

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

#### Nov 1, 2023 - 04:35 AM EDT

PDB ID	:	3HYX
Title	:	3-D X-Ray structure of the sulfide:quinone oxidoreductase from Aquifex aeoli-
		cus in complex with Aurachin C
Authors	:	Marcia, M.; Ermler, U.; Peng, G.H.; Michel, H.
Deposited on	:	2009-06-23
Resolution	:	2.90 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
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

## 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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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		
			2%		
1	А	430	83%	16%	
			2%		
1	В	430	83%	16%	•
			.% •		
1	С	430	79%	20%	
			8%		
1	D	430	82%	17%	•
			3%		
1	E	430	82%	17%	•



Mol	Chain	Length	Quality of chain	
			2%	
1	F	430	82%	18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	D	432	-	-	Х	-
2	SO4	Е	434	-	-	Х	-
2	SO4	F	434	-	-	-	Х
4	AUK	А	501	-	-	-	Х
4	AUK	В	501	-	-	-	Х
4	AUK	С	501	-	-	Х	-
4	AUK	D	501	-	-	Х	-
4	AUK	Е	501	-	-	-	Х
4	AUK	F	501	-	-	-	Х
5	LMT	А	600	-	-	-	Х
5	LMT	В	600	-	-	-	Х
5	LMT	С	600	-	-	-	Х
5	LMT	Е	600	-	-	Х	Х
5	LMT	F	600	-	-	-	Х
7	PS9	А	800	-	-	Х	Х
7	PS9	В	800	-	-	Х	Х
7	PS9	С	800	-		Х	Х
7	PS9	D	800	-	-	Х	Х
7	PS9	Е	800	-		Х	Х
7	PS9	F	800	_	_	-	X



#### 3 HYX

## 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 21163 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	Δ	420	Total	С	Ν	0	S	0	1	0	
	A	429	3345	2165	553	604	23	0	4	0	
1	В	420	Total	С	Ν	0	S	0	6	0	
1	D	429	3357	2173	553	608	23	0	0	U	
1	С	420	Total	С	Ν	0	S	0	Б	0	
1		429	3351	2169	553	606	23	0	5	0	
1	Л	420	Total	С	Ν	0	S	0	Б	0	
1	D	429	3351	2169	553	606	23	0	5	0	
1	F	420	Total	С	Ν	0	S	0	Б	0	
1		429	3351	2169	553	606	23	0	5	0	
1	Б	420	Total	С	Ν	0	S	0	1	0	
	Г	429	3345	2165	553	604	23	U	4		

• Molecule 1 is a protein called Sulfide-quinone reductase.

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
3	Δ	1	Total	С	Ν	Ο	Р	0	0
5	A	L	53	27	9	15	2	0	0
3	В	1	Total	С	Ν	Ο	Р	0	0
5	D	I	53	27	9	15	2	0	0
3	С	1	Total	С	Ν	Ο	Р	0	0
5		1	53	27	9	15	2	0	0
3	Л	1	Total	С	Ν	Ο	Р	0	0
5	D	I	53	27	9	15	2	0	0
2	F	1	Total	С	Ν	Ο	Р	0	0
5		L	53	27	9	15	2	0	0
3	F	1	Total	С	Ν	Ο	Р	0	0
	Ľ		53	27	9	15	2	0	

• Molecule 4 is 1-hydroxy-2-methyl-3-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl]quinol in-4(1H)-one (three-letter code: AUK) (formula:  $C_{25}H_{33}NO_2$ ).





Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
4	Λ	1	Total	С	Ν	Ο	0	0
4	Л	1	28	25	1	2	0	0
4	В	1	Total	С	Ν	Ο	0	0
4	D	1	28	25	1	2	0	0
4	С	1	Total	С	Ν	Ο	0	0
4	U	1	28	25	1	2	0	0
4	Л	1	Total	С	Ν	Ο	0	0
4	D	I	28	25	1	2	0	0
4	F	1	Total	С	Ν	Ο	0	0
4	Ľ	T	28	25	1	2	0	0
4	F	1	Total	С	N	0	0	0
4	T,	1	28	25	1	2	0	

• Molecule 5 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $\rm C_{24}H_{46}O_{11}).$ 





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Δ	1	Total C O	0	0
0	Л	1	35 24 11	0	0
5	В	1	Total C O	0	0
0	D	1	35 24 11	0	0
5	С	1	Total C O	0	0
0	U	T	35 24 11	0	0
5	Л	1	Total C O	0	0
0	D	1	35 24 11	0	0
5	F	1	Total C O	0	0
0	Ľ	I	35 24 11	0	0
5	F	1	Total C O	0	0
0	Ľ	1	35 24 11		0

• Molecule 6 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H<sub>2</sub>S).



	H2S		
H	2 <b>S</b>	S	

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total S 1 1	0	0
6	В	1	Total S 1 1	0	0
6	С	1	Total S 1 1	0	0
6	D	1	Total S 1 1	0	0
6	Ε	1	Total S 1 1	0	0
6	F	1	Total S 1 1	0	0

- Molecule 7 is octathiocane (three-letter code: PS9) (formula: S $_8).$ 





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total S 7 7	0	0
7	В	1	Total S 8 8	0	0
7	С	1	TotalS88	0	0
7	D	1	TotalS88	0	0
7	Е	1	Total S 8 8	0	0
7	F	1	Total S 8 8	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	0	0
8	В	33	Total         O           33         33	0	0
8	С	33	Total O 33 33	0	0
8	D	22	Total O 22 22	0	0
8	Е	25	$\begin{array}{cc} \text{Total} & \text{O} \\ 25 & 25 \end{array}$	0	0
8	F	34	$\begin{array}{cc} \text{Total} & \text{O} \\ 34 & 34 \end{array}$	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.



• Molecule 1: Sulfide-quinone reductase





• Molecule 1: Sulfide-quinone reductase





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	111.18Å 154.23Å 176.53Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	20.13 - 2.90	Depositor
Resolution (A)	20.13 - 2.90	EDS
% Data completeness	98.9 (20.13-2.90)	Depositor
(in resolution range)	98.9 (20.13-2.90)	EDS
$R_{merge}$	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.23 (at 2.88 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
B B.	0.181 , $0.240$	Depositor
II, II free	0.217 , $0.261$	DCC
$R_{free}$ test set	3388 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.4	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33, $39.6$	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	21163	wwPDB-VP
Average B, all atoms $(Å^2)$	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.59% 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: PS9, FAD, SO4, LMT, AUK, CSS, H2S

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 Chair		Bo	ond lengths	Bond angles	
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.50	1/3439~(0.0%)	0.58	0/4668
1	В	0.48	0/3457	0.56	0/4692
1	С	0.48	0/3448	0.58	0/4680
1	D	0.50	4/3448~(0.1%)	0.58	1/4680~(0.0%)
1	Е	0.45	0/3448	0.56	0/4680
1	F	0.45	0/3439	0.56	0/4668
All	All	0.48	5/20679~(0.0%)	0.57	1/28068~(0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	430	CYS	CB-SG	5.94	1.92	1.82
1	D	82	ASP	C-O	5.66	1.34	1.23
1	D	86	ASN	C-N	5.40	1.46	1.34
1	D	84	ASP	CG-OD2	5.23	1.37	1.25
1	D	98	TYR	CE2-CZ	5.11	1.45	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	98	TYR	CB-CG-CD2	-6.01	117.40	121.00

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3345	0	3346	40	0
1	В	3357	0	3358	41	0
1	С	3351	0	3352	55	0
1	D	3351	0	3352	50	0
1	Е	3351	0	3352	52	0
1	F	3345	0	3346	57	0
2	А	15	0	0	1	0
2	В	25	0	0	2	0
2	С	20	0	0	2	0
2	D	25	0	0	4	0
2	Е	25	0	0	4	0
2	F	10	0	0	1	0
3	А	53	0	30	1	0
3	В	53	0	30	3	0
3	С	53	0	29	1	0
3	D	53	0	29	1	0
3	Е	53	0	29	2	0
3	F	53	0	29	2	0
4	А	28	0	33	16	0
4	В	28	0	33	15	0
4	С	28	0	33	25	0
4	D	28	0	33	26	0
4	Е	28	0	33	20	0
4	F	28	0	33	6	0
5	А	35	0	46	15	0
5	В	35	0	46	10	0
5	С	35	0	46	11	0
5	D	35	0	46	4	0
5	Е	35	0	46	26	0
5	F	35	0	46	5	0
6	А	1	0	0	1	0
6	В	1	0	0	1	0
6	С	1	0	0	1	0
6	D	1	0	0	0	0
6	Е	1	0	0	1	0
6	F	1	0	0	1	0
7	A	7	0	0	4	0
7	В	8	0	0	3	0
7	C	8	0	0	2	0
7	D	8	0	0	4	0
7	E	8	0	0	3	0

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
7	F	8	0	0	1	0
8	А	47	0	0	1	0
8	В	33	0	0	1	0
8	С	33	0	0	1	0
8	D	22	0	0	0	0
8	Е	25	0	0	1	0
8	F	34	0	0	3	0
All	All	21163	0	20756	372	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 9.

All (372) 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)
4:C:501:AUK:H23A	4:D:501:AUK:C25	1.18	1.59
4:C:501:AUK:C23	4:D:501:AUK:H25	1.31	1.58
4:E:501:AUK:C21	5:E:600:LMT:H12	1.56	1.33
4:E:501:AUK:H25B	5:E:600:LMT:O1'	1.27	1.30
4:C:501:AUK:C23	4:D:501:AUK:C25	1.95	1.29
4:C:501:AUK:C23	4:D:501:AUK:H22	1.66	1.25
4:C:501:AUK:H23	4:D:501:AUK:C22	1.66	1.24
4:C:501:AUK:C23	4:D:501:AUK:C22	2.24	1.07
4:E:501:AUK:C24	5:E:600:LMT:H61	1.82	1.07
4:C:501:AUK:C23	4:D:501:AUK:C21	2.35	1.04
2:C:434:SO4:O1	5:C:600:LMT:H5B	1.56	1.03
1:C:347[B]:CYS:SG	7:C:800:PS9:S8	2.57	1.02
1:A:381:PHE:HZ	4:A:501:AUK:H14	1.23	1.01
2:E:434:SO4:O2	5:E:600:LMT:H5B	1.61	1.00
1:F:283:ASN:HD22	1:F:286:TYR:H	1.10	1.00
4:C:501:AUK:H23A	4:D:501:AUK:C21	1.92	1.00
4:E:501:AUK:C21	5:E:600:LMT:C1	2.40	0.99
4:E:501:AUK:H25B	5:E:600:LMT:C1	1.92	0.98
4:C:501:AUK:C13	4:D:501:AUK:H22	1.93	0.97
1:C:327:ASN:HD21	1:C:339:TYR:H	1.08	0.96
1:B:327:ASN:HD21	1:B:339:TYR:H	1.14	0.96
4:B:501:AUK:C24	5:B:600:LMT:H52	1.94	0.96
4:E:501:AUK:C25	5:E:600:LMT:C1	2.43	0.95
4:E:501:AUK:C20	5:E:600:LMT:H12	1.97	0.94
1:D:327:ASN:HD21	1:D:339:TYR:H	0.93	0.93
4:A:501:AUK:H18	5:A:600:LMT:H42	1.51	0.91



