

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

#### Oct 12, 2021 - 10:20 am BST

PDB ID	:	7B2E
Title	:	quadruple mutant of oxalyl-CoA decarboxylase from Methylorubrum ex-
		torquens with bound TPP and ADP
Authors	:	Pfister, P.; Burgener, S.; Nattermann, M.; Zarzycki, J.; Erb, T.J.
Deposited on	:	2020-11-26
Resolution	:	2.80  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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

## 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 2.80 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 <sub>free</sub>	130704	3140 (2.80-2.80)			
Clashscore	141614	3569 (2.80-2.80)			
Ramachandran outliers	138981	3498 (2.80-2.80)			
Sidechain outliers	138945	3500 (2.80-2.80)			

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain		
1	А	583	86%	8%	6%
1	В	583	86%	8%	6%
1	С	583	88%	6%	6%
1	D	583	87%	7%	6%
1	Е	583	86%	8%	• 6%
1	F	583	85%	9%	6%
1	G	583	87%	6%	6%



Mol	Chain	Length	Quality of chain		
1	Н	583	87%	7%	6%



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 34264 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	548	Total	С	Ν	Ο	$\mathbf{S}$	0	1	0
	A	040	4069	2569	710	767	23	0	1	0
1	В	548	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	D	040	4064	2566	710	765	23	0	0	0
1	С	548	Total	С	Ν	Ο	$\mathbf{S}$	0	1	0
1	U	040	4069	2569	710	767	23	0	I	0
1	Л	548	Total	С	Ν	Ο	S	0	0	0
1	D	040	4064	2566	710	765	23		0	
1	F	548	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	Ľ	040	4064	2566	710	765	23	0	0	
1	F	548	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	Ľ	040	4064	2566	710	765	23	0	0	0
1	C	548	Total	С	Ν	Ο	$\mathbf{S}$	0	3	0
1	I G	040	4083	2577	711	772	23	0	5	0
1	1 U	548	Total	С	Ν	Ο	$\mathbf{S}$	0	2	0
	11	040	4083	2577	711	772	23	0	5	

• Molecule 1 is a protein called Putative oxalyl-CoA decarboxylase (Oxc, yfdU).

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	135	GLY	GLU	engineered mutation	UNP C5AX46
А	415	CYS	ALA	engineered mutation	UNP C5AX46
А	497	PHE	TYR	engineered mutation	UNP C5AX46
А	568	GLY	SER	engineered mutation	UNP C5AX46
В	135	GLY	GLU	engineered mutation	UNP C5AX46
В	415	CYS	ALA	engineered mutation	UNP C5AX46
В	497	PHE	TYR	engineered mutation	UNP C5AX46
В	568	GLY	SER	engineered mutation	UNP C5AX46
С	135	GLY	GLU	engineered mutation	UNP C5AX46
С	415	CYS	ALA	engineered mutation	UNP C5AX46
С	497	PHE	TYR	engineered mutation	UNP C5AX46
С	568	GLY	SER	engineered mutation	UNP C5AX46
D	135	GLY	GLU	engineered mutation	UNP C5AX46



Chain	Residue	Modelled	Actual	Comment	Reference
D	415	CYS	ALA	engineered mutation	UNP C5AX46
D	497	PHE	TYR	engineered mutation	UNP C5AX46
D	568	GLY	SER	engineered mutation	UNP C5AX46
Е	135	GLY	GLU	engineered mutation	UNP C5AX46
Е	415	CYS	ALA	engineered mutation	UNP C5AX46
Е	497	PHE	TYR	engineered mutation	UNP C5AX46
Е	568	GLY	SER	engineered mutation	UNP C5AX46
F	135	GLY	GLU	engineered mutation	UNP C5AX46
F	415	CYS	ALA	engineered mutation	UNP C5AX46
F	497	PHE	TYR	engineered mutation	UNP C5AX46
F	568	GLY	SER	engineered mutation	UNP C5AX46
G	135	GLY	GLU	engineered mutation	UNP C5AX46
G	415	CYS	ALA	engineered mutation	UNP C5AX46
G	497	PHE	TYR	engineered mutation	UNP C5AX46
G	568	GLY	SER	engineered mutation	UNP C5AX46
Н	135	GLY	GLU	engineered mutation	UNP C5AX46
Н	415	CYS	ALA	engineered mutation	UNP C5AX46
Н	497	PHE	TYR	engineered mutation	UNP C5AX46
Н	568	GLY	SER	engineered mutation	UNP C5AX46

• Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	А	1	Total 26	C 12	N 4	O 7	Р 2	S 1	0	0



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Mol	Chain	Residues		Α	tom	ıs			ZeroOcc	AltConf		
0	Р	1	Total	С	Ν	0	Р	S	0	0		
	D	1	26	12	4	7	2	1	0	0		
9	С	C 1	Total	С	Ν	Ο	Р	$\mathbf{S}$	0	0		
	U		26	12	4	7	2	1	0	0		
9		П	Л	1	Total	С	Ν	Ο	Р	$\mathbf{S}$	0	0
	I	26	12	4	7	2	1	0	0			
9	9 F	E 1	Total	С	Ν	Ο	Р	$\mathbf{S}$	0	0		
	Ľ		26	12	4	7	2	1	0	0		
9	F	1	Total	С	Ν	Ο	Р	$\mathbf{S}$	0	0		
	T,	1	26	12	4	7	2	1	0	0		
9	С	1	Total	С	Ν	Ο	Р	S	0	0		
2 G	1	26	12	4	7	2	1	0	0			
2	Ч	1	Total	С	Ν	0	Р	S	0	0		
	Н	Η	1	26	12	4	7	2	1	U	U	

• Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf		
3 A	Λ	1	Total	С	Ν	Ο	Р	0	0		
	1	27	10	5	10	2	0	0			
3	3 B	В	1	Total	С	Ν	Ο	Р	0	0	
D D	1	27	10	5	10	2	0	0			
2	С	1	Total	С	Ν	Ο	Р	0	0		
0	U	1	27	10	5	10	2	0	0		
3	Л	D 1	Total	С	Ν	Ο	Р	0	0		
	D		27	10	5	10	2	0	U		



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Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
3	F	1	Total	С	Ν	Ο	Р	0	0
<u> </u>	T	27	10	5	10	2	0	0	
3	3 F	1	Total	С	Ν	Ο	Р	0	0
5 F	L	27	10	5	10	2	0	0	
2	С	1	Total	С	Ν	Ο	Р	0	0
3 G	1	27	10	5	10	2	0	0	
3	Ц	1	Total	С	Ν	Ο	Р	0	0
	П	1	27	10	5	10	2	0	U

#### • Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Mg 1 1	0	0
4	В	1	Total Mg 1 1	0	0
4	С	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	Е	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	Н	1	Total Mg 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	167	Total O 167 167	0	0
5	В	158	Total O 158 158	0	0
5	С	152	Total         O           152         152	0	0
5	D	146	Total         O           146         146	0	0
5	Е	159	Total O 159 159	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	171	Total O 171 171	0	0
5	G	166	Total O 166 166	0	0
5	Н	153	Total O 153 153	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. 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. 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: Putative oxalyl-CoA decarboxylase (Oxc, yfdU)



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• Molecule 1: Putative oxalyl-CoA decarboxylase (Oxc, yfdU)

Chain E:	86%	8% • 6%
MET THR VILL VILL VILL VILL CLN CLN VILA VILA VILA VILA VILA VILA VILA VILA	148 162 162 163 163 168 168 168 196 1146 1147 1147 1147 1147 1147 1147	Y179 Y179 D1180 D1180 X225 S226 S226 S226 S226 S226 S245
4249 L250 L268 P269 P269 P269 H303 H303 H303 H303 H303 H371 V345 V345 V345 V345 V345 V345 V345 V345	P380 D426 D426 1444 1444 E464 D466 D466 S465 C465 C465 C465 C465 C465 C466 C465 C466 C466	S566 E567 E567 G568 G1Y ASN ILE ASN ASN ASN PRO
LLVS LLVS LLVS LLVS SGLM		
• Molecule 1: Putative oxalyl-CoA	decarboxylase (Oxc, yfdU)	
Chain F:	85%	9% 6%
MET TAR VIA VIA VIA CUN CUN VIA VIA VIA VIA VIA VIA VIA VIA VIA	P44 1150 1150 152 152 152 153 153 153 153 153 153 153 113 113 113	S119 R124 D128 Q131 F151 F151
L180 D181 A209 A213 A213 A214 A214 A246 A246 A246 A246 A246 A246 A246 A24	1341 V345 W363 W363 W363 W371 W363 W439 W439 W439 W439 W439 W439 W439 W43	D501 D538 D538 D542 D545 D545 D545 C568 C1Y
ASN CLLE OLLE CLEU ASN PRO PRO PRO LLV SER LLVS LLVS		
• Molecule 1: Putative oxalyl-CoA	decarboxylase (Oxc, yfdU)	
Chain G:	87%	6% 6%
MET TAR VIA CLN CLN CLN CLN CLN ALA ALA ALA ALA ALA ALA ALA ALA ALA A	E70 G31 K86 K86 K86 K93 F96 F96 F96 F96 F126 F126 F126 F131 F135 F134 F134 F134 F134 F134 F134 F134 F134	A213 A213 L221 L221 A238 L250 L250 L250
L297 N298 W298 W298 H303 H303 H303 N330 N330 N330 N336 N330 N336 N336 N	v441 1444 1446 1446 1446 1446 1446 1446	SAT SAT SAT

• Molecule 1: Putative oxalyl-CoA decarboxylase (Oxc, yfdU)





## 1180 1181 1181 1181 1181 1287 4238 4238 4238 4238 4238 4238 4238 4333 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1341 1438 1438 1438 1438 1438 1438 1438 1448 1458 1458 1458 1458 1458 1458 1458



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	161.09Å 180.34Å 202.01Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	29.94 - 2.80	Depositor
Resolution (A)	29.94 - 2.80	EDS
% Data completeness	99.5 (29.94-2.80)	Depositor
(in resolution range)	99.8 (29.94-2.80)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	0.27	Depositor
$< I/\sigma(I) > 1$	$2.91 (at 2.80 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
P. P.	0.202 , $0.232$	Depositor
$n, n_{free}$	0.205 , $0.233$	DCC
$R_{free}$ test set	1996 reflections $(1.38\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	28.7	Xtriage
Anisotropy	1.392	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$   <  L  > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	34264	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 57.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3297e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: ADP, MG, TPP

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	Bond lengths		angles
		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.25	0/4143	0.43	0/5620
1	В	0.25	0/4135	0.44	0/5609
1	С	0.25	0/4143	0.44	0/5620
1	D	0.25	0/4135	0.44	0/5609
1	Е	0.25	0/4135	0.44	0/5609
1	F	0.25	0/4135	0.44	0/5609
1	G	0.25	0/4160	0.43	0/5643
1	Н	0.25	0/4160	0.43	0/5643
All	All	0.25	0/33146	0.44	0/44962

There are no bond length outliers.

There are no bond angle outliers.

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	4069	0	4145	28	0
1	В	4064	0	4141	28	0
1	С	4069	0	4145	21	0
1	D	4064	0	4141	26	0
1	Е	4064	0	4141	32	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4064	0	4141	31	0
1	G	4083	0	4154	24	0
1	Н	4083	0	4154	23	0
2	А	26	0	16	4	0
2	В	26	0	16	2	0
2	С	26	0	16	2	0
2	D	26	0	16	2	0
2	Е	26	0	16	2	0
2	F	26	0	16	3	0
2	G	26	0	16	2	0
2	Н	26	0	16	1	0
3	А	27	0	12	0	0
3	В	27	0	12	1	0
3	С	27	0	12	0	0
3	D	27	0	12	0	0
3	Ε	27	0	12	2	0
3	F	27	0	12	1	0
3	G	27	0	12	0	0
3	Η	27	0	12	0	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
4	$\mathbf{C}$	1	0	0	0	0
4	D	1	0	0	0	0
4	Ε	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	Н	1	0	0	0	0
5	А	167	0	0	1	0
5	В	158	0	0	2	0
5	С	152	0	0	3	0
5	D	146	0	0	1	0
5	Ε	159	0	0	2	0
5	F	171	0	0	1	0
5	G	166	0	0	1	0
5	Н	153	0	0	0	0
All	All	$34\overline{264}$	0	33386	198	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 3.

