



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:31 AM GMT

PDB ID : 2XDO  
Title : STRUCTURE OF THE TETRACYCLINE DEGRADING MONOOXYGENASE TETX2 FROM BACTEROIDES THETA IOTA MICRON  
Authors : Volkers, G.; Palm, G.J.; Wright, G.D.; Hinrichs, W.  
Deposited on : 2010-05-05  
Resolution : 2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

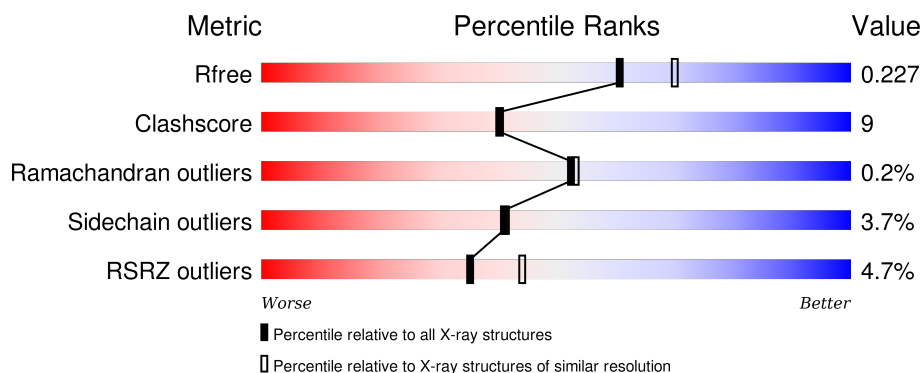
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	<div> <div>5%</div> <div>76%</div> <div>12%</div> <div>• •</div> <div>8%</div> </div>
1	B	398	<div> <div>3%</div> <div>77%</div> <div>13%</div> <div>• •</div> <div>8%</div> </div>
1	C	398	<div> <div>5%</div> <div>77%</div> <div>13%</div> <div>•</div> <div>8%</div> </div>
1	D	398	<div> <div>6%</div> <div>78%</div> <div>11%</div> <div>•</div> <div>9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12183 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TETX2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2857	1812	486	547	12			
1	B	366	Total	C	N	O	S	0	0	0
			2841	1801	480	548	12			
1	C	365	Total	C	N	O	S	0	0	0
			2826	1791	478	545	12			
1	D	364	Total	C	N	O	S	0	0	0
			2811	1781	477	541	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	EXPRESSION TAG	UNP Q93L51
A	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
A	-7	SER	-	EXPRESSION TAG	UNP Q93L51
A	-6	SER	-	EXPRESSION TAG	UNP Q93L51
A	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
A	0	HIS	-	EXPRESSION TAG	UNP Q93L51
A	1	SER	-	EXPRESSION TAG	UNP Q93L51
A	2	SER	-	EXPRESSION TAG	UNP Q93L51
A	3	GLY	-	EXPRESSION TAG	UNP Q93L51
A	4	LEU	-	EXPRESSION TAG	UNP Q93L51
A	5	VAL	-	EXPRESSION TAG	UNP Q93L51
A	6	PRO	-	EXPRESSION TAG	UNP Q93L51
A	7	ARG	-	EXPRESSION TAG	UNP Q93L51
A	8	GLY	-	EXPRESSION TAG	UNP Q93L51
A	9	SER	-	EXPRESSION TAG	UNP Q93L51
A	10	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-9	MET	-	EXPRESSION TAG	UNP Q93L51

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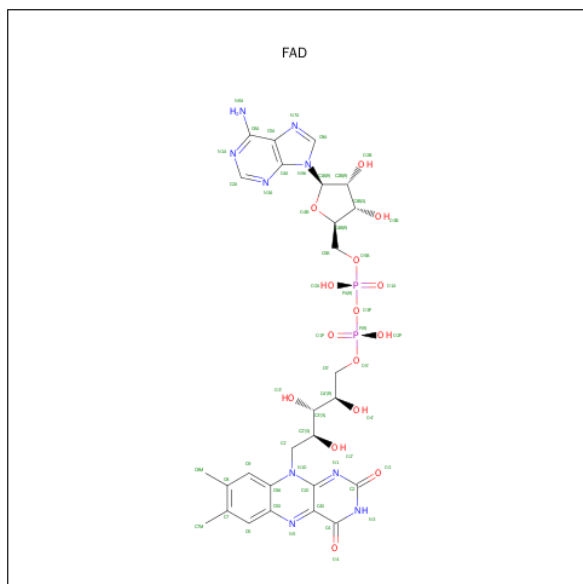
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
B	-7	SER	-	EXPRESSION TAG	UNP Q93L51
B	-6	SER	-	EXPRESSION TAG	UNP Q93L51
B	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
B	0	HIS	-	EXPRESSION TAG	UNP Q93L51
B	1	SER	-	EXPRESSION TAG	UNP Q93L51
B	2	SER	-	EXPRESSION TAG	UNP Q93L51
B	3	GLY	-	EXPRESSION TAG	UNP Q93L51
B	4	LEU	-	EXPRESSION TAG	UNP Q93L51
B	5	VAL	-	EXPRESSION TAG	UNP Q93L51
B	6	PRO	-	EXPRESSION TAG	UNP Q93L51
B	7	ARG	-	EXPRESSION TAG	UNP Q93L51
B	8	GLY	-	EXPRESSION TAG	UNP Q93L51
B	9	SER	-	EXPRESSION TAG	UNP Q93L51
B	10	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-9	MET	-	EXPRESSION TAG	UNP Q93L51
C	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
C	-7	SER	-	EXPRESSION TAG	UNP Q93L51
C	-6	SER	-	EXPRESSION TAG	UNP Q93L51
C	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
C	0	HIS	-	EXPRESSION TAG	UNP Q93L51
C	1	SER	-	EXPRESSION TAG	UNP Q93L51
C	2	SER	-	EXPRESSION TAG	UNP Q93L51
C	3	GLY	-	EXPRESSION TAG	UNP Q93L51
C	4	LEU	-	EXPRESSION TAG	UNP Q93L51
C	5	VAL	-	EXPRESSION TAG	UNP Q93L51
C	6	PRO	-	EXPRESSION TAG	UNP Q93L51
C	7	ARG	-	EXPRESSION TAG	UNP Q93L51
C	8	GLY	-	EXPRESSION TAG	UNP Q93L51
C	9	SER	-	EXPRESSION TAG	UNP Q93L51
C	10	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-9	MET	-	EXPRESSION TAG	UNP Q93L51
D	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
D	-7	SER	-	EXPRESSION TAG	UNP Q93L51