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:283:ASN:HD22	1:B:286:TYR:H	1.16	0.90
4:E:501:AUK:C25	5:E:600:LMT:O1'	2.17	0.90
4:E:501:AUK:H24B	5:E:600:LMT:H61	1.53	0.89
1:E:347[B]:CYS:SG	7:E:800:PS9:S5	2.71	0.89
4:C:501:AUK:H23	4:D:501:AUK:C21	2.00	0.88
1:A:327:ASN:HD21	1:A:339:TYR:H	1.15	0.88
1:F:327:ASN:HD21	1:F:339:TYR:H	1.23	0.87
1:A:283:ASN:HD22	1:A:286:TYR:H	1.21	0.86
4:B:501:AUK:C24	5:B:600:LMT:C5	2.53	0.86
1:D:347[B]:CYS:SG	7:D:800:PS9:S8	2.75	0.85
4:E:501:AUK:C25	5:E:600:LMT:H12	2.06	0.84
4:E:501:AUK:C24	5:E:600:LMT:C6	2.56	0.83
1:F:347[B]:CYS:SG	7:F:800:PS9:S5	2.77	0.83
1:C:124[A]:CYS:SG	6:C:700:H2S:S	2.63	0.82
1:D:367:ARG:H	1:F:214:ASN:HD22	1.28	0.81
1:B:204:ARG:HB2	1:B:204:ARG:HH11	1.45	0.80
4:B:501:AUK:H24	5:B:600:LMT:H52	1.63	0.80
1:D:327:ASN:HD21	1:D:339:TYR:N	1.76	0.79
4:A:501:AUK:H16	5:A:600:LMT:H61	1.64	0.79
1:D:90:THR:HG22	1:D:94:LYS:H	1.47	0.79
1:F:124[A]:CYS:SG	6:F:700:H2S:S	2.74	0.78
1:F:283:ASN:ND2	1:F:286:TYR:H	1.79	0.78
4:C:501:AUK:C14	4:D:501:AUK:H22	2.13	0.77
5:A:600:LMT:H12	5:A:600:LMT:O2'	1.82	0.77
1:F:381:PHE:HZ	4:F:501:AUK:H14	1.49	0.77
4:A:501:AUK:C18	5:A:600:LMT:H42	2.15	0.76
1:F:294:VAL:HA	1:F:312:LYS:HD3	1.68	0.76
1:C:392:LYS:HG2	1:C:397:ASN:O	1.86	0.76
1:A:381:PHE:CZ	4:A:501:AUK:H14	2.15	0.76
4:B:501:AUK:H24B	5:B:600:LMT:C5	2.16	0.75
4:B:501:AUK:H24B	5:B:600:LMT:H51	1.67	0.75
5:F:600:LMT:O2B	5:F:600:LMT:H4'	1.86	0.73
2:E:434:SO4:O2	5:E:600:LMT:C5B	2.34	0.73
1:E:283:ASN:HD22	1:E:286:TYR:H	1.36	0.72
1:D:327:ASN:ND2	1:D:339:TYR:H	1.79	0.72
1:E:327:ASN:HD21	1:E:339:TYR:H	1.38	0.72
1:A:327:ASN:HD21	1:A:339:TYR:N	1.88	0.72
1:C:293:GLY:HA2	1:C:317:ILE:HG12	1.72	0.71
1:C:347[B]:CYS:SG	7:C:800:PS9:S5	2.89	0.71
5:C:600:LMT:H82	5:D:600:LMT:H111	1.74	0.70
1:C:185:ILE:HD11	1:C:223:VAL:HG23	1.74	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
4:A:501:AUK:H25B	5:A:600:LMT:C1	2.23	0.69
1:F:341:PRO:HB2	1:F:343:LEU:HD13	1.75	0.69
1:A:283:ASN:ND2	1:A:286:TYR:H	1.90	0.69
5:F:600:LMT:H12	5:F:600:LMT:O2'	1.92	0.69
2:D:434:SO4:O1	5:D:600:LMT:H4B	1.92	0.68
1:D:6:VAL:HG12	1:D:98:TYR:HB3	1.75	0.68
1:C:283:ASN:HD22	1:C:286:TYR:H	1.40	0.67
1:B:283:ASN:ND2	1:B:286:TYR:H	1.90	0.67
1:A:156[A]:CSS:SG	7:A:800:PS9:S2	2.93	0.66
1:D:148:ILE:O	1:D:184:PHE:HA	1.94	0.66
1:F:283:ASN:HD22	1:F:286:TYR:N	1.89	0.66
5:A:600:LMT:H3'	5:B:600:LMT:H3'	1.76	0.65
1:C:420:LYS:HE3	1:C:430:CYS:OXT	1.95	0.65
1:B:402:PHE:O	1:B:406:VAL:HG23	1.97	0.65
1:E:381:PHE:HZ	4:E:501:AUK:H14	1.62	0.65
1:C:327:ASN:HD21	1:C:339:TYR:N	1.90	0.64
1:B:293:GLY:HA2	1:B:317:ILE:HG12	1.80	0.64
1:B:294:VAL:HA	1:B:312:LYS:HD3	1.80	0.64
4:A:501:AUK:H25B	5:A:600:LMT:O1'	1.97	0.64
4:C:501:AUK:H23	4:D:501:AUK:H22B	1.73	0.63
1:B:381:PHE:HE2	4:B:501:AUK:H1	1.63	0.63
1:E:144:GLY:O	1:E:180:VAL:HG13	1.99	0.63
1:D:6:VAL:HG12	1:D:98:TYR:CB	2.29	0.62
4:A:501:AUK:H18	5:A:600:LMT:H61	1.81	0.62
1:D:407:LEU:HD21	4:D:501:AUK:H11A	1.81	0.62
1:F:293:GLY:HA2	1:F:317:ILE:HG12	1.81	0.62
5:C:600:LMT:H92	4:D:501:AUK:C19	2.29	0.62
1:F:25:MET:HG2	1:F:28:LEU:HB2	1.81	0.62
1:C:373:LYS:HD2	5:C:600:LMT:H6E	1.81	0.61
1:D:394:ARG:NH1	2:D:432:SO4:O3	2.33	0.61
1:E:294:VAL:HA	1:E:312:LYS:HD3	1.83	0.61
4:B:501:AUK:H28B	8:B:469:HOH:O	2.01	0.61
1:B:144:GLY:HA3	1:B:246:LYS:HD2	1.83	0.61
1:A:367:ARG:H	1:E:214:ASN:ND2	1.99	0.61
1:C:25:MET:HG2	1:C:28:LEU:HB2	1.82	0.60
4:C:501:AUK:H14A	4:D:501:AUK:H22	1.83	0.60
1:D:6:VAL:CG1	1:D:98:TYR:HB3	2.32	0.60
1:D:19:TYR:HD2	1:D:398:ILE:HG12	1.68	0.59
5:C:600:LMT:H92	4:D:501:AUK:H19	1.85	0.59
1:E:293:GLY:HA2	1:E:317:ILE:HG12	1.85	0.59
1:B:327:ASN:HD21	1:B:339:TYR:N	1.94	0.59



	A L	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
4:A:501:AUK:H25B	5:A:600:LMT:H11	1.85	0.58	
1:D:338:LYS:HD2	1:D:422:CYS:SG	2.42	0.58	
3:A:441:FAD:HN3	4:A:501:AUK:H5	1.67	0.58	
1:D:158:GLY:HA3	7:D:800:PS9:S4	2.43	0.58	
1:E:388:TYR:CE2	1:E:392:LYS:HE2	2.38	0.58	
1:B:113:ALA:HB3	1:B:116:GLN:HB2	1.85	0.58	
1:D:11:GLY:HA3	3:D:441:FAD:O1A	2.03	0.58	
1:A:347[B]:CYS:SG	7:A:800:PS9:S8	3.01	0.58	
1:E:345:ALA:HB1	1:E:347[A]:CYS:SG	2.44	0.58	
1:E:9:GLY:O	1:E:14:GLY:HA3	2.04	0.57	
1:A:391:TRP:HH2	1:B:391:TRP:HH2	1.53	0.57	
1:F:381:PHE:CZ	4:F:501:AUK:H14	2.35	0.57	
1:D:283:ASN:HD22	1:D:286:TYR:H	1.53	0.56	
1:E:16:ALA:O	1:E:20:ASN:HB2	2.05	0.56	
1:F:196:VAL:CG2	1:F:363:VAL:HG12	2.35	0.56	
1:C:256:GLY:HA3	1:C:273:LYS:O	2.06	0.56	
1:F:63:ALA:HB3	1:F:64:PRO:HD3	1.87	0.56	
1:E:148:ILE:O	1:E:184:PHE:HA	2.05	0.56	
1:A:278:ASN:HB2	1:A:422:CYS:O	2.06	0.56	
1:D:388:TYR:CE2	4:D:501:AUK:H23	2.41	0.56	
4:A:501:AUK:C18	5:A:600:LMT:C4	2.84	0.55	
1:C:143:PRO:HB3	1:C:180:VAL:HG22	1.89	0.55	
1:C:403:GLU:HG3	4:D:501:AUK:H25A	1.88	0.55	
5:C:600:LMT:H122	4:D:501:AUK:H14A	1.89	0.55	
4:E:501:AUK:H24	5:E:600:LMT:H61	1.82	0.55	
1:F:236:LEU:HD11	1:F:305:PRO:HB3	1.88	0.55	
1:B:158:GLY:HA3	7:B:800:PS9:S4	2.46	0.55	
1:D:168:HIS:ND1	1:D:177:ARG:HD3	2.21	0.55	
1:D:256:GLY:HA3	1:D:273:LYS:O	2.06	0.55	
1:F:141:ALA:O	1:F:143:PRO:HD3	2.07	0.55	
1:B:315:MET:O	1:B:319:GLN:HG3	2.06	0.55	
1:E:345:ALA:HB2	1:E:363:VAL:CG2	2.37	0.55	
1:D:52:TRP:CZ3	1:D:166:MET:HG2	2.41	0.55	
1:C:185:ILE:CD1	1:C:221:VAL:HG23	2.36	0.54	
1:F:257:PRO:HB2	1:F:259:VAL:HG12	1.89	0.54	
1:C:283:ASN:ND2	1:C:286:TYR:H	2.04	0.54	
1:E:60:VAL:HG11	1:E:65:LEU:HD22	1.89	0.54	
4:A:501:AUK:C18	5:A:600:LMT:H61	2.36	0.54	
1:D:350:ASP:OD2	1:D:379:HIS:HD2	1.90	0.54	
1:C:346:ILE:HD11	1:C:411:LEU:CD1	2.38	0.54	
4:E:501:AUK:H19A	5:E:600:LMT:H32	1.89	0.53	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:F:196:VAL:HG21	1:F:363:VAL:CG1	2.38	0.53	
1:F:196:VAL:HG21	1:F:363:VAL:HG12	1.90	0.53	
1:C:151:ILE:HB	1:C:152:PRO:HD2	1.89	0.53	
5:B:600:LMT:H12	5:B:600:LMT:O2'	2.08	0.53	
1:E:278:ASN:HB2	1:E:422:CYS:O	2.09	0.53	
1:E:373:LYS:NZ	5:E:600:LMT:H6D	2.24	0.53	
1:B:165:LEU:HD12	1:B:213:ARG:HD2	1.91	0.52	
4:C:501:AUK:H14A	4:D:501:AUK:C22	2.39	0.52	
8:E:440:HOH:O	1:F:394:ARG:HD2	2.10	0.52	
1:C:147:VAL:HG13	1:C:248:THR:HG22	1.92	0.52	
1:B:12:VAL:HB	3:B:441:FAD:H5'2	1.92	0.52	
1:E:345:ALA:HB2	1:E:363:VAL:HG21	1.92	0.52	
1:A:298:ILE:HD12	1:A:312:LYS:HD2	1.91	0.52	
1:A:347[B]:CYS:SG	7:A:800:PS9:S6	3.07	0.52	
1:D:151:ILE:HD11	1:D:253:SER:H	1.74	0.52	
2:A:434:SO4:O4	5:A:600:LMT:H2B	2.10	0.51	
1:C:214:ASN:ND2	1:E:367:ARG:H	2.07	0.51	
1:C:358:PHE:HD1	1:C:372:THR:HG22	1.75	0.51	
1:B:317:ILE:CD1	3:B:441:FAD:H5'1	2.40	0.51	
5:C:600:LMT:C8	5:D:600:LMT:H111	2.40	0.51	
1:C:230:LYS:HE3	1:C:232:ILE:HD11	1.93	0.51	
1:C:359:PHE:HB3	1:C:371:ILE:HB	1.93	0.51	
1:B:257:PRO:HB2	1:B:259:VAL:HG12	1.93	0.51	
1:F:269:ASN:HB3	1:F:272:ASN:OD1	2.10	0.51	
1:B:407:LEU:HD11	4:B:501:AUK:H12	1.92	0.51	
1:A:358:PHE:HD1	1:A:372:THR:HG22	1.76	0.51	
4:E:501:AUK:H24A	5:E:600:LMT:C6	2.40	0.51	
4:B:501:AUK:H15A	5:B:600:LMT:H82	1.92	0.51	
1:F:148:ILE:O	1:F:184:PHE:HA	2.10	0.51	
1:A:359:PHE:HB3	1:A:371:ILE:HB	1.93	0.50	
1:B:79:GLU:HG3	1:B:91:GLN:HA	1.94	0.50	
1:E:199:ILE:O	1:E:202:SER:HB3	2.09	0.50	
1:A:394:ARG:NH1	2:B:432:SO4:O2	2.43	0.50	
1:E:283:ASN:HD22	1:E:286:TYR:N	2.08	0.50	
1:E:225:ALA:HB3	1:E:232:ILE:HB	1.93	0.50	
4:E:501:AUK:H24	5:E:600:LMT:C6	2.39	0.50	
1:B:369:ARG:NH1	2:D:431:SO4:O4	2.44	0.50	
4:A:501:AUK:H16	5:A:600:LMT:C6	2.38	0.50	
4:C:501:AUK:C23	4:D:501:AUK:H25A	2.24	0.50	
1:B:348:ILE:HA	1:B:356:GLY:O	2.13	0.49	
1:D:81:ILE:HG12	1:D:88:VAL:HG22	1.93	0.49	