All (198) 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:G:298:ASN:HD21	1:G:300:LEU:HD12	1.61	0.66
1:G:48:ILE:O	1:G:93:VAL:HG22	1.97	0.64
1:C:127:VAL:HG22	1:C:136:GLU:HG3	1.81	0.62
1:G:316:ARG:NH2	5:G:704:HOH:O	2.32	0.62
1:E:35:LYS:HG2	1:E:62:LEU:HD21	1.82	0.62
1:E:341:ILE:HG13	3:E:602:ADP:C2	2.36	0.61
1:C:346:GLU:OE1	5:C:701:HOH:O	2.16	0.60
1:E:95:ALA:HB3	1:E:96:PRO:HD3	1.84	0.60
1:E:278:ALA:HB3	1:E:371:ARG:HG3	1.82	0.60
1:E:48:ILE:O	1:E:93:VAL:HG22	2.01	0.60
1:A:127:VAL:HG22	1:A:136:GLU:HG3	1.85	0.59
1:F:124:ARG:NH1	1:F:128:ASP:OD1	2.35	0.59
1:F:48:ILE:O	1:F:93:VAL:HG22	2.02	0.59
1:B:209:ALA:HB3	1:G:213:ALA:HB2	1.85	0.59
1:C:48:ILE:O	1:C:93:VAL:HG22	2.03	0.59
1:B:278:ALA:HB3	1:B:371:ARG:HG3	1.84	0.58
1:E:96:PRO:HG3	1:H:439:TRP:HB3	1.85	0.58
1:E:96:PRO:HB3	1:H:441:VAL:HG22	1.86	0.58
1:F:439:TRP:HB3	1:G:96:PRO:HG3	1.86	0.57
1:G:95:ALA:HB3	1:G:96:PRO:HD3	1.85	0.57
1:E:226:SER:OG	1:E:316:ARG:NH2	2.37	0.57
1:C:274:LEU:HD23	1:C:364:LEU:HD21	1.87	0.56
1:E:501:ASP:OD2	1:H:55:ARG:NH2	2.37	0.56
1:B:48:ILE:O	1:B:93:VAL:HG22	2.06	0.56
1:A:152:ARG:HB3	1:G:128:ASP:HB3	1.87	0.56
1:D:209:ALA:HB3	1:H:213:ALA:HB2	1.88	0.56
1:F:278:ALA:HB3	1:F:371:ARG:HG3	1.88	0.55
1:F:96:PRO:HB3	1:G:441:VAL:HG22	1.87	0.55
1:H:238:ALA:HA	1:H:341:ILE:HD13	1.88	0.55
1:D:541:LYS:NZ	1:D:545:ASP:OD2	2.37	0.54
1:A:133:ASP:OD1	1:A:134:TYR:N	2.40	0.54
1:C:96:PRO:HB3	1:D:441:VAL:HG22	1.89	0.54
1:B:213:ALA:HB2	1:G:209:ALA:HB3	1.90	0.54
1:F:316:ARG:NH1	5:F:709:HOH:O	2.40	0.54
1:G:238:ALA:HA	1:G:341:ILE:HD13	1.89	0.53
1:G:466:ASP:OD1	1:G:466:ASP:N	2.38	0.53
1:G:278:ALA:O	1:G:374:ASN:ND2	2.41	0.53
1:H:368:ARG:O	1:H:372:GLU:HG2	2.08	0.53
1:A:213:ALA:HB2	1:F:209:ALA:HB3	1.91	0.53
2:H:601:TPP:HN42	2:H:601:TPP:C2	2.22	0.53
1:E:250:LEU:HD22	1:E:345:VAL:HG13	1.91	0.52
1:D:48:ILE:O	1:D:93:VAL:HG22	2.08	0.52



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:278:ALA:HB3	1:D:371:ARG:HG3	1.91	0.52
2:B:601:TPP:HN42	2:B:601:TPP:C2	2.22	0.52
1:C:133:ASP:OD1	1:C:134:TYR:N	2.41	0.52
1:B:431:ARG:NH2	5:B:712:HOH:O	2.42	0.52
1:A:209:ALA:HB3	1:F:213:ALA:HB2	1.92	0.52
1:D:174:ARG:HH12	1:D:326:GLU:HG2	1.75	0.51
1:B:133:ASP:OD1	1:B:134:TYR:N	2.44	0.51
1:F:466:ASP:OD1	1:F:466:ASP:N	2.43	0.51
1:B:498:ARG:HH11	1:B:567:GLU:HB2	1.76	0.51
1:D:174:ARG:NH1	1:D:326:GLU:HG2	2.26	0.51
1:C:362:ASN:OD1	1:C:362:ASN:N	2.42	0.50
1:A:274:LEU:HD23	1:A:364:LEU:HD11	1.94	0.50
1:B:129:LEU:HD23	1:F:151:PHE:HB3	1.92	0.50
1:E:225:LYS:NZ	1:E:355:ASP:OD2	2.43	0.50
1:F:231:LEU:HD11	1:F:259:VAL:HG23	1.93	0.50
2:C:601:TPP:C2	2:C:601:TPP:HN42	2.24	0.49
1:F:538:ASP:HB3	1:F:542:ARG:NH1	2.27	0.49
1:A:259:VAL:HG11	1:A:280:ARG:HG3	1.94	0.49
1:A:221:LEU:HD11	1:A:351:GLY:HA3	1.95	0.49
1:B:221:LEU:HD11	1:B:351:GLY:HA3	1.95	0.49
1:C:296:ARG:NH1	5:C:706:HOH:O	2.32	0.48
1:F:248:ARG:HG3	1:F:268:LEU:HG	1.96	0.48
1:C:278:ALA:HB3	1:C:371:ARG:HG3	1.94	0.48
1:E:466:ASP:OD1	1:E:466:ASP:N	2.44	0.48
1:F:501:ASP:OD2	1:G:55:ARG:NH2	2.47	0.48
2:F:601:TPP:C2	2:F:601:TPP:HN42	2.25	0.48
1:D:350:ASP:OD1	5:D:701:HOH:O	2.20	0.48
1:E:248:ARG:HA	1:E:268:LEU:HD11	1.96	0.48
2:G:601:TPP:C2	2:G:601:TPP:HN42	2.27	0.48
2:A:601:TPP:HN42	2:A:601:TPP:C2	2.27	0.47
1:F:43:TYR:O	1:F:90:CYS:HA	2.14	0.47
1:F:541:LYS:NZ	1:F:545:ASP:OD2	2.43	0.47
1:H:91:LEU:HA	1:H:118:ILE:O	2.14	0.47
1:C:466:ASP:N	1:C:466:ASP:OD1	2.45	0.47
1:E:464:GLU:HB2	1:E:490:ILE:HD13	1.96	0.47
1:E:467:SER:HB3	2:E:601:TPP:PA	2.54	0.47
1:F:496:ILE:HG23	2:F:601:TPP:H62	1.97	0.47
1:F:179:TYR:CE2	1:F:181:ASP:HB2	2.50	0.47
1:A:278:ALA:HB3	1:A:371:ARG:HG3	1.96	0.47
1:A:179:TYR:CE2	1:A:181:ASP:HB2	2.50	0.46
1:F:341:ILE:HG13	3:F:602:ADP:C2	2.50	0.46