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	EXPRESSION TAG	UNP Q93L51
D	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
D	0	HIS	-	EXPRESSION TAG	UNP Q93L51
D	1	SER	-	EXPRESSION TAG	UNP Q93L51
D	2	SER	-	EXPRESSION TAG	UNP Q93L51
D	3	GLY	-	EXPRESSION TAG	UNP Q93L51
D	4	LEU	-	EXPRESSION TAG	UNP Q93L51
D	5	VAL	-	EXPRESSION TAG	UNP Q93L51
D	6	PRO	-	EXPRESSION TAG	UNP Q93L51
D	7	ARG	-	EXPRESSION TAG	UNP Q93L51
D	8	GLY	-	EXPRESSION TAG	UNP Q93L51
D	9	SER	-	EXPRESSION TAG	UNP Q93L51
D	10	HIS	-	EXPRESSION TAG	UNP Q93L51

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

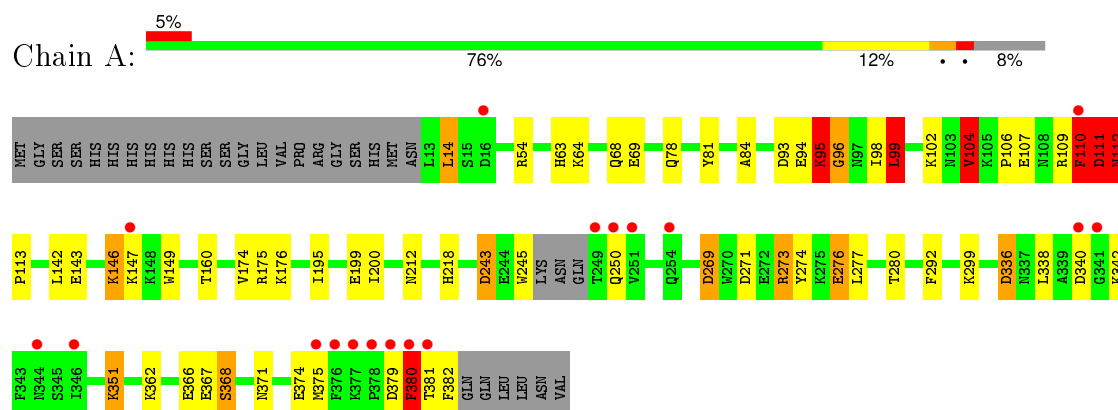
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		
4	B	174	Total	O	0	0
			174	174		
4	C	113	Total	O	0	0
			113	113		
4	D	106	Total	O	0	0
			106	106		

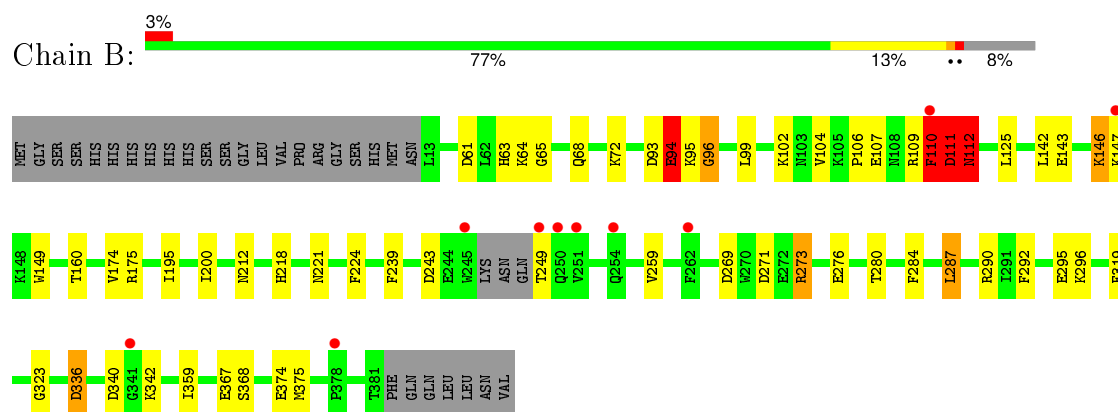
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

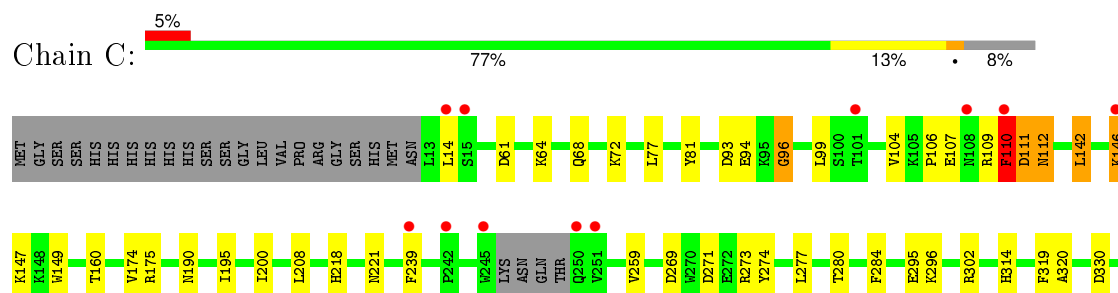
#### • Molecule 1: TETX2 PROTEIN



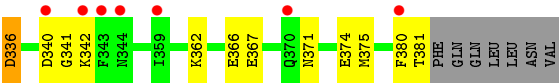
#### • Molecule 1: TETX2 PROTEIN



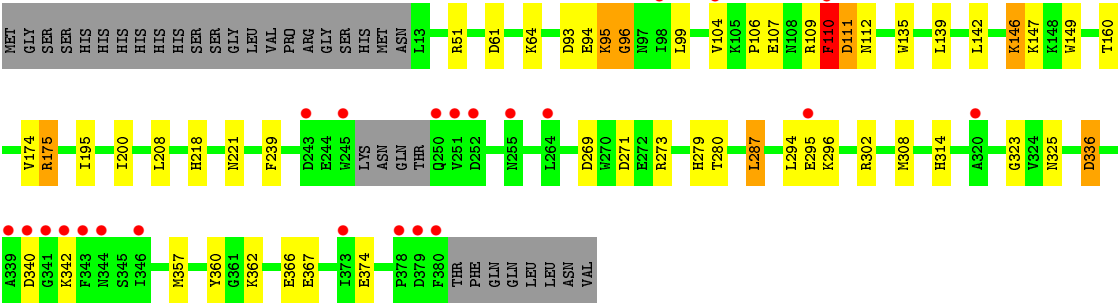
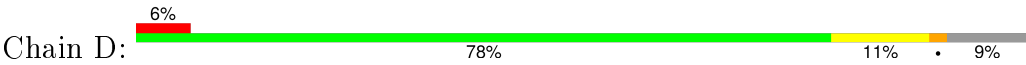
#### • Molecule 1: TETX2 PROTEIN