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
4:E:501:AUK:C20	5:E:600:LMT:H32	2.43	0.49
1:A:7:VAL:HG22	1:A:102:VAL:HB	1.93	0.49
1:C:391:TRP:HH2	1:D:391:TRP:HH2	1.59	0.49
1:D:162:GLU:OE2	1:D:382:LYS:HE2	2.12	0.49
1:B:256:GLY:HA3	1:B:273:LYS:O	2.13	0.49
1:C:381:PHE:CZ	4:C:501:AUK:H14	2.48	0.49
1:F:196:VAL:HG22	1:F:367:ARG:NH1	2.27	0.49
1:F:301:ILE:HG12	1:F:364:ILE:HG23	1.95	0.49
1:C:19:TYR:CE2	1:C:396:GLY:HA2	2.47	0.49
1:E:11:GLY:HA3	3:E:441:FAD:O1A	2.13	0.49
1:E:391:TRP:HH2	1:F:391:TRP:HH2	1.60	0.49
1:B:149:GLY:HA3	1:B:185:ILE:O	2.13	0.49
4:C:501:AUK:H23B	4:D:501:AUK:C25	2.26	0.48
1:A:165:LEU:HD13	1:A:351:PHE:CD1	2.48	0.48
5:C:600:LMT:H92	4:D:501:AUK:H19A	1.94	0.48
1:D:19:TYR:CD2	1:D:398:ILE:HG12	2.48	0.48
1:C:381:PHE:HZ	4:C:501:AUK:H14	1.78	0.48
1:D:33:ILE:HG12	1:D:74:ILE:HB	1.95	0.48
4:F:501:AUK:H16	5:F:600:LMT:H51	1.95	0.48
1:D:277:VAL:HG23	1:D:426:PRO:HG3	1.95	0.48
1:D:367:ARG:N	1:F:214:ASN:HD22	2.05	0.48
1:A:116:GLN:HG3	1:A:226:ILE:HD12	1.95	0.48
1:B:124[A]:CYS:SG	6:B:700:H2S:S	3.10	0.48
1:D:52:TRP:HZ3	1:D:166:MET:HG2	1.79	0.48
1:A:5:VAL:HG22	1:A:100:TYR:HB2	1.96	0.48
1:E:149:GLY:HA3	1:E:185:ILE:O	2.14	0.48
4:D:501:AUK:H24B	5:D:600:LMT:H122	1.96	0.48
4:F:501:AUK:H19	4:F:501:AUK:H24	1.62	0.47
1:A:147:VAL:O	1:A:248:THR:HA	2.15	0.47
1:B:214:ASN:HD22	1:F:367:ARG:H	1.62	0.47
4:C:501:AUK:H23A	4:D:501:AUK:C22	2.22	0.47
1:E:405:LYS:HD3	1:F:387:LYS:HD2	1.96	0.47
1:D:149:GLY:HA3	1:D:185:ILE:O	2.14	0.47
4:B:501:AUK:H24	5:B:600:LMT:C5	2.33	0.47
4:C:501:AUK:H24	4:C:501:AUK:H19	1.55	0.47
5:E:600:LMT:H3'	5:F:600:LMT:H3'	1.95	0.47
1:F:3:LYS:O	1:F:28:LEU:HD12	2.15	0.47
1:F:196:VAL:HG22	1:F:367:ARG:HH11	1.79	0.47
1:A:410:PHE:O	1:A:411:LEU:HD23	2.14	0.47
1:E:35:ASP:OD1	1:E:36:ARG:N	2.47	0.47
1:E:124[A]:CYS:SG	6:E:700:H2S:S	3.09	0.47



A + a 1		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:F:277:VAL:O	1:F:426:PRO:HD3	2.15	0.47	
1:F:327:ASN:HD21	1:F:339:TYR:N	2.03	0.47	
1:E:283:ASN:ND2	1:E:286:TYR:H	2.06	0.47	
1:D:98:TYR:CZ	1:D:101:LEU:HB2	2.50	0.47	
4:B:501:AUK:C24	5:B:600:LMT:H51	2.30	0.47	
1:C:11:GLY:HA3	3:C:441:FAD:O5B	2.14	0.47	
1:C:358:PHE:CD1	1:C:372:THR:HG22	2.50	0.47	
1:E:269:ASN:HB3	1:E:272:ASN:OD1	2.15	0.47	
1:D:159:PRO:HD3	7:D:800:PS9:S2	2.55	0.46	
1:F:60:VAL:HG11	1:F:65:LEU:HD22	1.98	0.46	
1:A:113:ALA:HB3	1:A:116:GLN:HB2	1.98	0.46	
1:E:196:VAL:HA	1:E:301:ILE:HD13	1.97	0.46	
1:E:373:LYS:CE	5:E:600:LMT:H6D	2.45	0.46	
1:A:121:THR:CG2	1:A:135:LYS:HD3	2.46	0.46	
1:F:300:PRO:HA	1:F:310:VAL:HG23	1.96	0.46	
1:A:128:HIS:HD2	1:A:131:GLU:OE2	1.99	0.46	
1:A:347[B]:CYS:SG	7:A:800:PS9:S4	3.13	0.46	
1:B:278:ASN:HB2	1:B:422:CYS:O	2.16	0.46	
1:C:235:ASP:OD2	1:C:241:HIS:HE1	1.99	0.46	
3:F:441:FAD:H8A	8:F:439:HOH:O	2.16	0.46	
1:C:5:VAL:HG11	1:C:21:LEU:HD13	1.98	0.46	
1:C:411:LEU:HD11	4:C:501:AUK:H24A	1.98	0.46	
1:D:90:THR:CG2	1:D:94:LYS:HB3	2.46	0.46	
1:A:111:PHE:CD2	1:A:117:GLU:HG3	2.51	0.45	
1:A:327:ASN:ND2	1:A:339:TYR:H	1.98	0.45	
1:F:199:ILE:O	1:F:202:SER:HB3	2.16	0.45	
1:C:350:ASP:OD1	1:C:379:HIS:HD2	2.00	0.45	
1:D:234:GLU:HA	1:D:239:ASN:O	2.16	0.45	
1:C:209:LEU:HD21	1:C:351:PHE:CE2	2.52	0.45	
1:C:373:LYS:HD2	5:C:600:LMT:C6'	2.46	0.45	
1:D:387:LYS:HA	1:D:387:LYS:HD3	1.84	0.45	
1:B:204:ARG:HB2	1:B:204:ARG:NH1	2.24	0.45	
1:B:407:LEU:HD21	4:B:501:AUK:H28A	1.98	0.45	
1:C:166:MET:HE2	1:C:350:ASP:HB3	1.98	0.45	
4:A:501:AUK:C16	5:A:600:LMT:H61	2.42	0.45	
1:E:345:ALA:CB	1:E:363:VAL:CG2	2.94	0.45	
1:B:39:PHE:O	1:B:59:SER:HA	2.17	0.45	
1:D:367:ARG:H	1:F:214:ASN:ND2	2.05	0.45	
1:B:407:LEU:CD1	4:B:501:AUK:H12	2.46	0.44	
1:B:388:TYR:CE2	1:B:392:LYS:HE2	2.53	0.44	
1:D:65:LEU:O	1:D:68:LYS:HB2	2.17	0.44	



			Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:D:150:ALA:HB1	1:D:154:VAL:HG21	1.98	0.44	
1:A:124[A]:CYS:SG	6:A:700:H2S:S	3.13	0.44	
1:B:233:TYR:CZ	1:B:241:HIS:HB2	2.52	0.44	
1:C:185:ILE:HD13	1:C:221:VAL:HG23	1.98	0.44	
1:C:151:ILE:HB	1:C:152:PRO:CD	2.47	0.44	
1:F:83:PRO:HB2	1:F:286:TYR:CD2	2.53	0.44	
1:B:381:PHE:HZ	4:B:501:AUK:H15	1.83	0.44	
1:D:345:ALA:HB3	1:D:363:VAL:CG2	2.47	0.44	
1:C:147:VAL:CG1	1:C:245:ALA:HB2	2.47	0.44	
2:C:431:SO4:O3	1:E:369:ARG:NH1	2.51	0.44	
1:A:348:ILE:HD12	4:A:501:AUK:H1	1.99	0.43	
1:E:346:ILE:HG23	1:E:346:ILE:O	2.18	0.43	
1:E:347[B]:CYS:SG	7:E:800:PS9:S8	3.17	0.43	
1:F:407:LEU:HD11	4:F:501:AUK:H11A	2.01	0.43	
1:A:148:ILE:O	1:A:184:PHE:HA	2.18	0.43	
4:B:501:AUK:H24	4:B:501:AUK:H19	1.71	0.43	
1:B:120:SER:HB2	1:B:226:ILE:HG21	2.01	0.43	
1:E:381:PHE:CZ	4:E:501:AUK:H14	2.48	0.43	
1:C:301:ILE:HD11	1:C:364:ILE:HG12	2.01	0.43	
1:C:381:PHE:HE2	4:C:501:AUK:O27	2.01	0.43	
1:E:151:ILE:HB	1:E:152:PRO:CD	2.49	0.43	
4:E:501:AUK:C22	5:E:600:LMT:H12	2.36	0.43	
2:B:435:SO4:O3	1:F:369:ARG:HD3	2.18	0.43	
1:C:188:GLU:HB3	1:C:193:HIS:HB3	2.00	0.43	
4:C:501:AUK:H18	5:C:600:LMT:H42	2.01	0.43	
1:A:149:GLY:HA3	1:A:185:ILE:O	2.19	0.43	
1:D:365:PRO:HB3	1:F:214:ASN:HD21	1.84	0.43	
1:E:226:ILE:HD13	1:E:231:VAL:HG13	2.01	0.43	
1:A:16:ALA:HA	1:A:398:ILE:HG13	2.01	0.42	
1:A:313:THR:O	1:A:317:ILE:HG13	2.18	0.42	
1:A:366:PRO:HA	1:E:214:ASN:HD21	1.83	0.42	
1:C:6:VAL:HG23	1:C:101:LEU:HD12	2.02	0.42	
4:E:501:AUK:H24	4:E:501:AUK:H19A	1.63	0.42	
1:F:328:ILE:O	1:F:332:ILE:HG13	2.19	0.42	
1:A:191:LEU:O	1:A:203:LYS:HA	2.19	0.42	
2:E:434:SO4:O2	5:E:600:LMT:H6'1	2.20	0.42	
1:B:347[B]:CYS:HB3	7:B:800:PS9:S6	2.59	0.42	
1:B:365:PRO:HA	1:B:366:PRO:C	2.39	0.42	
1:E:347[A]:CYS:HB3	7:E:800:PS9:S5	2.59	0.42	
1:E:410:PHE:CE1	5:E:600:LMT:H52	2.54	0.42	
1:C:214:ASN:HD21	1:E:366:PRO:HA	1.85	0.42	