	<b>A A A</b>	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:G:133:ASP:OD1	1:G:134:TYR:N	2.45	0.46	
1:D:79:ILE:HG21	1:D:448:PHE:HA	1.96	0.46	
1:A:496:ILE:HG23	2:A:601:TPP:H62	1.96	0.46	
1:B:405:ARG:NE	5:B:701:HOH:O	2.47	0.46	
1:B:464:GLU:HB2	1:B:490:ILE:HD13	1.97	0.46	
2:D:601:TPP:HN42	2:D:601:TPP:C2	2.28	0.46	
1:D:79:ILE:HD11	1:D:434:LEU:HD22	1.98	0.46	
1:D:464:GLU:HB2	1:D:490:ILE:HD13	1.97	0.46	
1:F:464:GLU:HB2	1:F:490:ILE:HD13	1.97	0.46	
1:A:467:SER:HB3	2:A:601:TPP:PA	2.56	0.46	
1:H:466:ASP:N	1:H:466:ASP:OD1	2.47	0.46	
2:E:601:TPP:HN42	2:E:601:TPP:C2	2.27	0.46	
1:H:50:ILE:HG12	1:H:92:THR:O	2.16	0.46	
1:B:43:TYR:O	1:B:90:CYS:HA	2.15	0.46	
1:B:76:ALA:HB1	1:B:451:ALA:HB2	1.97	0.46	
1:E:81:GLY:HA2	1:E:86:LYS:O	2.16	0.46	
1:A:66:SER:HB2	1:A:481:ARG:HH22	1.81	0.46	
1:C:524:MET:CE	1:C:555:LEU:HB2	2.46	0.45	
1:F:467:SER:HB3	2:F:601:TPP:PA	2.56	0.45	
1:B:79:ILE:HD12	1:B:79:ILE:HA	1.78	0.45	
1:E:43:TYR:O	1:E:90:CYS:HA	2.16	0.45	
1:D:76:ALA:HB1	1:D:451:ALA:HB2	1.97	0.45	
1:B:168:ARG:NH1	1:B:204:ILE:O	2.47	0.45	
1:H:81:GLY:HA2	1:H:86:LYS:O	2.17	0.45	
1:A:40:GLU:OE2	5:A:701:HOH:O	2.20	0.45	
1:B:122:SER:OG	1:B:134:TYR:O	2.22	0.45	
1:G:81:GLY:HA2	1:G:86:LYS:O	2.17	0.45	
1:E:441:VAL:HG22	1:H:96:PRO:HB3	1.98	0.44	
1:A:238:ALA:HA	1:A:341:ILE:HD13	1.99	0.44	
1:B:105:LEU:HD13	1:B:117:LEU:HB2	1.98	0.44	
1:E:93:VAL:HB	5:E:702:HOH:O	2.17	0.44	
1:G:417:THR:OG1	2:G:601:TPP:O2B	2.33	0.44	
1:H:69:HIS:HB3	1:H:72:ASN:ND2	2.33	0.44	
1:H:278:ALA:O	1:H:374:ASN:ND2	2.36	0.44	
1:D:91:LEU:HA	1:D:118:ILE:O	2.16	0.44	
1:D:467:SER:HB3	2:D:601:TPP:PA	2.56	0.44	
1:C:179:TYR:CE2	1:C:181:ASP:HB2	2.52	0.44	
1:C:297:LEU:O	1:C:303:HIS:HA	2.18	0.44	
1:H:110:THR:HG22	1:H:438:THR:HB	1.99	0.44	
1:H:121:SER:OG	1:H:181:ASP:OD2	2.34	0.44	
1:F:131:GLN:HB3	1:G:330:ASN:OD1	2.18	0.44	



	i agem	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:50:ILE:HD13	1:B:91:LEU:HG	1.98	0.43		
1:F:270:ASP:HB2	1:F:426:ASP:HB3	1.99	0.43		
1:A:79:ILE:HG12	1:A:434:LEU:HD13	2.00	0.43		
1:E:497:PHE:HB3	1:E:567:GLU:HA	1.99	0.43		
1:B:466:ASP:N	1:B:466:ASP:OD1	2.50	0.43		
1:H:297:LEU:O	1:H:303:HIS:HA	2.17	0.43		
1:G:221:LEU:HD11	1:G:351:GLY:HA3	1.99	0.43		
1:G:250:LEU:HD22	1:G:345:VAL:HG13	2.01	0.43		
1:A:217:ILE:HG23	1:A:348:LEU:HD23	2.00	0.43		
1:B:238:ALA:HB2	1:B:293:VAL:HG12	2.00	0.43		
1:D:133:ASP:OD1	1:D:134:TYR:N	2.49	0.43		
1:E:270:ASP:HB2	1:E:426:ASP:HB3	2.00	0.43		
1:F:92:THR:HG1	1:F:119:SER:HG	1.61	0.43		
1:A:126:ILE:HG23	1:A:131:GLN:HB2	2.00	0.43		
1:E:322:ILE:HB	3:E:602:ADP:C2	2.54	0.43		
1:G:126:ILE:HG23	1:G:131:GLN:HB2	2.01	0.43		
1:G:409:ILE:HD11	1:G:456:THR:HG21	2.00	0.43		
1:C:330:ASN:OD1	1:D:131:GLN:HB3	2.19	0.43		
1:D:323:GLU:HG3	1:D:325:ARG:H	1.84	0.43		
1:E:514:PHE:HA	1:H:481:ARG:HD3	2.02	0.42		
1:F:50:ILE:HD13	1:F:91:LEU:HG	2.01	0.42		
1:D:81:GLY:HA2	1:D:86:LYS:O	2.19	0.42		
1:G:297:LEU:O	1:G:303:HIS:HA	2.20	0.42		
1:E:248:ARG:HG3	1:E:268:LEU:HG	2.02	0.42		
1:B:521:ASP:OD1	1:B:521:ASP:N	2.52	0.42		
1:D:129:LEU:HD23	1:E:151:PHE:HB3	1.99	0.42		
1:D:179:TYR:CE2	1:D:181:ASP:HB2	2.53	0.42		
1:H:166:ALA:HA	1:H:178:VAL:HG11	2.01	0.42		
1:A:409:ILE:HD11	1:A:456:THR:HG21	2.02	0.42		
1:B:139:GLN:NE2	1:B:179:TYR:OH	2.52	0.42		
1:E:498:ARG:HH21	1:E:566:SER:HA	1.84	0.42		
1:A:91:LEU:HA	1:A:118:ILE:O	2.19	0.42		
1:E:377:LYS:O	1:E:380:PRO:HD2	2.19	0.42		
1:H:43:TYR:O	1:H:90:CYS:HA	2.20	0.42		
1:C:464:GLU:HB2	1:C:490:ILE:HD13	2.01	0.42		
1:E:297:LEU:O	1:E:303:HIS:HA	2.20	0.42		
1:F:267:LEU:HA	1:F:430:PRO:HG3	2.02	0.42		
1:B:495:GLY:HA2	1:B:514:PHE:CD2	2.55	0.42		
1:C:68:ARG:NH1	1:D:466:ASP:O	2.53	0.42		
1:C:124:ARG:HD2	5:C:731:HOH:O	2.19	0.42		
1:D:496:ILE:HB	1:D:512:THR:HB	2.02	0.41		



