



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:32 am GMT

PDB ID : 1GXF  
Title : CRYSTAL STRUCTURE OF TRYPANOSOMA CRUZI TRYPANOTHIONE  
REDUCTASE IN COMPLEX WITH THE INHIBITOR QUINACRINE MUS-  
TARD  
Authors : Bond, C.S.; Peterson, M.R.; Vickers, T.J.; Fairlamb, A.H.; Hunter, W.N.  
Deposited on : 2002-04-04  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

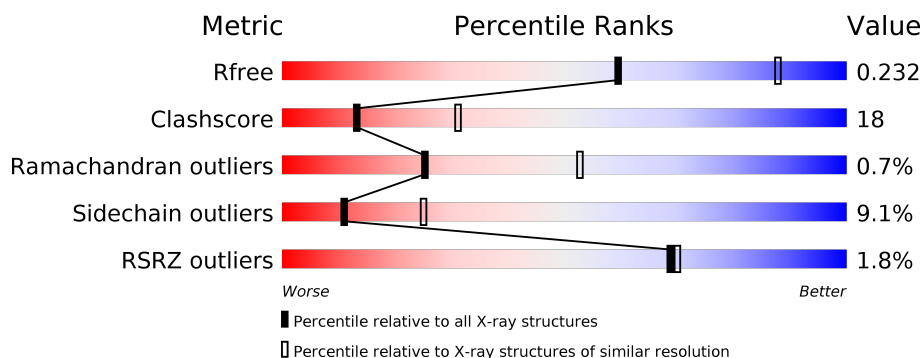
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	492	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 27%, yellow 27%, yellow 67%, green 67%, green 100%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 27%, yellow 27%, yellow 67%, green 67%, green 100%);"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 27%, yellow 27%, yellow 67%, green 67%, green 100%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 27%, yellow 27%, yellow 67%, green 67%, green 100%);"></div> <div style="position: absolute; 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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAE	A	1500	-	-	-	X
4	QUM	A	1501	-	-	X	X
4	QUM	A	1502	-	-	X	X
4	QUM	B	1501	-	-	X	X
4	QUM	B	1502	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7726 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.

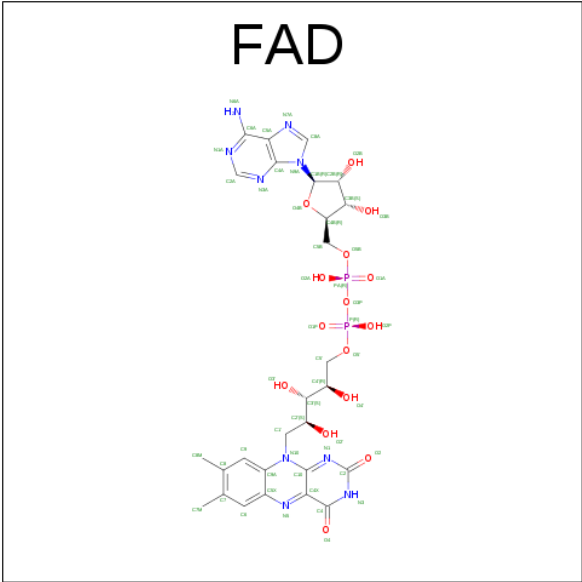
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE (OXIDIZED FORM).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	1
			3727	2370	635	701	21			
1	B	484	Total	C	N	O	S	0	0	1
			3718	2364	633	700	21			

There are 14 discrepancies between the modelled and reference sequences:

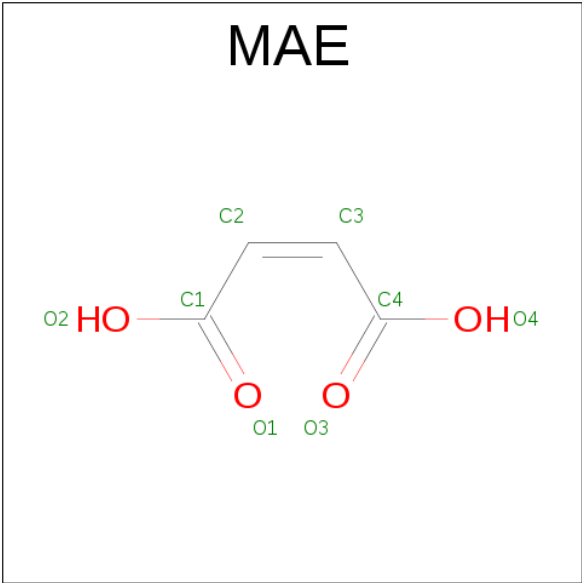
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ASN	LYS	VARIANT	UNP P28593
A	112	ASP	GLU	VARIANT	UNP P28593
A	156	HIS	ASN	VARIANT	UNP P28593
A	353	THR	ASN	VARIANT	UNP P28593
A	402	LYS	ASN	VARIANT	UNP P28593
A	403	VAL	ILE	VARIANT	UNP P28593
A	441	ILE	VAL	VARIANT	UNP P28593
B	95	ASN	LYS	VARIANT	UNP P28593
B	112	ASP	GLU	VARIANT	UNP P28593
B	156	HIS	ASN	VARIANT	UNP P28593
B	353	THR	ASN	VARIANT	UNP P28593
B	402	LYS	ASN	VARIANT	UNP P28593
B	403	VAL	ILE	VARIANT	UNP P28593
B	441	ILE	VAL	VARIANT	UNP P28593

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



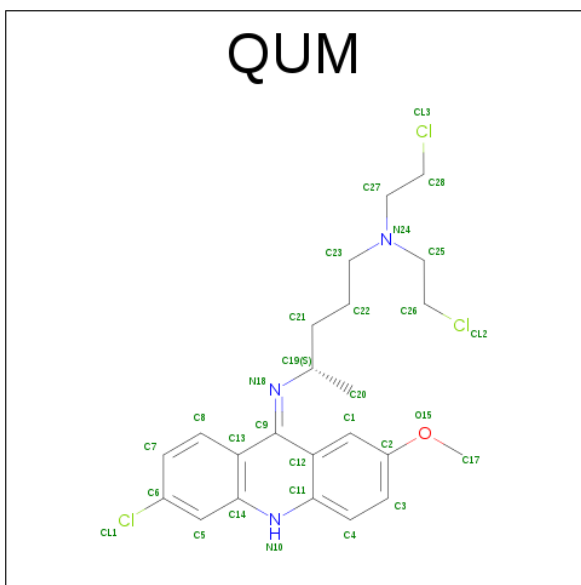
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is MALEIC ACID (three-letter code: MAE) (formula: C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			8	4 4		

- Molecule 4 is QUINACRINE MUSTARD (three-letter code: QUM) (formula: C<sub>23</sub>H<sub>28</sub>Cl<sub>3</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			28	23	1	3	1		
4	A	1	Total	C	Cl	N	O	0	0
			29	23	2	3	1		
4	B	1	Total	C	Cl	N	O	0	0
			28	23	1	3	1		
4	B	1	Total	C	Cl	N	O	0	0
			29	23	2	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	25	Total	O	0	0
			25	25		

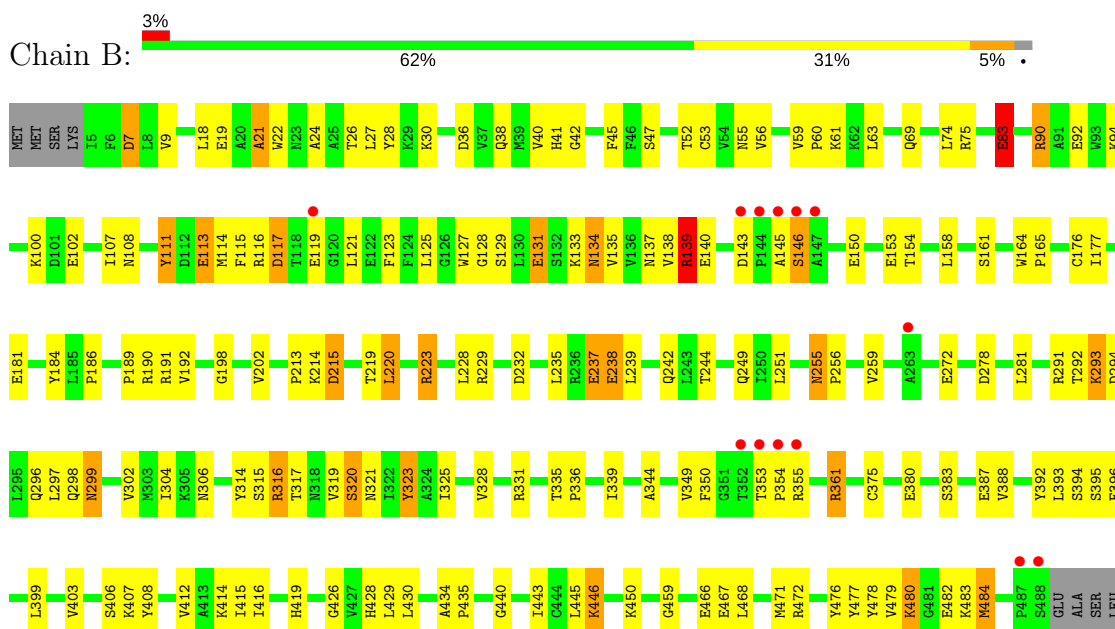
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: TRYPTANOTHIONE REDUCTASE (OXIDIZED FORM)