● Molecule 1: TETX2 PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.11Å 80.27Å 86.89Å 111.00° 90.23° 93.43°	Depositor
Resolution (Å)	40.54 – 2.09 40.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.5 (40.54-2.09) 58.7 (40.54-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.190 , 0.230 0.187 , 0.227	Depositor DCC
$R_{free}$ test set	3252 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63538 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.23	14/2915 (0.5%)	1.10	16/3949 (0.4%)
1	B	1.16	11/2898 (0.4%)	1.08	14/3929 (0.4%)
1	C	1.00	2/2883 (0.1%)	0.93	6/3912 (0.2%)
1	D	0.98	2/2868 (0.1%)	0.94	7/3892 (0.2%)
All	All	1.10	29/11564 (0.3%)	1.02	43/15682 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	4
1	D	0	3
All	All	0	16

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	PHE	CE1-CZ	-11.22	1.16	1.37
1	A	380	PHE	CG-CD2	-9.91	1.23	1.38
1	A	380	PHE	CE2-CZ	-8.96	1.20	1.37
1	B	174	VAL	CB-CG2	-7.57	1.36	1.52
1	B	96	GLY	N-CA	7.37	1.57	1.46
1	A	276	GLU	CD-OE1	6.98	1.33	1.25
1	D	96	GLY	N-CA	6.83	1.56	1.46
1	C	96	GLY	N-CA	6.83	1.56	1.46
1	A	174	VAL	CB-CG2	-6.75	1.38	1.52
1	A	95	LYS	N-CA	6.64	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	SER	CB-OG	-6.50	1.33	1.42
1	A	143	GLU	CD-OE1	6.41	1.32	1.25
1	A	380	PHE	CG-CD1	-6.26	1.29	1.38
1	B	276	GLU	CD-OE1	6.14	1.32	1.25
1	B	368	SER	CB-OG	-6.06	1.34	1.42
1	B	111	ASP	CA-CB	-6.01	1.40	1.53
1	B	94	GLU	CD-OE2	-5.98	1.19	1.25
1	B	95	LYS	N-CA	5.89	1.58	1.46
1	A	96	GLY	CA-C	5.77	1.61	1.51
1	A	199	GLU	CG-CD	5.53	1.60	1.51
1	B	143	GLU	CD-OE1	5.29	1.31	1.25
1	C	110	PHE	N-CA	5.27	1.56	1.46
1	A	112	ASN	CG-ND2	-5.26	1.19	1.32
1	D	110	PHE	N-CA	5.22	1.56	1.46
1	B	292	PHE	CD2-CE2	5.18	1.49	1.39
1	B	96	GLY	CA-C	5.12	1.60	1.51
1	B	94	GLU	CD-OE1	-5.06	1.20	1.25
1	A	292	PHE	CE1-CZ	5.04	1.47	1.37
1	A	269	ASP	CB-CG	-5.03	1.41	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ARG	NE-CZ-NH1	16.75	128.67	120.30
1	A	175	ARG	NE-CZ-NH1	15.97	128.29	120.30
1	B	175	ARG	NE-CZ-NH2	-14.85	112.88	120.30
1	A	175	ARG	NE-CZ-NH2	-14.60	113.00	120.30
1	D	175	ARG	NE-CZ-NH2	-11.75	114.43	120.30
1	C	175	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	D	175	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	B	94	GLU	OE1-CD-OE2	-8.30	113.34	123.30
1	B	287	LEU	CA-CB-CG	8.07	133.87	115.30
1	D	302	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	D	111	ASP	N-CA-C	-7.68	90.27	111.00
1	B	111	ASP	N-CA-C	-7.54	90.65	111.00
1	A	95	LYS	N-CA-C	7.48	131.19	111.00
1	A	99	LEU	CB-CG-CD1	7.23	123.30	111.00
1	B	290	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	273	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	287	LEU	CA-CB-CG	7.14	131.72	115.30
1	B	125	LEU	CB-CG-CD1	-6.89	99.29	111.00
1	B	64	LYS	C-N-CA	-6.66	108.32	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ASP	N-CA-C	-6.62	93.12	111.00
1	C	99	LEU	CA-CB-CG	6.46	130.15	115.30
1	B	96	GLY	N-CA-C	6.38	129.06	113.10
1	C	111	ASP	N-CA-C	-6.31	93.97	111.00
1	B	175	ARG	CD-NE-CZ	6.20	132.28	123.60
1	C	175	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	380	PHE	CB-CG-CD1	6.16	125.11	120.80
1	C	302	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	64	LYS	C-N-CA	-5.92	109.87	122.30
1	A	96	GLY	N-CA-C	5.91	127.86	113.10
1	A	269	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	110	PHE	N-CA-CB	5.79	121.03	110.60
1	A	380	PHE	CD1-CG-CD2	-5.71	110.87	118.30
1	A	380	PHE	CZ-CE2-CD2	5.71	126.95	120.10
