CZ2	2.54	0.41
1:E:215:ARG:HA	1:E:358:TRP:CG	2.55	0.41
4:E:703:TDL:H4'1	4:E:703:TDL:CLA	2.31	0.41
1:F:438:LEU:HB2	1:F:439:PRO:HD3	2.01	0.41
1:C:480:LYS:N	1:C:480:LYS:HD2	2.35	0.41
1:F:104:ASN:ND2	1:F:168:GLU:OE2	2.38	0.41
1:B:591:PRO:HG2	1:B:594:VAL:CG2	2.51	0.41
4:C:703:TDL:H4'1	4:C:703:TDL:C2	2.34	0.41
1:D:292:ILE:HB	1:D:293:PRO:HD3	2.03	0.41
1:E:195:LEU:HD11	1:E:339:ALA:HB2	2.01	0.41
1:F:239:LYS:HG2	1:F:344:LEU:HD13	2.03	0.41
1:D:215:ARG:HA	1:D:358:TRP:CG	2.55	0.41
1:B:17:GLU:HA	1:B:44:TYR:CE2	2.56	0.41
1:F:264:ARG:N	1:F:264:ARG:HD3	2.36	0.41
1:B:3:ASP:N	6:B:802:HOH:O	2.53	0.41
1:C:236:LEU:HD22	1:C:337:ILE:HG23	2.02	0.41
1:F:12:VAL:HG13	1:F:150:LEU:HD11	2.03	0.41
1:F:258:HIS:CG	1:F:259:PRO:HD2	2.56	0.41
1:A:378:ASP:HA	1:A:379:PRO:HD3	1.85	0.40
1:D:303:ALA:HB1	1:D:306:ALA:HB3	2.04	0.40
1:E:435:GLY:O	1:E:465:ASN:ND2	2.41	0.40
1:D:529:ALA:HA	1:D:553:ILE:O	2.21	0.40
1:E:522:ALA:HB2	1:E:553:ILE:HD12	2.03	0.40
1:F:480:LYS:N	1:F:480:LYS:HD2	2.37	0.40
1:D:12:VAL:HG13	1:D:150:LEU:CD1	2.51	0.40
4:D:703:TDL:C6'	4:D:703:TDL:HM41	2.51	0.40
1:B:571:VAL:O	1:B:571:VAL:CG2	2.70	0.40
1:E:438:LEU:HD22	1:E:472[A]:MET:SD	2.61	0.40
1:F:278:GLN:HG3	1:F:584:GLU:HB3	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	605/619~(98%)	592~(98%)	12 (2%)	1 (0%)	47	72
1	В	612/619~(99%)	595~(97%)	17 (3%)	0	100	100
1	С	605/619~(98%)	587~(97%)	18 (3%)	0	100	100
1	D	612/619~(99%)	593~(97%)	19 (3%)	0	100	100
1	Е	607/619~(98%)	587~(97%)	20 (3%)	0	100	100
1	F	598/619~(97%)	575~(96%)	23~(4%)	0	100	100
All	All	3639/3714~(98%)	3529 (97%)	109 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	379	PRO

#### 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	Perce	ntiles
1	А	492/500~(98%)	485 (99%)	7 (1%)	67	85
1	В	494/500~(99%)	483 (98%)	11 (2%)	52	78
1	С	492/500~(98%)	486 (99%)	6 (1%)	71	88
1	D	494/500~(99%)	487 (99%)	7 (1%)	67	85
1	Ε	494/500~(99%)	490 (99%)	4 (1%)	81	92
1	F	485/500~(97%)	480 (99%)	5 (1%)	76	90



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2951/3000~(98%)	2911 (99%)	40 (1%)	67 85