#### • Molecule 1: TRYPTANOTHIONE REDUCTASE (OXIDIZED FORM)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.10Å 93.10Å 156.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.70 29.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	79.0 (21.00-2.70) 79.5 (29.96-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.190 , 0.250 0.188 , 0.232	Depositor DCC
$R_{free}$ test set	1466 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: QUM, MAE, 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	0.41	0/3804	1.15	23/5154 (0.4%)
1	B	0.41	0/3795	1.20	23/5143 (0.4%)
All	All	0.41	0/7599	1.18	46/10297 (0.4%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	ARG	CD-NE-CZ	26.14	160.19	123.60
1	A	472	ARG	CD-NE-CZ	23.57	156.60	123.60
1	B	361	ARG	NE-CZ-NH2	11.73	126.17	120.30
1	A	139	ARG	CD-NE-CZ	11.66	139.92	123.60
1	B	139	ARG	CD-NE-CZ	10.80	138.72	123.60
1	A	361	ARG	CD-NE-CZ	9.87	137.42	123.60
1	A	361	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	361	ARG	CD-NE-CZ	9.07	136.30	123.60
1	B	238	GLU	OE1-CD-OE2	-8.57	113.02	123.30
1	B	361	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	A	482	GLU	OE1-CD-OE2	-7.67	114.09	123.30
1	A	131	GLU	OE1-CD-OE2	-7.54	114.26	123.30
1	A	111	TYR	CB-CG-CD1	7.29	125.37	121.00
1	A	83	GLU	OE1-CD-OE2	-7.27	114.58	123.30
1	B	131	GLU	OE1-CD-OE2	-7.25	114.60	123.30
1	B	380	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	A	238	GLU	OE1-CD-OE2	-6.94	114.97	123.30
1	A	361	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	380	GLU	OE1-CD-OE2	-6.70	115.26	123.30
1	B	482	GLU	OE1-CD-OE2	-6.66	115.31	123.30
1	B	69	GLN	CB-CG-CD	6.53	128.57	111.60
1	B	83	GLU	OE1-CD-OE2	-6.52	115.47	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	150	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	A	408	TYR	CB-CG-CD1	6.18	124.71	121.00
1	B	150	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	A	111	TYR	CZ-CE2-CD2	6.06	125.25	119.80
1	B	111	TYR	CB-CG-CD2	5.91	124.55	121.00
1	B	134	ASN	N-CA-CB	5.87	121.16	110.60
1	A	223	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	117	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	478	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	321	ASN	CB-CA-C	-5.67	99.07	110.40
1	A	55	ASN	N-CA-C	5.53	125.94	111.00
1	B	316	ARG	CD-NE-CZ	5.43	131.21	123.60
1	B	223	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	69	GLN	CB-CG-CD	5.35	125.51	111.60
1	A	117	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	150	GLU	CA-CB-CG	5.22	124.89	113.40
1	B	472	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	150	GLU	CB-CG-CD	5.15	128.11	114.20
1	B	408	TYR	CB-CG-CD1	5.09	124.05	121.00
1	B	220	LEU	CA-CB-CG	5.06	126.95	115.30
1	A	70	TYR	CB-CG-CD2	5.03	124.02	121.00
1	A	476	TYR	CB-CG-CD1	5.02	124.01	121.00
1	A	321	ASN	CA-CB-CG	5.01	124.41	113.40

There are no chirality outliers.