1	C	99	LEU	CB-CG-CD2	5.69	120.67	111.00
1	B	112	ASN	CB-CA-C	5.61	121.62	110.40
1	A	175	ARG	CD-NE-CZ	5.59	131.43	123.60
1	B	95	LYS	N-CA-C	5.58	126.06	111.00
1	D	95	LYS	N-CA-C	5.41	125.61	111.00
1	A	104	VAL	CA-CB-CG2	5.40	119.00	110.90
1	A	112	ASN	CB-CA-C	5.37	121.13	110.40
1	B	110	PHE	N-CA-CB	5.20	119.96	110.60
1	B	273	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	D	208	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Peptide
1	A	110	PHE	Peptide
1	A	111	ASP	Peptide
1	A	94	GLU	Peptide
1	B	109	ARG	Peptide
1	B	110	PHE	Peptide
1	B	111	ASP	Peptide
1	B	249	THR	Peptide
1	B	94	GLU	Peptide
1	C	109	ARG	Peptide
1	C	110	PHE	Peptide
1	C	111	ASP	Peptide
1	C	94	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	D	109	ARG	Peptide
1	D	111	ASP	Peptide
1	D	94	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2857	0	2760	71	0
1	B	2841	0	2735	52	0
1	C	2826	0	2710	43	0
1	D	2811	0	2688	41	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
3	A	15	0	0	1	0
3	B	20	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	178	0	0	10	0
4	B	174	0	0	13	0
4	C	113	0	0	5	0
4	D	106	0	0	5	0
All	All	12183	0	11017	197	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 (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLY:HA2	4:A:2045:HOH:O	1.28	1.26
1:B:96:GLY:HA2	4:B:2042:HOH:O	1.24	1.25
1:C:96:GLY:HA2	4:C:2030:HOH:O	1.37	1.22
1:D:96:GLY:HA2	4:D:2031:HOH:O	1.35	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD23	4:A:2040:HOH:O	1.39	1.16
1:A:104:VAL:HG23	1:A:106:PRO:HD2	1.33	1.11
1:D:104:VAL:HG12	1:D:106:PRO:HD2	1.17	1.11
1:B:104:VAL:HG12	1:B:106:PRO:HD2	1.26	1.10
1:C:104:VAL:HG12	1:C:106:PRO:HD2	1.11	1.08
1:A:380:PHE:CD1	1:A:382:PHE:HB3	1.94	1.03
1:A:146:LYS:HD2	1:A:147:LYS:H	1.24	0.99
1:B:146:LYS:HD2	1:B:147:LYS:H	1.26	0.97
1:A:98:ILE:HG21	1:B:359:ILE:HG23	1.49	0.95
1:D:146:LYS:HD2	1:D:147:LYS:H	1.31	0.91
1:A:104:VAL:CG2	1:A:106:PRO:HD2	2.01	0.91
1:A:98:ILE:CG2	1:B:359:ILE:HG23	2.00	0.90
1:A:99:LEU:CD2	4:A:2040:HOH:O	2.04	0.90
1:C:146:LYS:HD2	1:C:147:LYS:H	1.36	0.89
1:A:375:MET:HA	1:A:380:PHE:CD2	2.08	0.89
1:A:99:LEU:HD12	4:B:2162:HOH:O	1.74	0.86
1:A:379:ASP:O	1:A:381:THR:N	2.10	0.84
1:C:104:VAL:CG1	1:C:106:PRO:HD2	2.03	0.82
1:C:104:VAL:HG12	1:C:106:PRO:CD	2.04	0.82
1:A:379:ASP:CB	1:B:65:GLY:HA3	2.12	0.79
1:D:271:ASP:OD1	1:D:273:ARG:HD3	1.84	0.77
1:A:218:HIS:HD2	4:B:2165:HOH:O	1.70	0.75
1:D:61:ASP:HB2	1:D:112:ASN:HB2	1.71	0.73
1:A:271:ASP:OD1	1:A:273:ARG:HD3	1.88	0.72
1:D:362:LYS:O	1:D:366:GLU:HG2	1.89	0.72
1:A:381:THR:N	1:A:382:PHE:HA	2.04	0.72
1:D:104:VAL:HG12	1:D:106:PRO:CD	2.10	0.71
1:B:271:ASP:OD1	1:B:273:ARG:HD3	1.89	0.71
1:C:61:ASP:HB2	1:C:112:ASN:HB2	1.73	0.71
1:D:104:VAL:CG1	1:D:106:PRO:HD2	2.10	0.70
1:B:110:PHE:HA	4:B:2048:HOH:O	1.91	0.70
1:D:107:GLU:HA	1:D:110:PHE:HB3	1.72	0.70
1:A:107:GLU:CA	4:A:2051:HOH:O	2.38	0.70
1:A:99:LEU:CD1	4:B:2162:HOH:O	2.34	0.70
1:C:341:GLY:HA3	4:C:2105:HOH:O	1.92	0.70
1:D:195:ILE:HD12	1:D:280:THR:HG23	1.73	0.70
1:A:195:ILE:HD12	1:A:280:THR:HG23	1.72	0.70
1:A:95:LYS:O	4:A:2045:HOH:O	2.08	0.69
1:C:107:GLU:HA	1:C:110:PHE:HB3	1.73	0.69
1:A:380:PHE:CE1	1:A:382:PHE:HB3	2.27	0.69
1:A:107:GLU:CB	4:A:2051:HOH:O	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:HG12	1:B:106:PRO:CD	2.16	0.68
1:A:362:LYS:O	1:A:366:GLU:HG2	1.94	0.68
1:A:95:LYS:H	1:A:95:LYS:HD2	1.59	0.68
1:C:195:ILE:HD12	1:C:280:THR:HG23	1.74	0.67
1:C:96:GLY:HA3	4:C:2031:HOH:O	1.93	0.67