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:345:ALA:H	1:B:363:VAL:HG23	1.83	0.42	
1:C:384:ALA:HB1	1:D:406:VAL:HG22	2.02	0.42	
1:E:147:VAL:O	1:E:248:THR:HA	2.20	0.42	
5:E:600:LMT:H92	1:F:381:PHE:CE1	2.55	0.42	
1:C:185:ILE:HD13	1:C:221:VAL:CG2	2.50	0.42	
1:D:157:PHE:CE1	1:D:188:GLU:HG3	2.55	0.42	
1:F:278:ASN:ND2	1:F:422:CYS:HB3	2.35	0.42	
1:A:225:ALA:HB3	1:A:232:ILE:HB	2.01	0.42	
1:C:149:GLY:HA3	1:C:185:ILE:O	2.20	0.42	
1:F:411:LEU:HB2	1:F:413:VAL:HG23	2.02	0.42	
1:A:208:ASP:OD1	1:C:204:ARG:NE	2.50	0.42	
1:F:327:ASN:ND2	1:F:339:TYR:H	2.02	0.41	
4:A:501:AUK:H18	5:A:600:LMT:C4	2.35	0.41	
1:B:347[A]:CYS:HB3	7:B:800:PS9:S5	2.61	0.41	
1:E:46:PRO:HB2	1:E:166:MET:HE1	2.01	0.41	
1:E:329:VAL:HG13	1:E:333:ARG:HD2	2.03	0.41	
3:F:441:FAD:H9	3:F:441:FAD:H1'1	1.86	0.41	
1:C:9:GLY:O	1:C:14:GLY:HA3	2.20	0.41	
1:D:394:ARG:HD2	2:D:432:SO4:O4	2.20	0.41	
1:E:222:ALA:HB2	1:E:306:ILE:HD12	2.02	0.41	
2:E:434:SO4:O2	5:E:600:LMT:C6B	2.67	0.41	
1:F:209:LEU:HD12	1:F:209:LEU:HA	1.89	0.41	
4:C:501:AUK:H16	5:C:600:LMT:H61	2.01	0.41	
3:E:441:FAD:H9	3:E:441:FAD:H1'1	1.84	0.41	
1:F:20:ASN:HD21	1:F:322:MET:HG2	1.85	0.41	
1:F:403:GLU:OE2	4:F:501:AUK:H28B	2.20	0.41	
1:F:146:VAL:HG22	1:F:247:PHE:HB3	2.02	0.41	
1:F:412:LYS:NZ	8:F:465:HOH:O	2.52	0.41	
1:C:41:PHE:CE2	1:C:386:GLU:HG3	2.56	0.41	
1:C:282:GLN:NE2	1:C:287:LYS:O	2.49	0.41	
1:A:22:ARG:NH2	1:A:70:ASN:O	2.36	0.41	
1:B:298:ILE:HG12	1:B:426:PRO:HG2	2.03	0.41	
1:C:277:VAL:HB	1:C:281:PHE:HA	2.02	0.41	
1:C:322:MET:O	1:C:326:HIS:HD2	2.04	0.41	
1:D:165:LEU:HD13	1:D:351:PHE:CD1	2.55	0.41	
1:F:221:VAL:HG12	1:F:235:ASP:HA	2.02	0.41	
3:B:441:FAD:H9	3:B:441:FAD:H1'1	1.75	0.41	
1:D:347[A]:CYS:SG	7:D:800:PS9:S8	3.17	0.41	
1:E:154:VAL:CG1	1:E:155:SER:N	2.84	0.41	
1:F:277:VAL:HB	1:F:281:PHE:HA	2.02	0.41	
1:F:278:ASN:HB2	1:F:422:CYS:O	2.21	0.41	



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:F:434:SO4:O3	5:F:600:LMT:H3B	2.21	0.41
1:A:25:MET:HG2	1:A:28:LEU:HB2	2.02	0.40
1:D:427:GLY:O	1:D:429:ARG:NH2	2.53	0.40
1:E:170:GLU:OE2	1:E:174:ARG:NE	2.54	0.40
1:C:277:VAL:O	1:C:426:PRO:HD3	2.21	0.40
4:C:501:AUK:H23	4:D:501:AUK:H22	1.38	0.40
1:E:11:GLY:O	1:E:15:ILE:HG12	2.22	0.40
1:E:135:LYS:O	1:E:138:GLU:HB2	2.22	0.40
1:F:16:ALA:HA	1:F:398:ILE:HG13	2.03	0.40
1:F:33:ILE:HD11	1:F:96:ILE:HD12	2.02	0.40
1:F:66:LEU:HD12	1:F:73:PHE:HB2	2.03	0.40
1:B:25:MET:HG3	1:B:333:ARG:HH21	1.87	0.40
1:D:299:PRO:HA	1:D:300:PRO:HD2	1.89	0.40
1:E:74:ILE:O	1:E:74:ILE:HG13	2.20	0.40
1:D:151:ILE:HB	1:D:152:PRO:CD	2.52	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	429/430~(100%)	414 (96%)	14 (3%)	1 (0%)	47	78
1	В	431/430~(100%)	417 (97%)	14 (3%)	0	100	100
1	С	430/430~(100%)	421 (98%)	9 (2%)	0	100	100
1	D	430/430~(100%)	416 (97%)	12 (3%)	2 (0%)	29	61
1	Е	430/430~(100%)	413 (96%)	17 (4%)	0	100	100
1	F	429/430~(100%)	413 (96%)	15 (4%)	1 (0%)	47	78
All	All	2579/2580~(100%)	2494 (97%)	81 (3%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	D	334	ASN
1	F	287	LYS
1	А	158	GLY
1	D	284	PRO

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	358/356~(101%)	347~(97%)	11 (3%)	40	74
1	В	360/356~(101%)	342~(95%)	18 (5%)	24	57
1	$\mathbf{C}$	359/356~(101%)	338~(94%)	21 (6%)	20	50
1	D	359/356~(101%)	348~(97%)	11 (3%)	40	74
1	Ε	359/356~(101%)	347~(97%)	12 (3%)	38	72
1	F	358/356~(101%)	350~(98%)	8 (2%)	52	81
All	All	2153/2136~(101%)	2072~(96%)	81 (4%)	34	67

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	24	LEU
1	А	42	THR
1	А	120	SER
1	А	137	GLN
1	А	177	ARG
1	А	214	ASN
1	А	224	LYS
1	А	343	LEU
1	А	373	LYS
1	А	390	LEU
1	А	413	VAL
1	В	28	LEU
1	В	42	THR
1	В	56[A]	GLU
1	В	56[B]	GLU



Mol	Chain	Res	Type
1	В	97	GLU
1	В	122	SER
1	В	138	GLU
1	В	165	LEU
1	В	177	ARG
1	В	191	LEU
1	В	204	ARG
1	В	240	THR
1	В	265	ASP
1	В	308	THR
1	В	331	ASP
1	В	353	GLU
1	В	407	LEU
1	В	409	ILE
1	С	42	THR
1	С	56[A]	GLU
1	С	56[B]	GLU
1	С	114[A]	GLU
1	С	114[B]	GLU
1	С	147	VAL
1	С	171	LEU
1	С	172	LYS
1	С	177	ARG
1	С	185	ILE
1	С	191	LEU
1	С	240	THR
1	С	246	LYS
1	С	285	THR
1	С	310	VAL
1	С	313	THR
1	С	338	LYS
1	С	343	LEU
1	С	344	SER
1	С	390	LEU
1	C	423	GLU
1	D	8	ILE
1	D	24	LEU
1	D	25	MET
1	D	27	ASP
1	D	48	LEU
1	D	90	THR
1	D	171	LEU



Mol	Chain	Res	Type
1	D	177	ARG
1	D	292	VAL
1	D	294	VAL
1	D	404	GLU
1	Е	20	ASN
1	Е	28	LEU
1	Е	74	ILE
1	Е	147	VAL
1	Е	165	LEU
1	Е	171	LEU
1	Е	172	LYS
1	Е	177	ARG
1	Е	191	LEU
1	Е	205	LEU
1	Е	407	LEU
1	Е	409	ILE
1	F	56	GLU
1	F	142	ASN
1	F	165	LEU
1	F	177	ARG
1	F	191	LEU
1	F	205	LEU
1	F	292	VAL
1	F	343	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	23	ASN
1	А	86	ASN
1	А	128	HIS
1	А	133	GLN
1	А	239	ASN
1	А	283	ASN
1	А	326	HIS
1	А	327	ASN
1	А	379	HIS
1	В	23	ASN
1	В	214	ASN
1	В	237	ASN
1	В	241	HIS
1	В	283	ASN



Mol	Chain	Res	Type
1	В	327	ASN
1	С	23	ASN
1	С	214	ASN
1	С	237	ASN
1	С	241	HIS
1	С	283	ASN
1	С	326	HIS
1	С	327	ASN
1	С	379	HIS
1	С	395	ASN
1	D	91	GLN
1	D	128	HIS
1	D	214	ASN
1	D	283	ASN
1	D	327	ASN
1	D	379	HIS
1	D	395	ASN
1	Е	214	ASN
1	Е	237	ASN
1	Е	283	ASN
1	Е	327	ASN
1	Е	379	HIS
1	F	20	ASN
1	F	214	ASN
1	F	237	ASN
1	F	283	ASN
1	F	327	ASN
1	F	379	HIS

Continued from previous page...

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



Mal	Trune	Chain	Dec	Tinle	В	ond leng	gths	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSS	В	156[B]	7	$4,\!6,\!7$	1.11	0	$1,\!6,\!8$	1.36	0
1	CSS	С	156[B]	7	4,6,7	1.12	0	1,6,8	1.45	0
1	CSS	В	156[A]	-	$4,\!5,\!7$	1.22	0	$1,\!5,\!8$	0.97	0
1	CSS	D	156[B]	7	4,6,7	1.09	0	1,6,8	0.36	0
1	CSS	F	156[B]	7	4,6,7	1.21	0	1,6,8	0.90	0
1	CSS	Е	156[B]	7	$4,\!6,\!7$	0.99	0	$1,\!6,\!8$	1.39	0
1	CSS	А	156[B]	7	4,6,7	1.16	0	1,6,8	0.46	0
1	CSS	С	156[A]	-	4,5,7	1.14	0	1,5,8	0.24	0
1	CSS	Е	156[A]	-	4,5,7	1.04	0	1,5,8	0.05	0
1	CSS	А	156[A]	-	4,5,7	1.15	0	1,5,8	1.09	0
1	CSS	D	156[A]	-	4,5,7	1.28	0	1,5,8	1.80	0
1	CSS	F	156[A]	-	4,5,7	1.22	0	1,5,8	0.74	0

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).