	A + 0	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:245:GLU:OE2	5:E:701:HOH:O	2.22	0.41	
1:F:250:LEU:HD22	1:F:345:VAL:HG13	2.01	0.41	
1:F:82:PHE:HB2	1:F:113:PHE:CD1	2.55	0.41	
1:G:278:ALA:HB3	1:G:371:ARG:HG3	2.02	0.41	
1:A:225:LYS:NZ	1:A:355:ASP:O	2.43	0.41	
1:C:238:ALA:HA	1:C:341:ILE:HD13	2.02	0.41	
1:B:467:SER:HB3	2:B:601:TPP:PA	2.60	0.41	
1:C:467:SER:HB3	2:C:601:TPP:PA	2.61	0.41	
1:D:221:LEU:HD11	1:D:351:GLY:HA3	2.02	0.41	
1:D:498:ARG:HG3	1:D:567:GLU:OE2	2.21	0.41	
1:E:131:GLN:HB3	1:H:330:ASN:OD1	2.20	0.41	
1:F:98:PHE:CZ	1:F:102:LEU:HD22	2.56	0.41	
1:A:76:ALA:HB1	1:A:451:ALA:HB2	2.03	0.41	
1:B:409:ILE:HD11	1:B:456:THR:HG21	2.02	0.41	
1:C:152:ARG:HD2	1:H:128:ASP:OD2	2.20	0.41	
1:E:179:TYR:CE2	1:E:181:ASP:HB2	2.55	0.41	
1:E:105:LEU:HD13	1:E:117:LEU:HB2	2.03	0.41	
1:D:521:ASP:OD1	1:D:521:ASP:N	2.53	0.41	
1:G:70:GLU:HB2	1:G:100:ASN:HB2	2.02	0.40	
1:B:322:ILE:HB	3:B:602:ADP:C2	2.56	0.40	
1:H:31:ILE:HD12	1:H:57:ALA:HB2	2.03	0.40	
1:A:48:ILE:HA	1:A:49:PRO:HA	1.93	0.40	
1:A:131:GLN:HB3	1:B:330:ASN:OD1	2.21	0.40	
1:A:140:LEU:O	1:A:144:LYS:HG3	2.21	0.40	
1:A:415:CYS:HB3	2:A:601:TPP:O2B	2.21	0.40	
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.94	0.40	
1:F:52:ASP:OD1	1:F:55:ARG:NH1	2.55	0.40	
1:F:229:ARG:HB3	1:F:363:TRP:CD2	2.56	0.40	
1:A:33:ALA:HB2	1:A:200:LEU:HD22	2.04	0.40	
1:C:497:PHE:CD2	1:C:567:GLU:HG2	2.56	0.40	
1:A:119:SER:HB2	1:A:179:TYR:HE1	1.87	0.40	
1:D:495:GLY:HA2	1:D:514:PHE:CD2	2.57	0.40	
1:H:179:TYR:CE2	1:H:181:ASP:HB2	2.57	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	ntiles
1	А	547/583~(94%)	532 (97%)	14 (3%)	1 (0%)	47	78
1	В	546/583~(94%)	528~(97%)	17 (3%)	1 (0%)	47	78
1	С	547/583~(94%)	533~(97%)	13 (2%)	1 (0%)	47	78
1	D	546/583~(94%)	$531 \ (97\%)$	14 (3%)	1 (0%)	47	78
1	Е	546/583~(94%)	534 (98%)	11 (2%)	1 (0%)	47	78
1	F	546/583~(94%)	533~(98%)	12 (2%)	1 (0%)	47	78
1	G	549/583~(94%)	532 (97%)	16 (3%)	1 (0%)	47	78
1	Н	549/583~(94%)	533~(97%)	15 (3%)	1 (0%)	47	78
All	All	4376/4664~(94%)	4256 (97%)	112 (3%)	8 (0%)	47	78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	95	ALA
1	В	95	ALA
1	С	95	ALA
1	D	95	ALA
1	Е	95	ALA
1	F	95	ALA
1	G	95	ALA
1	Н	95	ALA

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	425/452~(94%)	422~(99%)	3~(1%)	84	95
1	В	424/452~(94%)	422 (100%)	2~(0%)	88	96
1	С	425/452~(94%)	420 (99%)	5 (1%)	71	92
1	D	424/452~(94%)	422 (100%)	2 (0%)	88	96
1	Ε	424/452~(94%)	420 (99%)	4 (1%)	78	94
1	F	424/452~(94%)	422 (100%)	2~(0%)	88	96
1	G	427/452~(94%)	423~(99%)	4 (1%)	78	94
1	Η	427/452~(94%)	424 (99%)	3(1%)	84	95
All	All	3400/3616~(94%)	3375~(99%)	25 (1%)	84	95

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	44	ASN
1	А	364	LEU
1	А	524	MET
1	В	93	VAL
1	В	388	PRO
1	С	44	ASN
1	С	93	VAL
1	С	221	LEU
1	С	364	LEU
1	С	508	ASP
1	D	44	ASN
1	D	93	VAL
1	Е	44	ASN
1	Е	93	VAL
1	Е	444	ILE
1	Е	567	GLU
1	F	44	ASN
1	F	93	VAL
1	G	93	VAL
1	G	307	LYS
1	G	444	ILE
1	G	567	GLU
1	Н	93	VAL
1	Н	94	SER
1	Н	567	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are



no such sidechains identified.