1:C:271:ASP:OD1	1:C:273:ARG:HD3	1.94	0.67
1:B:104:VAL:CG1	1:B:106:PRO:HD2	2.15	0.67
1:A:107:GLU:HA	1:A:110:PHE:HB3	1.75	0.67
1:C:107:GLU:CA	1:C:110:PHE:HB3	2.26	0.66
1:B:195:ILE:HD12	1:B:280:THR:HG23	1.77	0.66
1:A:95:LYS:HB3	1:A:271:ASP:HB2	1.77	0.65
1:D:107:GLU:CA	1:D:110:PHE:HB3	2.27	0.65
1:D:146:LYS:HD2	1:D:147:LYS:N	2.10	0.65
1:C:342:LYS:HB2	1:C:342:LYS:NZ	2.12	0.65
1:B:218:HIS:HD2	4:B:2121:HOH:O	1.79	0.64
1:A:218:HIS:HE1	1:A:269:ASP:OD2	1.80	0.64
1:A:342:LYS:HB2	1:A:342:LYS:NZ	2.12	0.64
1:B:319:PHE:HB2	4:B:2167:HOH:O	1.98	0.64
1:D:96:GLY:HA3	4:D:2032:HOH:O	1.96	0.63
1:B:102:LYS:HD3	1:B:212:ASN:HD21	1.62	0.63
1:A:107:GLU:CA	1:A:110:PHE:HB3	2.29	0.63
1:A:375:MET:HA	1:A:380:PHE:CE2	2.33	0.63
1:B:342:LYS:HB2	1:B:342:LYS:NZ	2.13	0.63
1:D:342:LYS:HB2	1:D:342:LYS:NZ	2.13	0.63
1:A:54:ARG:HB2	3:A:391:SO4:O4	1.99	0.62
1:A:98:ILE:HG21	1:B:359:ILE:CG2	2.24	0.62
1:C:93:ASP:OD1	1:C:96:GLY:N	2.31	0.62
1:A:93:ASP:OD1	1:A:96:GLY:N	2.32	0.62
1:D:93:ASP:OD1	1:D:96:GLY:N	2.33	0.62
1:A:98:ILE:HG22	1:B:359:ILE:HG23	1.80	0.62
1:B:96:GLY:CA	4:B:2042:HOH:O	2.06	0.61
1:C:269:ASP:HB2	4:C:2081:HOH:O	2.01	0.60
1:B:146:LYS:HD2	1:B:147:LYS:N	2.07	0.60
1:B:93:ASP:OD1	1:B:96:GLY:N	2.35	0.59
1:A:146:LYS:HD2	1:A:147:LYS:N	2.06	0.59
1:B:107:GLU:HA	1:B:110:PHE:HB3	1.83	0.59
1:A:107:GLU:HB3	4:A:2051:HOH:O	2.01	0.59
1:B:107:GLU:CA	1:B:110:PHE:HB3	2.33	0.58
1:D:221:ASN:HD22	1:D:239:PHE:HB3	1.69	0.58
1:D:95:LYS:O	4:D:2031:HOH:O	2.17	0.57
1:C:295:GLU:HG3	1:C:296:LYS:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:HD2	1:A:95:LYS:N	2.19	0.57
1:A:69:GLU:OE2	4:A:2029:HOH:O	2.17	0.57
1:A:380:PHE:CE1	1:A:382:PHE:CB	2.87	0.57
1:C:362:LYS:O	1:C:366:GLU:HG2	2.04	0.57
1:A:99:LEU:HB2	1:B:359:ILE:HG12	1.86	0.57
1:C:380:PHE:O	1:C:381:THR:HG23	2.04	0.57
1:A:342:LYS:HB2	1:A:342:LYS:HZ2	1.69	0.56
1:B:94:GLU:OE2	1:B:218:HIS:CD2	2.58	0.56
1:A:98:ILE:CG2	1:B:359:ILE:HA	2.36	0.55
1:C:72:LYS:HG3	1:C:77:LEU:HD22	1.88	0.55
1:B:68:GLN:NE2	1:B:111:ASP:HA	2.22	0.55
1:A:95:LYS:CD	1:A:95:LYS:N	2.68	0.55
1:C:64:LYS:HD2	1:C:110:PHE:O	2.06	0.55
1:B:221:ASN:HD22	1:B:239:PHE:HB3	1.72	0.55
1:C:68:GLN:NE2	1:C:81:TYR:OH	2.40	0.55
1:C:221:ASN:HD22	1:C:239:PHE:HB3	1.71	0.55
1:A:102:LYS:CD	1:A:212:ASN:HD21	2.20	0.55
1:A:99:LEU:HD13	1:B:359:ILE:HD11	1.90	0.53
1:B:336:ASP:OD1	1:B:340:ASP:OD2	2.27	0.53
1:A:195:ILE:HD12	1:A:280:THR:CG2	2.38	0.53
1:C:146:LYS:HD2	1:C:147:LYS:N	2.15	0.53
1:D:271:ASP:OD1	1:D:273:ARG:CD	2.56	0.53
1:C:314:HIS:NE2	1:C:330:ASP:OD2	2.33	0.53
1:A:274:TYR:O	1:A:277:LEU:HB3	2.10	0.52
1:C:61:ASP:OD2	1:C:112:ASN:HB2	2.09	0.52
1:A:78:GLN:HG2	1:C:64:LYS:HB3	1.92	0.52
1:D:61:ASP:OD2	1:D:112:ASN:HB2	2.12	0.50
1:A:107:GLU:HA	4:A:2051:HOH:O	2.08	0.50
1:C:195:ILE:HD12	1:C:280:THR:CG2	2.41	0.50
1:A:380:PHE:CE1	1:A:382:PHE:CG	3.00	0.49
1:C:221:ASN:ND2	1:C:239:PHE:HB3	2.27	0.49
1:A:149:TRP:O	1:A:160:THR:HA	2.12	0.49
1:A:98:ILE:HG23	1:B:359:ILE:HA	1.94	0.48
1:A:380:PHE:CD1	1:A:382:PHE:CB	2.84	0.48
1:C:149:TRP:O	1:C:160:THR:HA	2.13	0.48
1:C:271:ASP:OD1	1:C:273:ARG:CD	2.61	0.48
1:B:218:HIS:CD2	4:B:2121:HOH:O	2.62	0.48
1:A:336:ASP:OD1	1:A:340:ASP:OD2	2.32	0.48
1:B:259:VAL:HG11	1:B:284:PHE:CG	2.49	0.48
1:D:139:LEU:HD21	1:D:142:LEU:HD13	1.95	0.48
1:A:271:ASP:OD1	1:A:273:ARG:CD	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PHE:CE1	1:A:382:PHE:CD2	3.02	0.47
1:D:195:ILE:CD1	1:D:280:THR:HG23	2.43	0.47
1:D:107:GLU:HA	1:D:110:PHE:CB	2.44	0.47
1:D:195:ILE:HD12	1:D:280:THR:CG2	2.43	0.47