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSS	В	156[B]	7	-	1/1/5/7	-
1	CSS	С	156[B]	7	-	1/1/5/7	-
1	CSS	В	156[A]	-	-	1/1/4/7	-
1	CSS	D	156[B]	7	-	0/1/5/7	-
1	CSS	F	156[B]	7	-	1/1/5/7	-
1	CSS	Е	156[B]	7	-	1/1/5/7	-
1	CSS	А	156[B]	7	-	0/1/5/7	-
1	CSS	С	156[A]	-	-	1/1/4/7	-
1	CSS	Е	156[A]	-	-	1/1/4/7	-
1	CSS	А	156[A]	-	-	1/1/4/7	-
1	CSS	D	156[A]	-	-	1/1/4/7	-
1	CSS	F	156[A]	-	-	1/1/4/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
1	А	156[A]	CSS	N-CA-CB-SG
1	С	156[B]	CSS	N-CA-CB-SG
1	D	156[A]	CSS	N-CA-CB-SG
1	Е	156[A]	CSS	N-CA-CB-SG
1	Е	156[B]	CSS	N-CA-CB-SG
1	F	156[A]	CSS	N-CA-CB-SG
1	В	156[A]	CSS	N-CA-CB-SG
1	В	156[B]	CSS	N-CA-CB-SG
1	С	156[A]	CSS	N-CA-CB-SG
1	F	156[B]	CSS	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	156[A]	CSS	1	0

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 6 are modelled with single atom - leaving 48 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 Type Chain	Chain	Dec	Tiple	Bo	ond leng	ths	Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	SO4	А	434	-	4,4,4	0.17	0	$6,\!6,\!6$	0.18	0	
3	FAD	Е	441	6	$53,\!58,\!58$	1.31	4 (7%)	$68,\!89,\!89$	1.48	12 (17%)	
4	AUK	D	501	-	28,29,29	2.06	3 (10%)	32,39,39	1.46	5 (15%)	
2	SO4	А	431	-	4,4,4	0.14	0	6,6,6	0.20	0	
2	SO4	F	433	-	4,4,4	0.13	0	$6,\!6,\!6$	0.26	0	
3	FAD	F	441	6	$53,\!58,\!58$	1.35	5 (9%)	68,89,89	1.48	13 (19%)	



	<b>T</b>		D	T 1.	Bo	ond leng	ths	B	ond ang	gles
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
7	PS9	D	800	1	8,8,8	0.81	0	8,8,8	1.15	0
5	LMT	В	600	-	36,36,36	0.61	1 (2%)	47,47,47	1.05	3 (6%)
2	SO4	А	433	-	4,4,4	0.14	0	6,6,6	0.14	0
5	LMT	F	600	-	36,36,36	0.64	1 (2%)	47,47,47	1.15	3 (6%)
2	SO4	В	434	-	4,4,4	0.12	0	6,6,6	0.20	0
7	PS9	Е	800	1	8,8,8	0.86	0	8,8,8	0.99	0
2	SO4	С	434	-	4,4,4	0.15	0	6,6,6	0.23	0
2	SO4	D	433	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	С	431	-	4,4,4	0.18	0	6,6,6	0.28	0
2	SO4	D	435	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	E	434	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	E	432	-	4,4,4	0.14	0	6,6,6	0.19	0
5	LMT	D	600	-	36,36,36	0.86	2 (5%)	47,47,47	1.00	1 (2%)
2	SO4	E	431	-	4,4,4	0.16	0	6,6,6	0.11	0
3	FAD	D	441	6	53, 58, 58	1.34	4 (7%)	68,89,89	1.40	9 (13%)
4	AUK	А	501	-	28,29,29	2.06	3 (10%)	32,39,39	1.53	5 (15%)
2	SO4	В	432	-	4,4,4	0.11	0	6,6,6	0.26	0
4	AUK	F	501	-	28,29,29	2.07	3 (10%)	32,39,39	1.69	<mark>5 (15%)</mark>
2	SO4	Е	433	-	4,4,4	0.13	0	6,6,6	0.17	0
7	PS9	А	800	1	4,6,8	1.54	0	3,5,8	1.26	0
2	SO4	D	434	-	4,4,4	0.13	0	6,6,6	0.13	0
7	PS9	F	800	1	8,8,8	0.86	0	8,8,8	0.96	0
2	SO4	В	433	-	4,4,4	0.17	0	6,6,6	0.39	0
4	AUK	В	501	-	28,29,29	2.03	4 (14%)	32,39,39	1.34	<mark>5 (15%)</mark>
7	PS9	С	800	1	8,8,8	0.88	0	8,8,8	1.11	0
3	FAD	С	441	6	53,58,58	1.30	4 (7%)	68,89,89	1.44	14 (20%)
2	SO4	F	434	-	4,4,4	0.12	0	6,6,6	0.33	0
4	AUK	Е	501	-	28,29,29	2.02	3 (10%)	32,39,39	1.60	5 (15%)
4	AUK	С	501	_	28,29,29	2.08	3 (10%)	32,39,39	1.51	5 (15%)
5	LMT	А	600	-	36,36,36	0.55	1 (2%)	47,47,47	1.01	3 (6%)
2	SO4	D	432	-	4,4,4	0.17	0	6,6,6	0.30	0
7	PS9	В	800	1	8,8,8	0.83	0	8,8,8	1.09	0
2	SO4	С	433	-	4,4,4	0.13	0	6,6,6	0.37	0
2	SO4	С	432	-	4,4,4	0.11	0	6,6,6	0.27	0
5	LMT	С	600	_	36,36,36	0.51	0	47,47,47	1.05	4 (8%)
2	SO4	В	435	-	4,4,4	0.16	0	6,6,6	0.24	0
5	LMT	Е	600	-	36,36,36	0.50	0	47,47,47	1.07	5 (10%)
2	SO4	D	431	-	4,4,4	0.13	0	6,6,6	0.14	0
3	FAD	А	441	6	53,58,58	1.37	3 (5%)	68,89,89	1.51	12 (17%)
2	SO4	Е	435	-	4,4,4	0.19	0	6,6,6	0.40	0



Mol Type Cha	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
2	SO4	В	431	-	4,4,4	0.14	0	6,6,6	0.31	0
3	FAD	В	441	6	53,58,58	1.35	6 (11%)	68,89,89	1.43	12 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	Е	441	6	-	5/30/50/50	0/6/6/6
4	AUK	D	501	-	-	4/17/17/17	0/2/2/2
3	FAD	F	441	6	-	10/30/50/50	0/6/6/6
7	PS9	D	800	1	-	-	0/1/1/1
5	LMT	В	600	-	-	14/21/61/61	0/2/2/2
5	LMT	F	600	-	-	12/21/61/61	0/2/2/2
7	PS9	Е	800	1	-	-	0/1/1/1
5	LMT	D	600	-	-	13/21/61/61	0/2/2/2
3	FAD	D	441	6	-	10/30/50/50	0/6/6/6
4	AUK	А	501	-	-	7/17/17/17	0/2/2/2
4	AUK	F	501	-	-	8/17/17/17	0/2/2/2
7	PS9	А	800	1	-	0/4/4/8	-
7	PS9	F	800	1	_	-	0/1/1/1
4	AUK	В	501	-	-	6/17/17/17	0/2/2/2
7	PS9	С	800	1	-	-	0/1/1/1
3	FAD	С	441	6	-	6/30/50/50	0/6/6/6
4	AUK	Е	501	-	-	7/17/17/17	0/2/2/2
4	AUK	С	501	-	-	7/17/17/17	0/2/2/2
5	LMT	А	600	-	-	9/21/61/61	0/2/2/2
7	PS9	В	800	1	-	-	0/1/1/1
5	LMT	С	600	-	-	15/21/61/61	0/2/2/2
5	LMT	Е	600	-	-	14/21/61/61	0/2/2/2
3	FAD	А	441	6	-	10/30/50/50	0/6/6/6
3	FAD	В	441	6	-	10/30/50/50	0/6/6/6

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	С	501	AUK	C9-C8	7.78	1.50	1.36



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Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
4	А	501	AUK	C9-C8	7.76	1.50	1.36
4	D	501	AUK	C9-C8	7.73	1.50	1.36
4	F	501	AUK	C9-C8	7.59	1.50	1.36
4	Ε	501	AUK	C9-C8	7.49	1.50	1.36
4	В	501	AUK	C9-C8	7.49	1.50	1.36
3	D	441	FAD	O4-C4	6.86	1.36	1.23
3	А	441	FAD	O4-C4	6.80	1.36	1.23
3	Е	441	FAD	O4-C4	6.77	1.36	1.23
3	F	441	FAD	O4-C4	6.76	1.36	1.23
3	С	441	FAD	O4-C4	6.55	1.36	1.23
3	В	441	FAD	O4-C4	6.54	1.36	1.23
4	F	501	AUK	C2-C3	5.77	1.49	1.41
4	D	501	AUK	C2-C3	5.76	1.49	1.41
4	В	501	AUK	C2-C3	5.74	1.49	1.41
4	А	501	AUK	C2-C3	5.50	1.49	1.41
4	Е	501	AUK	C2-C3	5.48	1.49	1.41
4	С	501	AUK	C2-C3	5.46	1.49	1.41
4	С	501	AUK	O26-N10	3.33	1.44	1.39
4	В	501	AUK	O26-N10	3.32	1.44	1.39
4	F	501	AUK	O26-N10	3.29	1.44	1.39
4	Е	501	AUK	O26-N10	3.25	1.44	1.39
4	D	501	AUK	O26-N10	3.19	1.43	1.39
4	А	501	AUK	O26-N10	3.15	1.43	1.39
5	D	600	LMT	C12-C11	2.93	1.74	1.49
3	F	441	FAD	C9A-N10	-2.68	1.36	1.41
3	В	441	FAD	C9A-N10	-2.60	1.36	1.41
3	В	441	FAD	C4X-N5	2.57	1.35	1.30
3	А	441	FAD	C5X-N5	-2.57	1.34	1.39
5	F	600	LMT	O1'-C1'	2.50	1.44	1.40
3	А	441	FAD	C9A-N10	-2.44	1.36	1.41
5	В	600	LMT	O1'-C1'	2.44	1.44	1.40
3	D	441	FAD	C9A-N10	-2.42	1.36	1.41
3	С	441	FAD	C4X-N5	2.41	1.35	1.30
3	Е	441	FAD	C5X-N5	-2.40	1.34	1.39
3	D	441	FAD	C4X-N5	2.39	1.35	1.30
5	D	600	LMT	01'-C1'	2.37	1.44	1.40
3	F	441	FAD	C5X-N5	-2.36	1.34	1.39
3	Е	441	FAD	C4X-N5	2.33	1.35	1.30
3	F	441	FAD	C4X-N5	2.33	1.35	1.30
3	Е	441	FAD	C9A-N10	-2.29	1.37	1.41
3	С	441	FAD	C5X-N5	-2.25	1.35	1.39
3	D	441	FAD	C5X-N5	-2.24	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	С	441	FAD	C9A-N10	-2.23	1.37	1.41
3	В	441	FAD	O4B-C1B	2.21	1.44	1.41
3	В	441	FAD	C4-N3	-2.18	1.34	1.38
3	В	441	FAD	C5X-N5	-2.14	1.35	1.39
3	F	441	FAD	O4B-C1B	2.10	1.44	1.41
5	А	600	LMT	O1'-C1'	2.07	1.43	1.40
4	В	501	AUK	C3-N10	2.04	1.42	1.39