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	264	ARG
1	А	380	GLU
1	А	393	ASN
1	А	425	PHE
1	А	464	MET
1	А	480	LYS
1	А	509	ARG
1	В	3	ASP
1	В	41	ARG
1	В	239	LYS
1	В	264	ARG
1	В	380	GLU
1	В	393	ASN
1	B	464	MET
1	В	476	ASN
1	В	549	THR
1	В	573	ARG
1	В	575	ASP
1	С	3	ASP
1	С	264	ARG
1	С	393	ASN
1	С	425	PHE
1	С	464	MET
1	С	480	LYS
1	D	264	ARG
1	D	393	ASN
1	D	464	MET
1	D	476	ASN
1	D	480	LYS
1	D	491	MET
1	D	549	THR
1	E	264	ARG
1	Е	393	ASN
1	Е	425	PHE
1	E	464	MET
1	F	264	ARG
1	F	393	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	F	464	MET
1	F	480	LYS
1	F	563	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	34	HIS
1	С	326	GLN
1	С	475	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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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).

Mal	Mol Tuno Chain		Tiple	Bo	ond leng	$_{\rm ths}$	B	ond ang	les	
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TDL	А	703	3	26,33,33	0.77	0	30,51,51	0.86	1 (3%)
2	FAD	F	701	-	53,58,58	0.48	0	68,89,89	0.51	1 (1%)



Mal	Turne	Chain	Dec	Link	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	2PE	В	703	-	27,27,27	0.15	0	26,26,26	1.03	1 (3%)
2	FAD	Е	701	-	$53,\!58,\!58$	0.50	0	68,89,89	0.57	2 (2%)
4	TDL	В	704	3	26,33,33	0.77	0	30,51,51	0.92	1 (3%)
2	FAD	С	701	-	53,58,58	0.50	0	68,89,89	0.53	1 (1%)
4	TDL	С	703	3	26,33,33	0.78	0	30,51,51	0.87	1 (3%)
2	FAD	D	701	-	53,58,58	0.48	0	68,89,89	0.48	1 (1%)
4	TDL	F	703	3	26,33,33	0.79	0	30,51,51	0.88	1 (3%)
4	TDL	Е	703	3	26,33,33	0.79	0	30,51,51	0.90	1 (3%)
2	FAD	А	701	-	53,58,58	0.54	0	68,89,89	0.49	1 (1%)
2	FAD	В	701	-	53,58,58	0.50	0	68,89,89	0.49	1 (1%)
4	TDL	D	703	3	26,33,33	0.76	0	30,51,51	0.84	1 (3%)

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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
4	TDL	А	703	3	-	2/22/29/29	0/2/2/2
2	FAD	F	701	-	-	9/30/50/50	0/6/6/6
5	2PE	В	703	-	-	7/25/25/25	-
2	FAD	Е	701	-	-	7/30/50/50	0/6/6/6
4	TDL	В	704	3	-	3/22/29/29	0/2/2/2
2	FAD	С	701	-	-	7/30/50/50	0/6/6/6
4	TDL	С	703	3	-	4/22/29/29	0/2/2/2
2	FAD	D	701	-	-	9/30/50/50	0/6/6/6
4	TDL	F	703	3	-	5/22/29/29	0/2/2/2
4	TDL	Е	703	3	-	6/22/29/29	0/2/2/2
2	FAD	А	701	-	-	8/30/50/50	0/6/6/6
2	FAD	В	701	-	-	7/30/50/50	0/6/6/6
4	TDL	D	703	3	-	4/22/29/29	0/2/2/2

There are no bond length outliers.