1:D:218:HIS:HE1	1:D:269:ASP:OD2	1.98	0.47
1:B:224:PHE:HZ	1:B:375:MET:HE1	1.79	0.47
1:A:110:PHE:CD1	1:A:110:PHE:O	2.67	0.47
1:D:279:HIS:CE1	4:D:2083:HOH:O	2.68	0.47
1:D:294:LEU:HD11	1:D:314:HIS:HB3	1.96	0.47
1:B:243:ASP:CB	4:B:2133:HOH:O	2.62	0.47
1:C:342:LYS:HB2	1:C:342:LYS:HZ3	1.79	0.46
1:B:342:LYS:HZ2	1:B:342:LYS:HB2	1.79	0.46
1:D:295:GLU:HG3	1:D:296:LYS:H	1.80	0.46
1:C:142:LEU:HD22	1:C:174:VAL:HG22	1.96	0.46
1:A:95:LYS:H	1:A:95:LYS:CD	2.27	0.46
1:B:107:GLU:HB2	1:B:110:PHE:CD2	2.51	0.46
1:C:107:GLU:HA	1:C:110:PHE:CB	2.45	0.46
1:D:149:TRP:O	1:D:160:THR:HA	2.16	0.46
1:B:107:GLU:O	1:B:110:PHE:HB3	2.17	0.45
1:B:243:ASP:HA	4:B:2133:HOH:O	2.16	0.45
1:B:218:HIS:HE1	1:B:269:ASP:OD2	2.00	0.45
1:B:221:ASN:ND2	1:B:239:PHE:HB3	2.32	0.45
1:C:274:TYR:O	1:C:277:LEU:HB3	2.16	0.45
1:D:221:ASN:ND2	1:D:239:PHE:HB3	2.30	0.45
1:B:149:TRP:O	1:B:160:THR:HA	2.17	0.45
1:C:61:ASP:HB2	1:C:112:ASN:CB	2.46	0.45
1:B:295:GLU:HG3	1:B:296:LYS:H	1.82	0.45
1:A:351:LYS:HA	1:A:351:LYS:HD3	1.31	0.44
1:A:176:LYS:O	1:A:299:LYS:NZ	2.47	0.44
1:A:63:HIS:HA	1:A:111:ASP:CB	2.48	0.44
1:A:243:ASP:OD1	1:A:243:ASP:N	2.51	0.44
1:A:68:GLN:NE2	1:A:81:TYR:OH	2.51	0.43
2:A:389:FAD:H9	2:A:389:FAD:H1'1	1.82	0.43
1:A:371:ASN:OD1	1:A:375:MET:SD	2.77	0.43
1:A:84:ALA:HB1	1:A:113:PRO:HB2	2.00	0.43
1:B:342:LYS:NZ	1:B:342:LYS:CB	2.81	0.43
1:C:371:ASN:OD1	1:C:375:MET:SD	2.77	0.43
1:D:336:ASP:OD1	1:D:340:ASP:OD2	2.36	0.43
1:C:320:ALA:HB2	1:C:371:ASN:CG	2.39	0.42
1:B:110:PHE:CA	4:B:2048:HOH:O	2.58	0.42
1:B:63:HIS:HA	1:B:111:ASP:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LYS:HD2	1:D:110:PHE:O	2.20	0.42
1:C:259:VAL:HG11	1:C:284:PHE:CG	2.55	0.42
1:D:175:ARG:HG2	1:D:308:MET:SD	2.60	0.42
1:D:146:LYS:HG3	1:D:146:LYS:HZ3	1.73	0.42
1:B:110:PHE:O	1:B:110:PHE:CD1	2.72	0.42
1:B:72:LYS:HE2	1:B:72:LYS:HB2	1.81	0.42
1:C:218:HIS:HE1	1:C:269:ASP:OD2	2.02	0.42
1:A:107:GLU:N	4:A:2051:HOH:O	2.52	0.42
1:D:325:ASN:HB2	4:D:2099:HOH:O	2.20	0.42
1:C:208:LEU:HD21	4:C:2030:HOH:O	2.20	0.41
1:B:61:ASP:OD2	1:B:112:ASN:HB2	2.19	0.41
1:B:271:ASP:OD1	1:B:273:ARG:CD	2.64	0.41
1:C:107:GLU:HB2	1:C:110:PHE:CD2	2.56	0.41
1:C:190:ASN:HD21	1:C:319:PHE:HZ	1.67	0.41
1:A:112:ASN:N	1:A:113:PRO:HD2	2.36	0.41
1:D:61:ASP:CB	1:D:112:ASN:HB2	2.47	0.41
1:D:342:LYS:HB2	1:D:342:LYS:HZ3	1.82	0.41
1:A:98:ILE:CG2	1:B:359:ILE:CG2	2.86	0.41
1:A:104:VAL:H	1:A:107:GLU:HG2	1.85	0.41
1:A:245:TRP:HA	1:A:250:GLN:HE21	1.86	0.41
1:C:336:ASP:OD1	1:C:340:ASP:OD2	2.38	0.41
1:D:357:MET:HA	1:D:360:TYR:CZ	2.56	0.41
1:B:243:ASP:CA	4:B:2133:HOH:O	2.69	0.41
1:A:14:LEU:HD11	1:A:338:LEU:HD22	2.03	0.41
1:D:104:VAL:H	1:D:107:GLU:HG2	1.86	0.40
1:D:142:LEU:HD22	1:D:174:VAL:HG22	2.03	0.40
1:D:323:GLY:HA3	2:D:389:FAD:H1'2	2.03	0.40
1:B:68:GLN:HE22	1:B:111:ASP:HA	1.85	0.40
1:D:51:ARG:HB3	1:D:135:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	363/398 (91%)	350 (96%)	12 (3%)	1 (0%)	46	45
1	B	362/398 (91%)	348 (96%)	12 (3%)	2 (1%)	30	24
1	C	361/398 (91%)	347 (96%)	14 (4%)	0	100	100
1	D	360/398 (90%)	346 (96%)	14 (4%)	0	100	100
All	All	1446/1592 (91%)	1391 (96%)	52 (4%)	3 (0%)	52	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	PHE
1	B	112	ASN
1	B	323	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/345 (88%)	287 (95%)	16 (5%)	28	25
1	B	301/345 (87%)	290 (96%)	11 (4%)	41	41
1	C	298/345 (86%)	289 (97%)	9 (3%)	48	51
1	D	295/345 (86%)	287 (97%)	8 (3%)	52	56
All	All	1197/1380 (87%)	1153 (96%)	44 (4%)	41	41