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	F	501	AUK	C11-C8-C7	6.09	125.02	118.50
3	Е	441	FAD	N3A-C2A-N1A	-5.26	120.46	128.68
3	А	441	FAD	N3A-C2A-N1A	-5.09	120.72	128.68
4	Е	501	AUK	C11-C8-C7	5.01	123.86	118.50
4	А	501	AUK	C11-C8-C7	5.00	123.86	118.50
3	D	441	FAD	N3A-C2A-N1A	-4.87	121.06	128.68
3	С	441	FAD	N3A-C2A-N1A	-4.68	121.37	128.68
3	В	441	FAD	N3A-C2A-N1A	-4.62	121.45	128.68
4	С	501	AUK	C11-C8-C7	4.57	123.39	118.50
3	F	441	FAD	N3A-C2A-N1A	-4.57	121.54	128.68
5	F	600	LMT	O1'-C1'-C2'	4.38	115.14	108.30
4	D	501	AUK	C11-C8-C7	4.00	122.78	118.50
5	В	600	LMT	O1'-C1'-C2'	3.98	114.52	108.30
5	F	600	LMT	O1B-C1B-C2B	3.60	117.43	108.10
4	В	501	AUK	C24-C17-C18	3.35	120.91	115.27
3	В	441	FAD	C4-N3-C2	-3.20	119.73	125.64
4	F	501	AUK	C24-C17-C18	3.20	120.65	115.27
3	Е	441	FAD	C1B-N9A-C4A	-3.19	121.05	126.64
3	D	441	FAD	P-O3P-PA	-3.18	121.90	132.83
4	Е	501	AUK	C24-C17-C18	3.16	120.59	115.27
5	А	600	LMT	O1'-C1'-C2'	3.11	113.15	108.30
3	А	441	FAD	C4X-C10-N1	-3.10	117.54	124.73
3	А	441	FAD	C4-N3-C2	-3.09	119.93	125.64
5	D	600	LMT	O5B-C5B-C6B	3.06	114.05	106.44
3	D	441	FAD	C4X-C10-N1	-3.06	117.63	124.73
4	С	501	AUK	C2-C3-N10	3.03	120.52	117.65
3	А	441	FAD	P-O3P-PA	-3.02	122.46	132.83
3	В	441	FAD	C4X-C10-N1	-3.02	117.73	124.73
3	В	441	FAD	C4X-C10-N10	3.00	120.87	116.48
3	С	441	FAD	C4X-C10-N10	2.95	120.80	116.48
3	С	441	FAD	C4-N3-C2	-2.94	120.22	125.64



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Mol	Chain	Res	Type	Atoms	Z	Observed( <sup>6</sup> )	Ideal(°)
3	F'	441	FAD	C4-N3-C2	-2.91	120.27	125.64
4	E	501	AUK	C2-C3-N10	2.89	120.39	117.65
4	D	501	AUK	C2-C3-N10	2.89	120.39	117.65
4	В	501	AUK	C2-C3-N10	2.87	120.37	117.65
3	E	441	FAD	C5X-C9A-N10	2.87	120.92	117.95
4	A	501	AUK	C2-C3-N10	2.85	120.35	117.65
3	В	441	FAD	C4X-C4-N3	2.84	120.40	113.19
4	F	501	AUK	C2-C3-N10	2.81	120.32	117.65
3	С	441	FAD	C4A-C5A-N7A	-2.81	106.47	109.40
3	D	441	FAD	C4-N3-C2	-2.80	120.48	125.64
5	В	600	LMT	C1-O1'-C1'	2.79	118.47	113.84
3	F	441	FAD	C4X-C10-N1	-2.75	118.36	124.73
3	А	441	FAD	O4-C4-C4X	-2.73	119.35	126.60
3	Е	441	FAD	P-O3P-PA	-2.73	123.47	132.83
4	D	501	AUK	C12-C11-C8	2.73	119.40	112.05
3	D	441	FAD	C4X-C4-N3	2.71	120.07	113.19
3	С	441	FAD	C4X-C4-N3	2.70	120.05	113.19
5	С	600	LMT	C4B-C3B-C2B	2.69	115.52	110.82
5	Е	600	LMT	C1'-O5'-C5'	-2.67	108.44	113.69
3	Е	441	FAD	C4X-C10-N10	2.67	120.38	116.48
3	Е	441	FAD	C4-N3-C2	-2.66	120.73	125.64
3	D	441	FAD	C4X-C10-N10	2.65	120.36	116.48
4	А	501	AUK	C24-C17-C18	2.65	119.73	115.27
3	С	441	FAD	C1B-N9A-C4A	-2.63	122.02	126.64
3	А	441	FAD	C4X-C4-N3	2.63	119.86	113.19
3	F	441	FAD	C4X-C4-N3	2.61	119.81	113.19
3	В	441	FAD	C5X-C9A-N10	2.60	120.64	117.95
3	В	441	FAD	P-O3P-PA	-2.56	124.03	132.83
3	Е	441	FAD	C9A-C5X-N5	-2.54	119.67	122.43
3	F	441	FAD	C4X-C10-N10	2.54	120.19	116.48
4	С	501	AUK	C24-C17-C18	2.52	119.51	115.27
3	Е	441	FAD	C4X-C4-N3	2.51	119.56	113.19
3	Е	441	FAD	C4X-C10-N1	-2.51	118.91	124.73
5	F	600	LMT	C1-O1'-C1'	2.49	117.97	113.84
3	С	441	FAD	C4X-C10-N1	-2.47	118.99	124.73
4	F	501	AUK	C12-C11-C8	2.45	118.65	112.05
3	Е	441	FAD	C4A-C5A-N7A	-2.45	106.84	109.40
3	D	441	FAD	C5X-C9A-N10	2.44	120.47	117.95
4	D	501	AUK	C23-C13-C14	2.42	119.34	115.27
5	C	600	LMT	C3B-C4B-C5B	2.41	114.54	110.24
3	D	441	FAD	C10-N1-C2	2.40	121.70	116.90
3	F	441	FAD	04-C4-C4X	-2.38	120.29	126.60

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$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$ $ Ideal( $^{o}$ )
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	В	441	FAD	C10-N1-C2	2.37	121.64	116.90
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	С	441	FAD	O2A-PA-O1A	2.37	123.95	112.24
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	4	В	501	AUK	C3-C2-C7	-2.36	119.06	121.44
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	F	441	FAD	C1B-N9A-C4A	-2.36	122.50	126.64
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	А	441	FAD	C4A-C5A-N7A	-2.34	106.96	109.40
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	С	600	LMT	O1B-C1B-C2B	2.33	114.14	108.10
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	А	501	AUK	C12-C11-C8	2.32	118.31	112.05
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	4	В	501	AUK	C23-C13-C14	2.29	119.12	115.27
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3	А	441	FAD	C1B-N9A-C4A	-2.29	122.62	126.64
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	F	441	FAD	O5'-P-O1P	-2.26	100.24	109.07
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	F	441	FAD	C4A-C5A-N7A	-2.26	107.05	109.40
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	С	600	LMT	O5B-C5B-C6B	2.26	112.05	106.44
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	Е	501	AUK	C3-C2-C7	-2.26	119.17	121.44
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	В	441	FAD	C5'-C4'-C3'	2.23	116.51	112.20
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	А	441	FAD	C4-C4X-C10	2.22	120.53	116.79
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	А	441	FAD	C4X-C10-N10	2.22	119.72	116.48
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	С	441	FAD	C10-C4X-N5	-2.22	120.15	124.86
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	А	600	LMT	C1B-O5B-C5B	2.20	118.01	113.69
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	С	441	FAD	O4-C4-C4X	-2.19	120.80	126.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	F	441	FAD	P-O3P-PA	-2.17	125.38	132.83
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	F	441	FAD	C9A-C5X-N5	-2.15	120.09	122.43
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	А	441	FAD	O2P-P-O1P	2.14	122.84	112.24
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	F	441	FAD	C10-C4X-N5	-2.14	120.32	124.86
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	D	501	AUK	C24-C17-C18	2.13	118.86	115.27
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	Е	441	FAD	O4-C4-C4X	-2.13	120.95	126.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	F	441	FAD	C10-N1-C2	2.12	121.14	116.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	С	441	FAD	O4'-C4'-C3'	-2.12	103.96	109.10
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	А	501	AUK	C3-C2-C7	-2.11	119.32	121.44
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	С	501	AUK	C3-C2-C7	-2.11	119.32	121.44
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	С	441	FAD	P-O3P-PA	-2.10	125.61	132.83
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	Е	600	LMT	O1'-C1'-C2'	2.10	111.58	108.30
3         D         441         FAD         O4-C4-C4X         -2.10         121.04         126.60           4         F         501         AUK         C28-C9-C8         -2.09         119.13         123.96           4         E         501         AUK         C23-C13-C14         2.09         118.78         115.27           3         B         441         FAD         C4A-C5A-N7A         -2.09         107.22         109.40           3         A         441         FAD         C10-N1-C2         2.09         121.07         116.90           5         A         600         LMT         C1-O1'-C1'         2.08         117.30         113.84           3         E         441         FAD         O4B-C1B-C2B         -2.05         103.93         106.93           3         B         441         FAD         O4-C4-C4X         -2.04         121.18         126.60           5         E         600         LMT         O5'-C5'-C6'         2.04         111.50         106.44           3         C         441         FAD         C10-N1-C2         2.04         120.97         116.90	4	В	501	AUK	C11-C8-C7	2.10	120.74	118.50
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	D	441	FAD	O4-C4-C4X	-2.10	121.04	126.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	501	AUK	C28-C9-C8	-2.09	119.13	123.96
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	Е	501	AUK	C23-C13-C14	2.09	118.78	115.27
3         A         441         FAD         C10-N1-C2         2.09         121.07         116.90           5         A         600         LMT         C1-O1'-C1'         2.08         117.30         113.84           3         E         441         FAD         O4B-C1B-C2B         -2.05         103.93         106.93           3         B         441         FAD         O4-C4-C4X         -2.04         121.18         126.60           5         E         600         LMT         O5'-C5'-C6'         2.04         111.50         106.44           3         C         441         FAD         C10-N1-C2         2.04         120.97         116.90	3	В	441	FAD	C4A-C5A-N7A	-2.09	107.22	109.40
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	А	441	FAD	C10-N1-C2	2.09	121.07	116.90
3         E         441         FAD         O4B-C1B-C2B         -2.05         103.93         106.93           3         B         441         FAD         O4-C4-C4X         -2.04         121.18         126.60           5         E         600         LMT         O5'-C5'-C6'         2.04         111.50         106.44           3         C         441         FAD         C10-N1-C2         2.04         120.97         116.90	5	А	600	LMT	C1-O1'-C1'	2.08	117.30	113.84
3         B         441         FAD         O4-C4-C4X         -2.04         121.18         126.60           5         E         600         LMT         O5'-C5'-C6'         2.04         111.50         106.44           3         C         441         FAD         C10-N1-C2         2.04         120.97         116.90	3	E	441	FAD	O4B-C1B-C2B	-2.05	103.93	106.93
5         E         600         LMT         O5'-C5'-C6'         2.04         111.50         106.44           3         C         441         FAD         C10-N1-C2         2.04         120.97         116.90	3	В	441	FAD	O4-C4-C4X	-2.04	121.18	126.60
3         C         441         FAD         C10-N1-C2         2.04         120.97         116.90	5	Е	600	LMT	O5'-C5'-C6'	2.04	111.50	106.44
	3	С	441	FAD	C10-N1-C2	2.04	120.97	116.90