#### 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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	Type	Chain	Dog	Link	Bo	Bond lengths			ond ang	les
WIOI	туре	Ullalli	1105		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	В	602	-	$24,\!29,\!29$	1.67	3 (12%)	29,45,45	2.24	6 (20%)
2	TPP	F	601	4	$22,\!27,\!27$	2.32	4 (18%)	29,40,40	1.72	7 (24%)
2	TPP	Н	601	4	$22,\!27,\!27$	2.33	3 (13%)	29,40,40	1.74	7 (24%)
3	ADP	А	602	-	$24,\!29,\!29$	1.68	3 (12%)	$29,\!45,\!45$	2.20	6 (20%)
2	TPP	А	601	4	$22,\!27,\!27$	2.31	3 (13%)	29,40,40	1.74	7 (24%)
3	ADP	D	602	-	$24,\!29,\!29$	1.64	3 (12%)	$29,\!45,\!45$	2.20	7 (24%)
2	TPP	D	601	4	$22,\!27,\!27$	2.32	3 (13%)	29,40,40	1.74	7 (24%)
2	TPP	Ε	601	4	$22,\!27,\!27$	2.32	4 (18%)	29,40,40	1.71	7 (24%)
3	ADP	G	602	-	$24,\!29,\!29$	1.66	3 (12%)	$29,\!45,\!45$	2.22	7 (24%)
2	TPP	В	601	4	$22,\!27,\!27$	2.35	3 (13%)	29,40,40	1.75	7 (24%)
2	TPP	С	601	4	22,27,27	2.31	3 (13%)	29,40,40	1.73	7 (24%)
3	ADP	F	602	-	24,29,29	1.68	3 (12%)	29,45,45	2.21	7 (24%)



Mol Type C	Chain	Dec	Tiple	Bo	ond leng	Bond angles				
INIOI	туре	Chan	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	TPP	G	601	4	22,27,27	2.35	4 (18%)	29,40,40	1.73	7 (24%)
3	ADP	Е	602	-	24,29,29	1.67	3 (12%)	29,45,45	2.24	6 (20%)
3	ADP	С	602	-	24,29,29	1.69	3 (12%)	29,45,45	2.22	7 (24%)
3	ADP	Н	602	-	24,29,29	1.62	3 (12%)	29,45,45	2.25	6 (20%)

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
3	ADP	В	602	-	-	2/12/32/32	0/3/3/3
2	TPP	F	601	4	-	2/16/17/17	0/2/2/2
2	TPP	Н	601	4	-	2/16/17/17	0/2/2/2
3	ADP	А	602	-	-	2/12/32/32	0/3/3/3
2	TPP	А	601	4	-	4/16/17/17	0/2/2/2
3	ADP	D	602	-	-	3/12/32/32	0/3/3/3
2	TPP	D	601	4	-	3/16/17/17	0/2/2/2
2	TPP	Е	601	4	-	3/16/17/17	0/2/2/2
3	ADP	G	602	-	-	2/12/32/32	0/3/3/3
2	TPP	В	601	4	-	5/16/17/17	0/2/2/2
2	TPP	С	601	4	-	5/16/17/17	0/2/2/2
3	ADP	F	602	-	-	2/12/32/32	0/3/3/3
2	TPP	G	601	4	-	4/16/17/17	0/2/2/2
3	ADP	Е	602	-	-	2/12/32/32	0/3/3/3
3	ADP	С	602	-	-	3/12/32/32	0/3/3/3
3	ADP	Н	602	-	-	3/12/32/32	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	С	601	TPP	C4-N3	-7.57	1.33	1.39
2	Ε	601	TPP	C4-N3	-7.55	1.33	1.39
2	А	601	TPP	C4-N3	-7.53	1.33	1.39
2	В	601	TPP	C4-N3	-7.53	1.33	1.39
2	F	601	TPP	C4-N3	-7.50	1.33	1.39
2	G	601	TPP	C4-N3	-7.47	1.33	1.39
2	D	601	TPP	C4-N3	-7.47	1.33	1.39



 $\mathbf{Mol}$ 2

3

3

3

3

3

Atoms	Z	Observed(Å)	Ideal(Å)
C4-N3	-7.41	1.33	1.39
PA-05'	6.26	1.84	1.59
PA-05'	6.19	1.84	1.59
PA-05'	6.19	1.84	1.59
PA-05'	6.18	1.84	1.59
PA-05'	6.15	1.84	1.59
PA-05'	6.09	1.84	1.59
PA-05'	5.99	1.83	1.59
PA-05'	5.92	1.83	1.59
C4'-N4'	4.52	1.45	1.34
C4'-N4'	4.51	1.45	1.34
C4'-N4'	4.51	1.45	1.34
C4'-N4'	4.51	1.45	1.34
C4'-N4'	4.51	1.45	1.34
C4'-N4'	4.50	1.45	1.34
C4'-N4'	4.48	1.45	1.34
C4'-N4'	4.45	1.45	1.34
C6-C5	4.28	1.52	1.50
C6-C5	4.17	1.52	1.50
C6-C5	4.08	1.52	1.50
C6-C5	4.02	1.52	1.50
C6-C5	3.97	1.52	1.50
CG CE	2 00	1 59	1 50

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Res

601

602

602

602

602

602

Type

TPP

ADP

ADP

ADP

ADP

ADP

Chain

Н

А

Е

F

С

G

3	В	602	ADP	PA-O5'	6.09	1.84	1.59
3	D	602	ADP	PA-05'	5.99	1.83	1.59
3	Н	602	ADP	PA-05'	5.92	1.83	1.59
2	С	601	TPP	C4'-N4'	4.52	1.45	1.34
2	В	601	TPP	C4'-N4'	4.51	1.45	1.34
2	А	601	TPP	C4'-N4'	4.51	1.45	1.34
2	Н	601	TPP	C4'-N4'	4.51	1.45	1.34
2	D	601	TPP	C4'-N4'	4.51	1.45	1.34
2	G	601	TPP	C4'-N4'	4.50	1.45	1.34
2	Ε	601	TPP	C4'-N4'	4.48	1.45	1.34
2	F	601	TPP	C4'-N4'	4.45	1.45	1.34
2	G	601	TPP	C6-C5	4.28	1.52	1.50
2	В	601	TPP	C6-C5	4.17	1.52	1.50
2	Н	601	TPP	C6-C5	4.08	1.52	1.50
2	D	601	TPP	C6-C5	4.02	1.52	1.50
2	F	601	TPP	C6-C5	3.97	1.52	1.50
2	А	601	TPP	C6-C5	3.88	1.52	1.50
2	Е	601	TPP	C6-C5	3.84	1.52	1.50
2	С	601	TPP	C6-C5	3.78	1.52	1.50
3	С	602	ADP	O5'-C5'	-2.37	1.35	1.44
3	В	602	ADP	O5'-C5'	-2.33	1.35	1.44
3	Н	602	ADP	O5'-C5'	-2.29	1.36	1.44
3	D	602	ADP	O5'-C5'	-2.28	1.36	1.44
3	Е	602	ADP	O5'-C5'	-2.27	1.36	1.44
3	G	602	ADP	O5'-C5'	-2.27	1.36	1.44
3	А	602	ADP	O5'-C5'	-2.26	1.36	1.44
3	F	602	ADP	O5'-C5'	-2.20	1.36	1.44
3	А	602	ADP	C2-N1	2.14	1.37	1.33
3	С	602	ADP	C2-N1	2.13	1.37	1.33
3	Е	602	ADP	C2-N1	2.11	1.37	1.33
3	G	602	ADP	C2-N1	2.08	1.37	1.33
3	F	602	ADP	C2-N1	2.08	1.37	1.33
3	В	602	ADP	C2-N1	2.06	1.37	1.33
2	G	601	TPP	C5'-C4'	-2.04	1.39	1.42
3	Н	602	ADP	C2-N1	2.03	1.37	1.33
2	Е	601	TPP	C5'-C4'	-2.03	1.39	1.42
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Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)	
3	D	602	ADP	C2-N1	2.03	1.37	1.33	
2	F	601	TPP	C5'-C4'	-2.01	1.39	1.42	