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	95	LYS
1	A	99	LEU
1	A	104	VAL
1	A	110	PHE
1	A	112	ASN
1	A	142	LEU
1	A	146	LYS

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Mol	Chain	Res	Type
1	A	200	ILE
1	A	243	ASP
1	A	276	GLU
1	A	336	ASP
1	A	351	LYS
1	A	367	GLU
1	A	368	SER
1	A	374	GLU
1	B	94	GLU
1	B	99	LEU
1	B	110	PHE
1	B	112	ASN
1	B	142	LEU
1	B	146	LYS
1	B	200	ILE
1	B	287	LEU
1	B	336	ASP
1	B	367	GLU
1	B	374	GLU
1	C	14	LEU
1	C	110	PHE
1	C	112	ASN
1	C	142	LEU
1	C	146	LYS
1	C	200	ILE
1	C	336	ASP
1	C	367	GLU
1	C	374	GLU
1	D	99	LEU
1	D	110	PHE
1	D	146	LYS
1	D	200	ILE
1	D	287	LEU
1	D	336	ASP
1	D	367	GLU
1	D	374	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	68	GLN

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Mol	Chain	Res	Type
1	A	130	ASN
1	A	190	ASN
1	A	218	HIS
1	A	221	ASN
1	A	250	GLN
1	A	370	GLN
1	B	130	ASN
1	B	190	ASN
1	B	201	ASN
1	B	212	ASN
1	B	218	HIS
1	B	221	ASN
1	C	68	GLN
1	C	130	ASN
1	C	190	ASN
1	C	201	ASN
1	C	218	HIS
1	C	221	ASN
1	D	130	ASN
1	D	190	ASN
1	D	201	ASN
1	D	207	GLN
1	D	218	HIS
1	D	221	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	A	389	-	48,58,58	1.39	6 (12%)	54,89,89	2.78	17 (31%)
3	SO4	A	391	-	4,4,4	0.40	0	6,6,6	0.66	0
3	SO4	A	392	-	4,4,4	0.29	0	6,6,6	0.39	0
3	SO4	A	393	-	4,4,4	0.30	0	6,6,6	0.20	0
2	FAD	B	389	-	48,58,58	1.11	4 (8%)	54,89,89	2.96	19 (35%)
3	SO4	B	391	-	4,4,4	0.18	0	6,6,6	0.41	0
3	SO4	B	392	-	4,4,4	0.14	0	6,6,6	0.48	0
3	SO4	B	393	-	4,4,4	0.59	0	6,6,6	0.33	0
3	SO4	B	394	-	4,4,4	0.57	0	6,6,6	0.18	0
2	FAD	C	389	-	48,58,58	1.47	8 (16%)	54,89,89	2.64	13 (24%)
3	SO4	C	391	-	4,4,4	0.27	0	6,6,6	0.80	0
3	SO4	C	392	-	4,4,4	0.25	0	6,6,6	0.86	0
3	SO4	C	393	-	4,4,4	0.32	0	6,6,6	0.26	0
2	FAD	D	389	-	48,58,58	1.71	9 (18%)	54,89,89	2.37	12 (22%)
3	SO4	D	391	-	4,4,4	0.27	0	6,6,6	0.54	0
3	SO4	D	392	-	4,4,4	0.20	0	6,6,6	0.26	0
3	SO4	D	393	-	4,4,4	0.20	0	6,6,6	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	389	-	-	0/30/50/50	0/6/6/6
3	SO4	A	391	-	-	0/0/0/0	0/0/0/0
3	SO4	A	392	-	-	0/0/0/0	0/0/0/0
3	SO4	A	393	-	-	0/0/0/0	0/0/0/0
2	FAD	B	389	-	-	0/30/50/50	0/6/6/6
3	SO4	B	391	-	-	0/0/0/0	0/0/0/0
3	SO4	B	392	-	-	0/0/0/0	0/0/0/0
3	SO4	B	393	-	-	0/0/0/0	0/0/0/0
3	SO4	B	394	-	-	0/0/0/0	0/0/0/0
2	FAD	C	389	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	391	-	-	0/0/0/0	0/0/0/0
3	SO4	C	392	-	-	0/0/0/0	0/0/0/0
3	SO4	C	393	-	-	0/0/0/0	0/0/0/0
2	FAD	D	389	-	-	0/30/50/50	0/6/6/6
3	SO4	D	391	-	-	0/0/0/0	0/0/0/0
3	SO4	D	392	-	-	0/0/0/0	0/0/0/0
3	SO4	D	393	-	-	0/0/0/0	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	389	FAD	C10-N10	-3.23	1.35	1.39
2	A	389	FAD	C10-N10	-2.71	1.36	1.39
2	A	389	FAD	P-O2P	-2.44	1.44	1.54
2	D	389	FAD	C6-C5X	-2.33	1.38	1.41
2	A	389	FAD	C10-N1	-2.30	1.31	1.35
2	C	389	FAD	C10-N1	2.02	1.39	1.35
2	C	389	FAD	C8A-N7A	2.04	1.38	1.34
2	C	389	FAD	C1'-N10	2.13	1.50	1.48
2	C	389	FAD	C4-N3	2.22	1.37	1.33
2	C	389	FAD	C5X-N5	2.44	1.39	1.35
2	B	389	FAD	C2A-N3A	2.47	1.36	1.32
2	D	389	FAD	C5X-N5	2.51	1.39	1.35
2	B	389	FAD	C2A-N1A	2.64	1.38	1.33
2	B	389	FAD	C5'-C4'	2.64	1.55	1.51
2	C	389	FAD	C2A-N1A	2.95	1.39	1.33
2	A	389	FAD	C4X-N5	2.98	1.38	1.33
2	A	389	FAD	C2A-N1A	3.02	1.39	1.33
2	D	389	FAD	C8A-N7A	3.22	1.40	1.34
2	D	389	FAD	C4X-N5	3.24	1.38	1.33
2	B	389	FAD	C4X-N5	3.37	1.38	1.33
2	C	389	FAD	C4X-N5	3.40	1.38	1.33
2	D	389	FAD	C4-N3	3.55	1.39	1.33
2	D	389	FAD	C2A-N1A	3.62	1.40	1.33
2	D	389	FAD	O4B-C1B	3.96	1.46	1.41
2	A	389	FAD	C2A-N3A	4.09	1.39	1.32
2	C	389	FAD	C2A-N3A	5.04	1.41	1.32
2	D	389	FAD	C2A-N3A	5.05	1.41	1.32