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Ε	600	LMT	O1B-C1B-C2B	2.02	113.34	108.10
5	В	600	LMT	C3B-C4B-C5B	2.02	113.85	110.24
5	Ε	600	LMT	C4B-C3B-C2B	2.01	114.34	110.82
3	С	441	FAD	C4-C4X-N5	2.01	121.09	118.23
4	С	501	AUK	C25-C21-C22	2.00	119.02	114.60
3	В	441	FAD	C10-C4X-N5	-2.00	120.61	124.86

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
3	А	441	FAD	C5B-O5B-PA-O3P
3	А	441	FAD	PA-O3P-P-O5'
3	В	441	FAD	C5B-O5B-PA-O1A
3	В	441	FAD	C5B-O5B-PA-O2A
3	В	441	FAD	C5B-O5B-PA-O3P
3	В	441	FAD	O4'-C4'-C5'-O5'
3	В	441	FAD	C5'-O5'-P-O3P
3	С	441	FAD	N10-C1'-C2'-C3'
3	D	441	FAD	C5B-O5B-PA-O1A
3	D	441	FAD	PA-O3P-P-O5'
3	Е	441	FAD	PA-O3P-P-O5'
3	F	441	FAD	C5B-O5B-PA-O3P
4	А	501	AUK	C12-C11-C8-C7
4	А	501	AUK	C12-C11-C8-C9
4	А	501	AUK	C24-C17-C18-C19
4	А	501	AUK	C17-C18-C19-C20
4	В	501	AUK	C13-C14-C15-C16
4	В	501	AUK	C16-C17-C18-C19
4	В	501	AUK	C24-C17-C18-C19
4	С	501	AUK	C12-C11-C8-C7
4	С	501	AUK	C12-C11-C8-C9
4	С	501	AUK	C17-C18-C19-C20
4	Е	501	AUK	C12-C11-C8-C7
4	Е	501	AUK	C12-C11-C8-C9
4	Е	501	AUK	C13-C14-C15-C16
4	Е	501	AUK	C17-C18-C19-C20
4	F	501	AUK	C12-C11-C8-C7
4	F	501	AUK	C12-C11-C8-C9
4	F	501	AUK	C17-C18-C19-C20
5	А	600	LMT	O5'-C1'-O1'-C1
5	В	600	LMT	O5'-C1'-O1'-C1

All (167) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
5	D	600	LMT	C2'-C1'-O1'-C1
5	D	600	LMT	O5'-C1'-O1'-C1
5	F	600	LMT	C2B-C1B-O1B-C4'
5	F	600	LMT	C2'-C1'-O1'-C1
5	F	600	LMT	O5'-C1'-O1'-C1
5	F	600	LMT	C2-C1-O1'-C1'
5	Е	600	LMT	O5B-C1B-O1B-C4'
5	С	600	LMT	O5B-C1B-O1B-C4'
4	А	501	AUK	C16-C17-C18-C19
5	Е	600	LMT	O5'-C5'-C6'-O6'
5	С	600	LMT	O5'-C5'-C6'-O6'
3	А	441	FAD	O4B-C4B-C5B-O5B
3	В	441	FAD	O4B-C4B-C5B-O5B
3	D	441	FAD	O4B-C4B-C5B-O5B
3	Е	441	FAD	O4B-C4B-C5B-O5B
3	F	441	FAD	O4B-C4B-C5B-O5B
4	С	501	AUK	C24-C17-C18-C19
4	Е	501	AUK	C24-C17-C18-C19
4	F	501	AUK	C24-C17-C18-C19
4	С	501	AUK	C16-C17-C18-C19
4	Е	501	AUK	C16-C17-C18-C19
4	F	501	AUK	C16-C17-C18-C19
5	В	600	LMT	C4'-C5'-C6'-O6'
4	В	501	AUK	C17-C18-C19-C20
4	D	501	AUK	C17-C18-C19-C20
5	F	600	LMT	O5'-C5'-C6'-O6'
3	А	441	FAD	O3'-C3'-C4'-C5'
3	А	441	FAD	C2'-C3'-C4'-C5'
3	С	441	FAD	C2'-C3'-C4'-C5'
5	D	600	LMT	O5B-C5B-C6B-O6B
5	А	600	LMT	C2'-C1'-O1'-C1
5	D	600	LMT	C4'-C5'-C6'-O6'
3	Е	441	FAD	C3B-C4B-C5B-O5B
5	D	600	LMT	O1'-C1-C2-C3
5	В	600	LMT	O5'-C5'-C6'-O6'
4	D	501	AUK	C13-C14-C15-C16
3	D	441	FAD	C2'-C3'-C4'-C5'
5	Е	600	LMT	C4'-C5'-C6'-O6'
3	А	441	FAD	O3'-C3'-C4'-O4'
3	С	441	FAD	O3'-C3'-C4'-O4'
3	D	441	FAD	O3'-C3'-C4'-O4'
3	D	441	FAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
5	В	600	LMT	C6-C7-C8-C9
5	D	600	LMT	C5-C6-C7-C8
5	B	600	LMT	C4-C5-C6-C7
5	C	600	LMT	C3-C4-C5-C6
5	F	600	LMT	C6-C7-C8-C9
3	A	441	FAD	C2'-C3'-C4'-O4'
3	C	441	FAD	C2'-C3'-C4'-O4'
3	D	441	FAD	C2'-C3'-C4'-O4'
5	F	600	LMT	C11-C10-C9-C8
5	Е	600	LMT	C7-C8-C9-C10
5	Е	600	LMT	C2'-C1'-O1'-C1
5	С	600	LMT	C11-C10-C9-C8
5	D	600	LMT	C3-C4-C5-C6
5	В	600	LMT	C3-C4-C5-C6
5	Е	600	LMT	C3-C4-C5-C6
5	В	600	LMT	C7-C8-C9-C10
5	А	600	LMT	C5-C6-C7-C8
5	Е	600	LMT	O5B-C5B-C6B-O6B
5	С	600	LMT	C2-C1-O1'-C1'
3	С	441	FAD	O3'-C3'-C4'-C5'
3	D	441	FAD	O3'-C3'-C4'-C5'
5	А	600	LMT	C7-C8-C9-C10
3	F	441	FAD	C2'-C3'-C4'-C5'
5	Е	600	LMT	C1-C2-C3-C4
5	С	600	LMT	C5-C6-C7-C8
5	D	600	LMT	C4-C5-C6-C7
3	F	441	FAD	O3'-C3'-C4'-O4'
5	D	600	LMT	O5'-C5'-C6'-O6'
3	F	441	FAD	C2'-C3'-C4'-O4'
5	С	600	LMT	C7-C8-C9-C10
5	С	600	LMT	O1'-C1-C2-C3
5	С	600	LMT	C2B-C1B-O1B-C4'
5	F	600	LMT	C3-C4-C5-C6
5	E	600	LMT	O5'-C1'-O1'-C1
5	В	600	LMT	C5-C6-C7-C8
5	С	600	LMT	C1-C2-C3-C4
5	Е	600	LMT	C2-C3-C4-C5
5	Е	600	LMT	O1'-C1-C2-C3
3	В	441	FAD	C3'-C4'-C5'-O5'
4	В	501	AUK	C12-C11-C8-C9
4	D	501	AUK	C12-C11-C8-C9
5	А	600	LMT	C1-C2-C3-C4

Continued from previous page...



Mol	Chain	$\mathbf{Res}$	Tvpe	Atoms
5	B	600	LMT	C11-C10-C9-C8
5	A	600	LMT	C9-C10-C11-C12
5	C	600	LMT	C9-C10-C11-C12
3	A	441	FAD	C3B-C4B-C5B-O5B
3	F	441	FAD	C3B-C4B-C5B-O5B
4	B	501	AUK	C12-C11-C8-C7
4	D	501	AUK	C12-C11-C8-C7
5	F	600	LMT	C9-C10-C11-C12
5	E	600	LMT	C9-C10-C11-C12
5	B	600	LMT	C2'-C1'-O1'-C1
5	A	600	LMT	C3-C4-C5-C6
3	B	441	FAD	C3B-C4B-C5B-O5B
5	С	600	LMT	C4'-C5'-C6'-O6'
5	B	600	LMT	C1-C2-C3-C4
5	A	600	LMT	C2-C1-O1'-C1'
5	В	600	LMT	C2-C1-O1'-C1'
5	Е	600	LMT	C2-C1-O1'-C1'
3	F	441	FAD	O3'-C3'-C4'-C5'
5	В	600	LMT	C2-C3-C4-C5
5	D	600	LMT	C4B-C5B-C6B-O6B
5	F	600	LMT	C2-C3-C4-C5
5	А	600	LMT	C4-C5-C6-C7
5	С	600	LMT	C2-C3-C4-C5
3	В	441	FAD	PA-O3P-P-O5'
3	F	441	FAD	PA-O3P-P-O5'
5	F	600	LMT	C4'-C5'-C6'-O6'
3	D	441	FAD	C5B-O5B-PA-O3P
5	Е	600	LMT	C11-C10-C9-C8
3	А	441	FAD	C5B-O5B-PA-O1A
3	А	441	FAD	C5B-O5B-PA-O2A
3	В	441	FAD	C5'-O5'-P-O1P
3	D	441	FAD	C5B-O5B-PA-O2A
3	F	441	FAD	C5B-O5B-PA-O1A
3	F	441	FAD	C5B-O5B-PA-O2A
3	Е	441	FAD	C2'-C3'-C4'-C5'
5	В	600	LMT	O1'-C1-C2-C3
4	F	501	AUK	C13-C14-C15-C16
5	С	600	LMT	C4-C5-C6-C7
4	С	501	AUK	C23-C13-C14-C15
4	F	501	AUK	C23-C13-C14-C15
3	C	441	FAD	O4B-C4B-C5B-O5B
5	D	600	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	А	501	AUK	C23-C13-C14-C15
5	С	600	LMT	O5B-C5B-C6B-O6B
4	С	501	AUK	C12-C13-C14-C15
3	Ε	441	FAD	C2'-C3'-C4'-O4'
5	F	600	LMT	C5-C6-C7-C8
4	А	501	AUK	C12-C13-C14-C15
4	F	501	AUK	C12-C13-C14-C15
5	D	600	LMT	C11-C10-C9-C8
5	D	600	LMT	C6-C7-C8-C9
4	Е	501	AUK	C23-C13-C14-C15

There are no ring outliers.

34 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	434	SO4	1	0
3	Е	441	FAD	2	0
4	D	501	AUK	26	0
3	F	441	FAD	2	0
7	D	800	PS9	4	0
5	В	600	LMT	10	0
5	F	600	LMT	5	0
7	Е	800	PS9	3	0
2	С	434	SO4	1	0
2	С	431	SO4	1	0
2	Е	434	SO4	4	0
5	D	600	LMT	4	0
3	D	441	FAD	1	0
4	А	501	AUK	16	0
2	В	432	SO4	1	0
4	F	501	AUK	6	0
7	А	800	PS9	4	0
2	D	434	SO4	1	0
7	F	800	PS9	1	0
4	В	501	AUK	15	0
7	С	800	PS9	2	0
3	С	441	FAD	1	0
2	F	434	SO4	1	0
4	Е	501	AUK	20	0
4	С	501	AUK	25	0
5	А	600	LMT	15	0
2	D	432	SO4	2	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	В	800	PS9	3	0
5	С	600	LMT	11	0
2	В	435	SO4	1	0
5	Е	600	LMT	26	0
2	D	431	SO4	1	0
3	А	441	FAD	1	0
3	В	441	FAD	3	0

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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.

