All (14) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	В	704	TDL	C5-C4-N3	2.76	113.42	107.66
4	F	703	TDL	C5-C4-N3	2.73	113.38	107.66
4	А	703	TDL	C5-C4-N3	2.69	113.29	107.66
4	С	703	TDL	C5-C4-N3	2.67	113.24	107.66
4	D	703	TDL	C5-C4-N3	2.67	113.24	107.66
4	Е	703	TDL	C5-C4-N3	2.60	113.10	107.66
2	D	701	FAD	C5A-C6A-N6A	2.33	123.89	120.35
2	Е	701	FAD	C5A-C6A-N6A	2.32	123.87	120.35
2	F	701	FAD	C5A-C6A-N6A	2.31	123.87	120.35
5	В	703	2PE	O19-C18-C17	-2.31	99.98	110.39
2	Е	701	FAD	P-O3P-PA	-2.28	125.00	132.83
2	С	701	FAD	C5A-C6A-N6A	2.23	123.74	120.35
2	В	701	FAD	C5A-C6A-N6A	2.23	123.74	120.35
2	А	701	FAD	C5A-C6A-N6A	2.18	123.67	120.35

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	701	FAD	C5B-O5B-PA-O1A
2	А	701	FAD	O4B-C4B-C5B-O5B
2	В	701	FAD	C5B-O5B-PA-O1A
2	С	701	FAD	C5B-O5B-PA-O1A
2	С	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	C5B-O5B-PA-O1A
2	D	701	FAD	O4B-C4B-C5B-O5B
2	Е	701	FAD	C5B-O5B-PA-O1A
2	Е	701	FAD	C5B-O5B-PA-O2A
2	F	701	FAD	C5B-O5B-PA-O1A
2	F	701	FAD	C5B-O5B-PA-O2A
4	А	703	TDL	OL1-CLA-CLC-OL2
4	В	704	TDL	OL1-CLA-CLC-OL2
4	В	704	TDL	C4'-C5'-C7'-N3
4	С	703	TDL	C4-C5-C6-C7
4	С	703	TDL	OL1-CLA-CLC-OL2
4	С	703	TDL	C4'-C5'-C7'-N3
4	D	703	TDL	C4-C5-C6-C7
4	D	703	TDL	OL1-CLA-CLC-OL2
4	D	703	TDL	C4'-C5'-C7'-N3
4	Е	703	TDL	C4-C5-C6-C7
4	Е	703	TDL	OL1-CLA-CLC-OL2
4	F	703	TDL	C4-C5-C6-C7
4	F	703	TDL	OL1-CLA-CLC-OL2



Mol	Chain	Res	Type	Atoms
2	А	701	FAD	C3B-C4B-C5B-O5B
2	В	701	FAD	O4B-C4B-C5B-O5B
2	С	701	FAD	C3B-C4B-C5B-O5B
2	Е	701	FAD	O4B-C4B-C5B-O5B
2	Е	701	FAD	C3B-C4B-C5B-O5B
2	F	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	C3B-C4B-C5B-O5B
5	В	703	2PE	O7-C8-C9-O10
2	В	701	FAD	C3B-C4B-C5B-O5B
2	D	701	FAD	C3B-C4B-C5B-O5B
4	Е	703	TDL	CLB-CLA-CLC-OL2
4	F	703	TDL	CLB-CLA-CLC-OL2
5	В	703	2PE	O13-C14-C15-O16
5	В	703	2PE	O16-C17-C18-O19
4	Е	703	TDL	CLB-CLA-CLC-OL3
4	F	703	TDL	CLB-CLA-CLC-OL3
2	В	701	FAD	C4'-C5'-O5'-P
2	D	701	FAD	C4'-C5'-O5'-P
2	Е	701	FAD	C4'-C5'-O5'-P
2	F	701	FAD	C4'-C5'-O5'-P
2	А	701	FAD	P-O3P-PA-O5B
2	В	701	FAD	P-O3P-PA-O5B
2	С	701	FAD	P-O3P-PA-O5B
2	D	701	FAD	P-O3P-PA-O5B
2	Е	701	FAD	P-O3P-PA-O5B
2	F	701	FAD	P-O3P-PA-O5B
4	Е	703	TDL	PB-O3A-PA-O7
2	А	701	FAD	C4'-C5'-O5'-P
2	А	701	FAD	C5B-O5B-PA-O3P
2	С	701	FAD	C5B-O5B-PA-O3P
2	D	701	FAD	C5B-O5B-PA-O3P
2	D	701	FAD	P-O3P-PA-O1A
2	F	701	FAD	P-O3P-PA-O1A
5	В	703	2PE	C21-C20-O19-C18
2	С	701	FAD	C4'-C5'-O5'-P
2	A	701	FAD	C5B-O5B-PA-O2A
2	В	701	FAD	C5B-O5B-PA-O2A
2	С	701	FAD	C5B-O5B-PA-O2A
2	D	701	FAD	C5B-O5B-PA-O2A
4	A	703	TDL	OL1-CLA-CLC-OL3
4	В	704	TDL	OL1-CLA-CLC-OL3
4	С	703	TDL	OL1-CLA-CLC-OL3