All (61) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	389	FAD	N3A-C2A-N1A	-15.35	117.14	128.89
2	C	389	FAD	N3A-C2A-N1A	-14.46	117.82	128.89
2	A	389	FAD	N3A-C2A-N1A	-12.81	119.08	128.89
2	D	389	FAD	N3A-C2A-N1A	-9.50	121.62	128.89
2	A	389	FAD	C4X-C4-N3	-4.81	117.01	123.59
2	C	389	FAD	P-O3P-PA	-4.29	120.68	132.73
2	D	389	FAD	C4X-C4-N3	-3.98	118.15	123.59
2	C	389	FAD	C1B-N9A-C4A	-3.86	121.12	126.94
2	D	389	FAD	C1B-N9A-C4A	-3.59	121.52	126.94
2	A	389	FAD	O4B-C1B-N9A	-3.39	101.01	108.10
2	A	389	FAD	C2B-C1B-N9A	-3.26	109.32	114.29
2	A	389	FAD	O3B-C3B-C4B	-3.03	101.95	111.05
2	A	389	FAD	C7-C6-C5X	-3.02	115.98	120.92
2	B	389	FAD	C4X-C4-N3	-2.92	119.60	123.59
2	A	389	FAD	C1B-N9A-C4A	-2.59	123.03	126.94
2	A	389	FAD	C9A-C5X-N5	-2.46	118.72	122.36
2	D	389	FAD	C6-C5X-N5	-2.43	115.83	118.96
2	B	389	FAD	C2B-C1B-N9A	-2.35	110.70	114.29
2	C	389	FAD	C9A-C5X-N5	-2.27	118.99	122.36
2	D	389	FAD	P-O3P-PA	-2.25	126.41	132.73
2	C	389	FAD	O3'-C3'-C2'	-2.20	103.20	108.75
2	B	389	FAD	C9A-C5X-N5	-2.20	119.10	122.36
2	A	389	FAD	O2'-C2'-C3'	-2.19	103.52	109.02
2	C	389	FAD	O3B-C3B-C4B	-2.16	104.56	111.05
2	B	389	FAD	C4B-O4B-C1B	-2.11	107.40	109.72
2	D	389	FAD	C2B-C1B-N9A	-2.11	111.07	114.29
2	B	389	FAD	O4B-C1B-N9A	-2.08	103.75	108.10
2	B	389	FAD	C4-C4X-C10	-2.07	118.62	119.94
2	B	389	FAD	C1B-N9A-C4A	-2.07	123.82	126.94
2	B	389	FAD	P-O3P-PA	-2.05	126.98	132.73
2	B	389	FAD	C7-C6-C5X	-2.04	117.59	120.92
2	D	389	FAD	O5B-PA-O1A	2.01	117.43	109.62
2	C	389	FAD	O3P-P-O5'	2.06	108.40	102.94
2	B	389	FAD	C4X-C10-N10	2.13	121.78	120.52
2	C	389	FAD	O5B-PA-O1A	2.25	118.35	109.62
2	B	389	FAD	O5B-PA-O1A	2.26	118.39	109.62
2	B	389	FAD	C6-C5X-C9A	2.30	122.01	118.98
2	D	389	FAD	C6-C5X-C9A	2.40	122.14	118.98
2	C	389	FAD	C5X-C9A-N10	2.45	119.48	117.62
2	A	389	FAD	C4X-N5-C5X	2.47	119.60	116.76
2	A	389	FAD	O2A-PA-O3P	2.47	116.29	105.09
2	A	389	FAD	C4X-C10-N10	2.55	122.02	120.52
2	A	389	FAD	O2'-C2'-C1'	2.74	116.67	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	389	FAD	O4'-C4'-C3'	2.74	115.91	109.02
2	A	389	FAD	C6-C5X-C9A	2.85	122.73	118.98
2	D	389	FAD	C4X-C10-N10	2.92	122.24	120.52
2	B	389	FAD	C2A-N1A-C6A	3.00	124.12	118.77
2	C	389	FAD	C4-C4X-N5	3.03	122.40	118.72
2	B	389	FAD	C5X-C9A-N10	3.45	120.24	117.62
2	D	389	FAD	C5X-C9A-N10	3.69	120.42	117.62
2	B	389	FAD	C4-C4X-N5	3.86	123.40	118.72
2	C	389	FAD	C4X-N5-C5X	3.91	121.26	116.76
2	A	389	FAD	C1'-N10-C9A	4.05	123.41	118.86
2	B	389	FAD	C4X-N5-C5X	4.26	121.67	116.76
2	C	389	FAD	C1'-N10-C9A	5.47	125.01	118.86
2	B	389	FAD	C4-N3-C2	5.78	120.24	115.25
2	A	389	FAD	C5X-C9A-N10	6.36	122.45	117.62
2	D	389	FAD	C4-N3-C2	6.41	120.79	115.25
2	A	389	FAD	C4-N3-C2	6.80	121.12	115.25
2	D	389	FAD	C1'-N10-C9A	6.86	126.56	118.86
2	B	389	FAD	C1'-N10-C9A	7.95	127.79	118.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	389	FAD	1	0
3	A	391	SO4	1	0
2	D	389	FAD	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	367/398 (92%)	0.13	18 (4%) 33 42	18, 32, 59, 84	0
1	B	366/398 (91%)	0.11	10 (2%) 58 65	17, 33, 58, 80	0
1	C	365/398 (91%)	0.21	18 (4%) 33 42	22, 42, 73, 95	0
1	D	364/398 (91%)	0.27	23 (6%) 23 31	22, 44, 76, 101	0
All	All	1462/1592 (91%)	0.18	69 (4%) 35 44	17, 38, 68, 101	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	PRO	6.9
1	A	110	PHE	5.9
1	B	110	PHE	5.3
1	A	381	THR	5.3
1	B	249	THR	5.2
1	C	110	PHE	5.1
1	C	251	VAL	5.0
1	B	250	GLN	4.8
1	A	377	LYS	4.6
1	B	378	PRO	4.3
1	A	249	THR	4.2
1	D	251	VAL	4.1
1	D	380	PHE	4.1
1	C	344	ASN	3.9
1	D	104	VAL	3.7
1	D	373	ILE	3.7
1	D	339	ALA	3.7
1	A	379	ASP	3.6
1	D	245	TRP	3.6
1	D	342	LYS	3.5
1	D	341	GLY	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	15	SER	3.4
1	D	110	PHE	3.4
1	C	340	ASP	3.3
1	A	341	GLY	3.3
1	A	380	PHE	3.2
1	D	378	PRO	3.1
1	D	344	ASN	3.1
1	C	342	LYS	3.0
1	C	343	PHE	2.9
1	D	346	ILE	2.9
1	B	245	TRP	2.9
1	A	251	VAL	2.8
1	D	340	ASP	2.8
1	C	250	GLN	2.8
1	D	379	ASP	2.8
1	A	340	ASP	2.6
1	D	243	ASP	2.6
1	D	295	GLU	2.6
1	D	255	ASN	2.6
1	C	245	TRP	2.6
1	C	14	LEU	2.6
1	A	254	GLN	2.5
1	C	370	GLN	2.5
1	C	146	LYS	2.5
1	D	343	PHE	2.5
1	D	264	LEU	2.5
1	B	341	GLY	2.4
1	D	252	ASP	2.4
1	A	16	ASP	2.4
1	B	147	LYS	2.4
1	C	242	PRO	2.3
1	B	251	VAL	2.3
1	D	98	ILE	2.3
1	D	320	ALA	2.3
1	C	239	PHE	2.3
1	A	250	GLN	2.2
1	A	344	ASN	2.2
1	B	254	GLN	2.1
1	C	359	ILE	2.1
1	A	147	LYS	2.1
1	A	375	MET	2.1
1	C	380	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	250	GLN	2.1
1	B	262	PHE	2.1
1	C	101	THR	2.0
1	C	108	ASN	2.0
1	A	346	ILE	2.0
1	A	376	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	394	5/5	0.97	0.14	0.95	61,63,66,67	0
2	FAD	A	389	53/53	0.99	0.12	0.08	15,22,25,27	0
2	FAD	C	389	53/53	0.98	0.12	0.01	18,24,33,37	0
2	FAD	D	389	53/53	0.98	0.12	0.00	20,26,35,38	0
2	FAD	B	389	53/53	0.99	0.13	-0.10	14,20,26,28	0
3	SO4	B	392	5/5	0.97	0.24	-	73,75,75,75	0
3	SO4	D	392	5/5	0.98	0.12	-	58,59,60,60	0
3	SO4	A	393	5/5	0.93	0.13	-	68,71,73,73	0
3	SO4	C	393	5/5	0.94	0.14	-	58,62,63,63	5
3	SO4	D	391	5/5	0.97	0.09	-	49,53,58,58	0
3	SO4	C	391	5/5	0.97	0.07	-	57,64,65,67	0
3	SO4	A	392	5/5	0.95	0.17	-	65,67,68,68	0
3	SO4	B	391	5/5	0.98	0.08	-	60,63,65,67	0
3	SO4	B	393	5/5	0.84	0.19	-	55,55,59,61	5
3	SO4	D	393	5/5	0.96	0.11	-	57,59,61,61	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	392	5/5	0.98	0.12	-	58,59,60,61	0
3	SO4	A	391	5/5	0.97	0.12	-	61,62,62,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.