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	F	602	ADP	PA-O3A-PB	-7.67	106.49	132.83
3	Е	602	ADP	PA-O3A-PB	-7.67	106.49	132.83
3	Н	602	ADP	PA-O3A-PB	-7.65	106.57	132.83
3	G	602	ADP	PA-O3A-PB	-7.63	106.65	132.83
3	С	602	ADP	PA-O3A-PB	-7.61	106.72	132.83
3	В	602	ADP	PA-O3A-PB	-7.60	106.75	132.83
3	D	602	ADP	PA-O3A-PB	-7.49	107.12	132.83
3	А	602	ADP	PA-O3A-PB	-7.47	107.21	132.83
3	Н	602	ADP	O5'-PA-O1A	-5.08	89.22	109.07
3	В	602	ADP	O5'-PA-O1A	-5.07	89.27	109.07
3	А	602	ADP	O5'-PA-O1A	-5.05	89.32	109.07
3	Е	602	ADP	O5'-PA-O1A	-5.02	89.47	109.07
2	G	601	TPP	C5-C4-N3	4.57	116.72	107.57
2	Е	601	TPP	C5-C4-N3	4.54	116.65	107.57
2	В	601	TPP	C5-C4-N3	4.53	116.64	107.57
2	С	601	TPP	C5-C4-N3	4.53	116.63	107.57
2	D	601	TPP	C5-C4-N3	4.52	116.61	107.57
2	F	601	TPP	C5-C4-N3	4.52	116.61	107.57
2	Н	601	TPP	C5-C4-N3	4.51	116.59	107.57
2	А	601	TPP	C5-C4-N3	4.50	116.58	107.57
3	F	602	ADP	O3B-PB-O2B	4.44	124.62	107.64
3	С	602	ADP	O3B-PB-O2B	4.43	124.57	107.64
3	D	602	ADP	O3B-PB-O2B	4.43	124.56	107.64
3	G	602	ADP	O3B-PB-O2B	4.40	124.45	107.64
3	С	602	ADP	O2A-PA-O5'	-4.11	88.64	107.75
3	G	602	ADP	O2A-PA-O5'	-4.01	89.10	107.75
3	F	602	ADP	O2A-PA-O5'	-3.96	89.34	107.75
3	D	602	ADP	O2A-PA-O5'	-3.88	89.70	107.75
2	В	601	TPP	CM4-C4-C5	-3.61	119.71	127.60
3	Е	602	ADP	O2B-PB-O1B	3.57	124.66	110.68
2	D	601	TPP	CM4-C4-C5	-3.55	119.84	127.60
3	Н	602	ADP	O2B-PB-O1B	3.54	124.55	110.68
3	В	602	ADP	O2B-PB-O1B	3.54	124.54	110.68
3	А	602	ADP	O2B-PB-O1B	3.52	124.48	110.68
2	Н	601	TPP	CM4-C4-C5	-3.52	119.90	127.60
2	G	601	TPP	CM4-C4-C5	-3.46	120.03	127.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Е	601	TPP	CM4-C4-C5	-3.45	120.06	127.60
2	F	601	TPP	CM4-C4-C5	-3.41	120.14	127.60
2	А	601	TPP	CM4-C4-C5	-3.38	120.22	127.60
2	С	601	TPP	CM4-C4-C5	-3.35	120.27	127.60
3	В	602	ADP	O3B-PB-O3A	-3.12	94.18	104.64
3	Н	602	ADP	O3B-PB-O3A	-3.08	94.29	104.64
3	F	602	ADP	O3A-PB-O1B	-3.05	94.27	111.19
3	D	602	ADP	O3A-PB-O1B	-3.04	94.33	111.19
3	Ε	602	ADP	O3B-PB-O3A	-3.03	94.46	104.64
3	G	602	ADP	O3A-PB-O1B	-3.03	94.36	111.19
3	С	602	ADP	O3A-PB-O1B	-3.03	94.36	111.19
2	С	601	TPP	C6'-N1'-C2'	3.00	121.06	115.96
2	G	601	TPP	PA-O3A-PB	-2.99	122.57	132.83
2	С	601	TPP	PA-O3A-PB	-2.99	122.58	132.83
2	А	601	TPP	C6'-N1'-C2'	2.98	121.04	115.96
3	А	602	ADP	O3B-PB-O3A	-2.97	94.66	104.64
2	F	601	TPP	PA-O3A-PB	-2.94	122.74	132.83
2	D	601	TPP	C6'-N1'-C2'	2.92	120.94	115.96
2	Н	601	TPP	C6'-N1'-C2'	2.91	120.92	115.96
2	F	601	TPP	C6'-N1'-C2'	2.89	120.88	115.96
2	В	601	TPP	C6'-N1'-C2'	2.88	120.86	115.96
2	А	601	TPP	PA-O3A-PB	-2.86	123.00	132.83
2	Н	601	TPP	PA-O3A-PB	-2.86	123.01	132.83
2	G	601	TPP	C6'-N1'-C2'	2.86	120.83	115.96
2	Ε	601	TPP	C6'-N1'-C2'	2.84	120.80	115.96
2	D	601	TPP	PA-O3A-PB	-2.80	123.21	132.83
2	В	601	TPP	PA-O3A-PB	-2.76	123.37	132.83
3	Ε	602	ADP	PA-O5'-C5'	-2.70	105.86	121.68
3	С	602	ADP	PA-O5'-C5'	-2.68	105.95	121.68
2	Ε	601	TPP	PA-O3A-PB	-2.68	123.62	132.83
3	F	602	ADP	PA-O5'-C5'	-2.67	106.01	121.68
3	Η	602	ADP	PA-O5'-C5'	-2.66	106.09	121.68
3	G	602	ADP	PA-O5'-C5'	-2.64	106.21	121.68
3	A	602	ADP	PA-O5'-C5'	-2.63	106.24	121.68
2	Н	601	TPP	C7'-N3-C2	-2.63	120.59	125.35
2	G	601	TPP	C7'-N3-C2	-2.63	120.60	125.35
3	D	602	ADP	PA-O5'-C5'	-2.63	106.26	121.68
3	В	602	ADP	PA-O5'-C5'	-2.60	106.41	121.68
2	A	601	TPP	C7'-N3-C2	-2.58	120.68	125.35
2	D	601	TPP	C7'-N3-C2	-2.57	120.70	125.35
2	Н	601	TPP	N1'-C2'-N3'	-2.54	121.17	125.54
2	F	601	TPP	C7'-N3-C2	-2.53	120.79	125.35