![](_page_45_Picture_4.jpeg)

![](_page_46_Figure_2.jpeg)

![](_page_46_Figure_3.jpeg)

![](_page_46_Picture_4.jpeg)

![](_page_47_Figure_3.jpeg)

![](_page_47_Picture_4.jpeg)

![](_page_48_Figure_3.jpeg)

![](_page_48_Picture_4.jpeg)

![](_page_49_Figure_2.jpeg)

![](_page_49_Picture_3.jpeg)

![](_page_50_Figure_2.jpeg)

![](_page_50_Figure_3.jpeg)

![](_page_50_Picture_4.jpeg)

![](_page_51_Figure_3.jpeg)

![](_page_51_Picture_4.jpeg)

![](_page_52_Figure_3.jpeg)

![](_page_52_Picture_4.jpeg)

![](_page_53_Figure_3.jpeg)

![](_page_53_Picture_4.jpeg)

![](_page_54_Figure_3.jpeg)

![](_page_54_Picture_4.jpeg)

![](_page_55_Figure_2.jpeg)

![](_page_55_Figure_3.jpeg)

![](_page_55_Picture_4.jpeg)

![](_page_56_Figure_3.jpeg)

![](_page_56_Picture_4.jpeg)

![](_page_57_Figure_3.jpeg)

![](_page_57_Picture_4.jpeg)

![](_page_58_Figure_3.jpeg)

### 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.

![](_page_58_Picture_8.jpeg)

# 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	< <b>RSRZ</b> >	# <b>RSRZ</b>	>2	$OWAB(Å^2)$	Q<0.9
1	А	428/430~(99%)	-0.05	7 (1%) 72	71	32, 41, 50, 54	0
1	В	428/430~(99%)	-0.05	7 (1%) 72	71	32, 41, 50, 54	0
1	С	428/430~(99%)	0.01	6 (1%) 75	75	32, 43, 53, 61	0
1	D	428/430~(99%)	0.32	34 (7%) 12	10	33, 43, 51, 56	0
1	Ε	428/430~(99%)	0.07	11 (2%) 56	52	32, 44, 51, 54	0
1	F	428/430~(99%)	-0.01	7 (1%) 72	71	35, 44, 51, 58	0
All	All	2568/2580~(99%)	0.05	72 (2%) 53	49	32, 42, 51, 61	0

All (72) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	С	430	CYS	5.9
1	D	430	CYS	5.0
1	Е	430	CYS	4.9
1	F	430	CYS	4.6
1	А	430	CYS	4.5
1	Е	84	ASP	3.9
1	В	430	CYS	3.9
1	В	237	ASN	3.5
1	Е	336	PRO	3.3
1	Е	141	ALA	3.1
1	D	334	ASN	3.1
1	D	141	ALA	3.1
1	F	2	ALA	3.0
1	D	93	GLY	3.0
1	D	97	GLU	3.0
1	D	117	GLU	3.0
1	D	92	SER	2.9
1	F	91	GLN	2.9
1	А	2	ALA	2.9

![](_page_59_Picture_10.jpeg)

Mol	Chain	Res	Type	RSRZ	
1	E	91	GLN	2.8	
1	D	86	ASN	2.8	
1	D	95	LYS	2.8	
1	D	236	LEU	2.8	
1	Е	85	ALA	2.8	
1	Е	353	GLU	2.8	
1	Е	27	ASP	2.8	
1	В	91	GLN	2.7	
1	С	92	SER	2.7	
1	Е	92	SER	2.7	
1	F	97	GLU	2.7	
1	D	138	GLU	2.7	
1	D	285	THR	2.7	
1	F	56	GLU	2.6	
1	D	239	ASN	2.6	
1	D	353	GLU	2.6	
1	D	303	LYS	2.6	
1	D	238	GLY	2.6	
1	D	423	GLU	2.6	
1	D	229	ASP	2.5	
1	А	92	SER	2.5	
1	В	420	LYS	2.5	
1	D	237	ASN	2.4	
1	D	2	ALA	2.4	
1	D	91	GLN	2.4	
1	А	237	ASN	2.4	
1	D	118	GLU	2.4	
1	А	423	GLU	2.4	
1	С	141	ALA	2.4	
1	D	79	GLU	2.3	
1	D	336	PRO	2.3	
1	С	408	GLU	2.3	
1	D	131	GLU	2.3	
1	D	27	ASP	2.3	
1	D	70	ASN	2.2	
1	D	173	LYS	2.2	
1	D	265	ASP	2.2	
1	В	27	ASP	2.2	
1	С	91	GLN	2.2	
1	F	235	ASP	2.2	
1	А	353	GLU	2.2	
1	В	236	LEU	2.1	

![](_page_60_Picture_6.jpeg)

Mol	Chain	Res	Type	RSRZ
1	F	114[A]	GLU	2.1
1	А	27	ASP	2.1
1	D	241	HIS	2.1
1	D	114[A]	GLU	2.1
1	В	423	GLU	2.1
1	D	89	THR	2.0
1	D	140	TYR	2.0
1	Ε	114[A]	GLU	2.0
1	C	421	ASP	2.0
1	D	262	SER	2.0
1	Е	271	ALA	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
1	CSS	В	156[A]	6/8	0.92	0.21	41,41,42,42	1
1	CSS	В	156[B]	7/8	0.92	0.21	41,41,42,45	2
1	CSS	С	156[A]	6/8	0.96	0.20	45,45,45,46	1
1	CSS	С	156[B]	7/8	0.96	0.20	45,45,46,48	2
1	CSS	D	156[A]	6/8	0.96	0.14	40,40,41,41	1
1	CSS	D	156[B]	7/8	0.96	0.14	40,40,41,43	2
1	CSS	Е	156[A]	6/8	0.96	0.18	47,47,47,48	1
1	CSS	E	156[B]	7/8	0.96	0.18	47,47,48,50	2
1	CSS	F	156[A]	6/8	0.97	0.17	45,45,45,46	1
1	CSS	F	156[B]	7/8	0.97	0.17	45,45,46,46	2
1	CSS	А	156[A]	6/8	0.98	0.17	40,40,40,43	1
1	CSS	A	156[B]	7/8	0.98	0.17	40,40,41,43	2

## 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,

![](_page_61_Picture_12.jpeg)

3H	YX	
011		

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	LMT	А	600	35/35	0.57	0.49	35,47,56,57	35
5	LMT	F	600	35/35	0.59	0.51	29,47,52,54	35
7	PS9	В	800	8/8	0.60	0.74	50,51,51,52	8
5	LMT	В	600	35/35	0.63	0.46	21,33,41,42	35
5	LMT	С	600	35/35	0.65	0.44	38,51,54,54	35
2	SO4	Е	431	5/5	0.66	0.40	52,53,53,53	5
4	AUK	Е	501	28/28	0.68	0.56	33,41,41,41	28
7	PS9	Е	800	8/8	0.68	0.77	54,55,55,56	8
5	LMT	Е	600	35/35	0.69	0.41	28,42,45,45	35
7	PS9	D	800	8/8	0.69	0.62	46,47,48,48	8
5	LMT	D	600	35/35	0.69	0.39	22,27,32,32	35
4	AUK	А	501	28/28	0.70	0.56	43,46,46,46	28
4	AUK	В	501	28/28	0.72	0.49	42,48,49,49	28
7	PS9	С	800	8/8	0.73	0.54	51,52,53,53	8
7	PS9	F	800	8/8	0.73	0.70	48,49,49,49	8
4	AUK	F	501	28/28	0.74	0.46	34,38,39,39	28
2	SO4	F	434	5/5	0.74	0.51	37,37,38,39	5
7	PS9	А	800	7/8	0.75	0.64	45,46,47,47	7
2	SO4	D	435	5/5	0.78	0.32	43,43,44,44	5
4	AUK	D	501	28/28	0.80	0.50	47,50,50,50	28
2	SO4	А	431	5/5	0.80	0.31	52,53,53,54	5
4	AUK	С	501	28/28	0.80	0.48	32,38,38,38	28
2	SO4	C	434	5/5	0.81	0.34	41,41,42,42	5
2	SO4	В	435	5/5	0.81	0.33	37,38,38,39	5
2	SO4	С	431	5/5	0.82	0.26	39,39,40,40	5
2	SO4	С	433	5/5	0.82	0.34	44,44,45,45	5
2	SO4	E	433	5/5	0.84	0.31	48,48,48,49	5
2	SO4	D	431	5/5	0.85	0.20	37,38,38,38	5
6	H2S	E	700	1/1	0.85	0.26	44,44,44,44	1
2	SO4	D	433	$\frac{5}{5}$	0.87	0.32	76,76,77,77	5
2	SO4	E	435	$\frac{5}{5}$	0.87	0.31	58,58,59,59	5
2	SO4	В	433	$\frac{5}{5}$	0.88	0.29	40,40,40,41	5
<u> </u>	H2S		700		0.88	0.28	43,43,43,43	
	H2S	B	700		0.89	0.23	42,42,42,42	
	<u>п25</u>		100		0.89	0.35	45,45,45,45	
	504 504	Б	434		0.90	0.25	39,40,40,40	о Б
	504 1199		434		0.91	0.27	39,40,40,40 36 36 36 36	0 1
	1125 SO4	A C	100	5/5	0.91	0.37	56 56 56 57	5
	SO4 SO4		402	5/5	0.91	$\begin{array}{c} 0.22 \\ 0.21 \end{array}$	38 38 38 38 38	5
	504	r	400	<u> </u>	0.91	0.21	00,00,00,00	5

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.

![](_page_62_Picture_6.jpeg)

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	В	432	5/5	0.92	0.24	44,44,45,45	5
2	SO4	D	434	5/5	0.92	0.38	45,45,46,46	5
2	SO4	А	434	5/5	0.93	0.21	33,33,34,34	5
2	SO4	Е	432	5/5	0.93	0.26	52,52,53,53	5
2	SO4	D	432	5/5	0.94	0.16	46,47,47,47	5
6	H2S	D	700	1/1	0.94	0.19	52,52,52,52	1
2	SO4	В	431	5/5	0.95	0.20	46,46,47,47	5
2	SO4	А	433	5/5	0.95	0.13	46,47,47,48	5
3	FAD	D	441	53/53	0.95	0.15	$39,\!50,\!52,\!52$	0
3	FAD	Е	441	53/53	0.95	0.15	32,38,46,46	0
3	FAD	А	441	53/53	0.96	0.13	23,30,34,34	0
3	FAD	В	441	53/53	0.96	0.14	30,38,41,41	0
3	FAD	F	441	53/53	0.96	0.14	33,41,46,47	0
3	FAD	С	441	53/53	0.97	0.13	28,34,41,42	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.

![](_page_63_Figure_6.jpeg)

![](_page_63_Picture_7.jpeg)

![](_page_64_Figure_3.jpeg)

![](_page_64_Picture_4.jpeg)

![](_page_65_Figure_3.jpeg)

![](_page_65_Picture_4.jpeg)

![](_page_66_Figure_3.jpeg)

![](_page_66_Picture_4.jpeg)

![](_page_67_Figure_3.jpeg)

![](_page_67_Picture_4.jpeg)

![](_page_68_Figure_3.jpeg)

![](_page_68_Picture_4.jpeg)

![](_page_69_Figure_3.jpeg)

![](_page_69_Picture_4.jpeg)

![](_page_70_Figure_3.jpeg)

![](_page_70_Picture_4.jpeg)

![](_page_71_Figure_3.jpeg)

![](_page_71_Picture_4.jpeg)




































## 6.5 Other polymers (i)

There are no such residues in this entry.