Continued from previous page...



OTOT T
--------

Mol	Chain	Res	Type	Atoms
4	D	703	TDL	OL1-CLA-CLC-OL3
4	Е	703	TDL	OL1-CLA-CLC-OL3
4	F	703	TDL	OL1-CLA-CLC-OL3
2	А	701	FAD	P-O3P-PA-O1A
5	В	703	2PE	C11-C12-O13-C14
5	В	703	2PE	O19-C20-C21-O22
2	В	701	FAD	C5B-O5B-PA-O3P
2	Е	701	FAD	C5B-O5B-PA-O3P
2	F	701	FAD	C5B-O5B-PA-O3P
2	D	701	FAD	O3'-C3'-C4'-C5'
2	F	701	FAD	O3'-C3'-C4'-C5'
5	В	703	2PE	O22-C23-C24-O25

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	703	TDL	3	0
2	F	701	FAD	3	0
5	В	703	2PE	2	0
4	В	704	TDL	4	0
4	С	703	TDL	4	0
4	F	703	TDL	4	0
4	Е	703	TDL	4	0
2	В	701	FAD	1	0
4	D	703	TDL	4	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.































## 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	605/619~(97%)	0.13	6 (0%) 82 83	40, 55, 75, 107	0
1	В	608/619~(98%)	0.18	10 (1%) 72 74	39, 56, 73, 99	0
1	С	605/619~(97%)	0.20	17 (2%) 53 54	44, 58, 81, 100	0
1	D	608/619~(98%)	0.21	12 (1%) 65 67	39, 53, 77, 117	0
1	Ε	605/619~(97%)	0.16	8 (1%) 77 78	42, 54, 74, 102	0
1	F	598/619~(96%)	0.44	32 (5%) 25 25	41, 71, 98, 126	0
All	All	3629/3714~(97%)	0.22	85 (2%) 60 62	39, 57, 86, 126	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	572	SER	5.0
1	А	347	ALA	5.0
1	F	233	LEU	4.7
1	Е	347	ALA	4.2
1	F	348	ASP	4.0
1	F	262	PHE	3.8
1	F	241	GLY	3.7
1	А	578	LEU	3.6
1	А	573	ARG	3.5
1	F	354	SER	3.3
1	Е	573	ARG	3.3
1	F	236	LEU	3.2
1	F	340	LEU	3.1
1	С	352	ILE	3.1
1	Е	571	VAL	3.1
1	D	574	ALA	3.0
1	F	232	LEU	2.9
1	Е	610	LEU	2.9
1	C	259	PRO	2.9