Mol	Chain	$\mathbf{Res}$	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	G	601	TPP	N1'-C2'-N3'	-2.51	121.21	125.54
2	В	601	TPP	C7'-N3-C2	-2.50	120.83	125.35
2	Ε	601	TPP	C7'-N3-C2	-2.50	120.83	125.35
2	С	601	TPP	N1'-C2'-N3'	-2.48	121.27	125.54
2	F	601	TPP	N1'-C2'-N3'	-2.45	121.32	125.54
2	Е	601	TPP	N1'-C2'-N3'	-2.44	121.35	125.54
2	С	601	TPP	C7'-N3-C2	-2.42	120.97	125.35
2	А	601	TPP	N1'-C2'-N3'	-2.41	121.40	125.54
2	В	601	TPP	N1'-C2'-N3'	-2.40	121.41	125.54
2	D	601	TPP	N1'-C2'-N3'	-2.36	121.47	125.54
2	А	601	TPP	C5'-C6'-N1'	-2.34	119.93	123.82
2	С	601	TPP	C5'-C6'-N1'	-2.31	119.97	123.82
2	D	601	TPP	C5'-C6'-N1'	-2.27	120.03	123.82
2	В	601	TPP	C5'-C6'-N1'	-2.25	120.07	123.82
2	F	601	TPP	C5'-C6'-N1'	-2.23	120.11	123.82
3	D	602	ADP	O5'-PA-O1A	-2.20	100.46	109.07
2	Ε	601	TPP	C5'-C6'-N1'	-2.20	120.16	123.82
3	А	602	ADP	C2-N1-C6	-2.19	115.00	118.75
3	С	602	ADP	C2-N1-C6	-2.19	115.01	118.75
3	С	602	ADP	O5'-PA-O1A	-2.19	100.52	109.07
3	G	602	ADP	O5'-PA-O1A	-2.19	100.53	109.07
3	В	602	ADP	C2-N1-C6	-2.15	115.07	118.75
2	Н	601	TPP	C5'-C6'-N1'	-2.13	120.27	123.82
3	F	602	ADP	C2-N1-C6	-2.13	115.11	118.75
3	Е	602	ADP	C2-N1-C6	-2.12	115.12	118.75
2	G	601	TPP	C5'-C6'-N1'	-2.12	120.29	123.82
3	D	602	ADP	C2-N1-C6	-2.06	115.22	118.75
3	G	602	ADP	C2-N1-C6	-2.05	115.25	118.75
3	Н	602	ADP	C2-N1-C6	-2.04	115.27	118.75
3	F	602	ADP	O5'-PA-O1A	-2.01	101.22	109.07

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There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	601	TPP	C4-C5-C6-C7
2	В	601	TPP	C4'-C5'-C7'-N3
2	В	601	TPP	C4-C5-C6-C7
2	В	601	TPP	C5-C6-C7-O7
2	В	601	TPP	PA-O3A-PB-O3B
2	С	601	TPP	C4-C5-C6-C7
2	С	601	TPP	PA-O3A-PB-O3B



Mol	Chain	Res	Type	Atoms
2	D	601	TPP	C4-C5-C6-C7
2	D	601	TPP	PA-O3A-PB-O2B
2	D	601	TPP	PA-O3A-PB-O3B
2	Е	601	TPP	C4-C5-C6-C7
2	F	601	TPP	C4-C5-C6-C7
2	G	601	TPP	C4-C5-C6-C7
2	Н	601	TPP	C4'-C5'-C7'-N3
2	Н	601	TPP	C4-C5-C6-C7
3	С	602	ADP	PA-O3A-PB-O3B
3	Е	602	ADP	O4'-C4'-C5'-O5'
3	Е	602	ADP	C3'-C4'-C5'-O5'
2	А	601	TPP	PA-O3A-PB-O1B
2	Е	601	TPP	PA-O3A-PB-O1B
3	F	602	ADP	O4'-C4'-C5'-O5'
3	D	602	ADP	O4'-C4'-C5'-O5'
3	G	602	ADP	O4'-C4'-C5'-O5'
2	А	601	TPP	PA-O3A-PB-O3B
2	С	601	TPP	PA-O3A-PB-O2B
2	Е	601	TPP	PA-O3A-PB-O3B
2	G	601	TPP	PA-O3A-PB-O2B
2	G	601	TPP	PA-O3A-PB-O3B
3	Н	602	ADP	O4'-C4'-C5'-O5'
3	F	602	ADP	C3'-C4'-C5'-O5'
2	В	601	TPP	PA-O3A-PB-O1B
3	G	602	ADP	C3'-C4'-C5'-O5'
3	А	602	ADP	PB-O3A-PA-O1A
3	А	602	ADP	O4'-C4'-C5'-O5'
2	С	601	TPP	C4'-C5'-C7'-N3
2	F	601	TPP	C4'-C5'-C7'-N3
2	G	601	TPP	C4'-C5'-C7'-N3
3	D	602	ADP	C3'-C4'-C5'-O5'
3	H	602	ADP	C3'-C4'-C5'-O5'
2	С	601	TPP	PA-O3A-PB-O1B
2	A	601	TPP	C5-C6-C7-O7
3	С	602	ADP	C5'-O5'-PA-O3A
3	С	602	ADP	O4'-C4'-C5'-O5'
3	В	602	ADP	PB-O3A-PA-O1A
3	D	$60\overline{2}$	ADP	PB-O3A-PA-O2A
3	Н	602	ADP	PB-O3A-PA-O1A
3	В	602	ADP	O4'-C4'-C5'-O5'

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There are no ring outliers.



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	602	ADP	1	0
2	F	601	TPP	3	0
2	Н	601	TPP	1	0
2	А	601	TPP	4	0
2	D	601	TPP	2	0
2	Е	601	TPP	2	0
2	В	601	TPP	2	0
2	С	601	TPP	2	0
3	F	602	ADP	1	0
2	G	601	TPP	2	0
3	Е	602	ADP	2	0

11 monomers are involved in 22 short contacts:

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 sufficient must be 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