8RPI
------

Mol	Chain	Res	Type	RSRZ	
1	С	236	LEU	2.9	
1	D	211	ALA	2.9	
1	D	575	ASP	2.8	
1	С	343	ARG	2.8	
1	В	254	LEU	2.8	
1	F	347	ALA	2.8	
1	F	337	ILE	2.8	
1	В	473	VAL	2.8	
1	С	235	PRO	2.8	
1	D	578	LEU	2.7	
1	F	341	LEU	2.7	
1	F	600	ILE	2.7	
1	D	3	ASP	2.7	
1	A	346	ALA	2.7	
1	Е	346	ALA	2.7	
1	В	383	ILE	2.7	
1	F	237	LEU	2.6	
1	F	266	GLY	2.6	
1	С	339	ALA	2.6	
1	С	372	VAL	2.6	
1	С	600	ILE	2.6	
1	F	362	CYS	2.5	
1	F	244	ALA	2.5	
1	F	218	LEU	2.5	
1	F	530	TYR	2.4	
1	С	272	ALA	2.4	
1	В	477	LEU	2.4	
1	С	453	VAL	2.4	
1	В	595	LEU	2.4	
1	F	190	PRO	2.3	
1	В	232	LEU	2.3	
1	F	263	GLY	2.3	
1	E	379	PRO	2.3	
1	F	210	LEU	2.3	
1	D	354	SER	2.3	
1	A	449	ASP	2.3	
1	E	569	GLY	2.2	
1	F	284	LEU	2.2	
1	C	610	LEU	2.2	
1	D	344	LEU	2.2	
1	F	549	THR	2.2	
1	С	261	VAL	2.2	



8RPI
------

Mol	Chain	Res	Type	RSRZ
1	F	346	ALA	2.2
1	F	352	ILE	2.2
1	С	244	ALA	2.2
1	D	351	ALA	2.2
1	С	521	LEU	2.2
1	С	276	ILE	2.2
1	F	4	ASN	2.2
1	С	536	ASP	2.1
1	F	521	LEU	2.1
1	В	610	LEU	2.1
1	F	253	MET	2.1
1	А	210	LEU	2.1
1	F	336 PHE		2.1
1	D	352	ILE	2.1
1	F	545	VAL	2.1
1	В	525	PHE	2.1
1	С	232	LEU	2.0
1	D	210	LEU	2.0
1	D	276	ILE	2.0
1	D	212	LYS	2.0
1	В	262	PHE	2.0
1	В	603	MET	2.0
1	F	482	PHE	2.0
1	F	207	LEU	2.0

Continued from previous page...

## 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 monosaccharides in this entry.

#### 6.4 Ligands (i)

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



8RPI	

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
5	2PE	В	703	28/28	0.79	0.27	75,100,122,123	0
3	MG	С	702	1/1	0.87	0.20	52,52,52,52	0
3	MG	F	702	1/1	0.89	0.20	60,60,60,60	0
3	MG	А	702	1/1	0.90	0.16	$55,\!55,\!55,\!55$	0
3	MG	Е	702	1/1	0.93	0.15	58, 58, 58, 58	0
2	FAD	F	701	53/53	0.95	0.17	65,74,87,92	0
4	TDL	В	704	32/32	0.96	0.17	45,50,56,60	0
2	FAD	В	701	53/53	0.97	0.16	46,52,63,65	0
2	FAD	С	701	53/53	0.97	0.20	$50,\!56,\!68,\!71$	0
4	TDL	А	703	32/32	0.97	0.17	46,54,58,60	0
3	MG	В	702	1/1	0.97	0.16	49,49,49,49	0
4	TDL	С	703	32/32	0.97	0.18	44,53,58,61	0
4	TDL	D	703	32/32	0.97	0.18	46, 49, 55, 56	0
4	TDL	Е	703	32/32	0.97	0.20	$48,\!55,\!59,\!62$	0
4	TDL	F	703	32/32	0.97	0.20	54,60,67,68	0
2	FAD	D	701	53/53	0.97	0.18	44,49,59,64	0
2	FAD	А	701	53/53	0.98	0.17	39,49,59,60	0
2	FAD	E	701	53/53	0.98	0.18	40,46,55,57	0
3	MG	D	702	1/1	0.98	0.18	$4\overline{9,49,49,49}$	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.

































# 6.5 Other polymers (i)

There are no such residues in this entry.