There are no planarity outliers.

## 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	3727	0	3739	130	1
1	B	3718	0	3726	142	1
2	A	53	0	31	1	0
2	B	53	0	31	3	0
3	A	8	0	2	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	57	0	48	33	0
4	B	57	0	48	14	0
5	A	28	0	0	4	0
5	B	25	0	0	5	0
All	All	7726	0	7625	278	1

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 18.

All (278) 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)
4:A:1502:QUM:H1	4:A:1502:QUM:C20	1.28	1.61
4:A:1502:QUM:C1	4:A:1502:QUM:C20	2.22	1.18
1:B:232:ASP:HB3	1:B:235:LEU:HD12	1.21	1.12
1:A:232:ASP:HB3	1:A:235:LEU:HD12	1.26	1.10
4:A:1502:QUM:H1	4:A:1502:QUM:H203	1.15	1.08
4:A:1502:QUM:C1	4:A:1502:QUM:H202	1.80	1.06
4:A:1502:QUM:C1	4:A:1502:QUM:H203	1.91	0.97
1:A:111:TYR:CE2	4:A:1502:QUM:H7	1.99	0.96
4:A:1502:QUM:H1	4:A:1502:QUM:H202	1.00	0.96
1:B:255:ASN:HD22	1:B:256:PRO:HD2	1.33	0.93
1:B:114:MET:HG3	4:B:1501:QUM:H231	1.52	0.92
1:A:387:GLU:HG3	1:A:480:LYS:HG3	1.52	0.91
4:B:1501:QUM:H173	4:B:1502:QUM:H8	1.53	0.89
1:B:55:ASN:HD21	1:B:108:ASN:HD21	1.20	0.88
1:B:41:HIS:HB3	1:B:55:ASN:HD22	1.39	0.86
1:B:235:LEU:HD23	1:B:430:LEU:HB2	1.57	0.86
1:B:387:GLU:HG3	1:B:480:LYS:HG3	1.58	0.86
1:A:235:LEU:HD11	1:A:428:HIS:HB3	1.57	0.85
1:B:297:LEU:HD22	1:B:302:VAL:HG21	1.59	0.85
1:B:320:SER:O	1:B:321:ASN:OD1	1.96	0.84
1:A:235:LEU:HD23	1:A:430:LEU:HB2	1.60	0.83
4:A:1501:QUM:H173	4:A:1502:QUM:H8	1.62	0.81
1:A:114:MET:HG3	4:A:1501:QUM:H231	1.61	0.81
1:A:111:TYR:CE2	4:A:1502:QUM:C7	2.63	0.81
1:B:36:ASP:OD1	2:B:1492:FAD:H1B	1.81	0.81
1:A:111:TYR:HE2	4:A:1502:QUM:H8	1.46	0.80
1:B:189:PRO:HB2	1:B:192:VAL:HG12	1.63	0.80
1:B:235:LEU:HD11	1:B:428:HIS:HB3	1.64	0.79
1:A:111:TYR:HE2	4:A:1502:QUM:C8	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:HG	1:B:63:LEU:HD21	1.66	0.76
1:A:94:LYS:NZ	1:A:186:PRO:HA	2.01	0.76
1:A:439:GLN:HE22	1:B:459:GLY:HA2	1.50	0.76
1:B:298:GLN:HG2	1:B:299:ASN:HD22	1.50	0.76
1:A:75:ARG:NH2	1:A:406:SER:OG	2.18	0.76
1:A:297:LEU:HD22	1:A:302:VAL:HG21	1.69	0.74
1:A:19:GLU:OE1	4:A:1501:QUM:H4	1.86	0.74
1:B:19:GLU:OE1	4:B:1501:QUM:H4	1.88	0.74
1:A:111:TYR:CD2	4:A:1502:QUM:H7	2.22	0.73
1:B:335:THR:HB	1:B:336:PRO:HD3	1.71	0.73
1:B:107:ILE:O	1:B:111:TYR:HD2	1.72	0.73
3:A:1500:MAE:O2	3:A:1500:MAE:O4	2.08	0.72
1:B:479:VAL:HB	1:B:484:MET:HE2	1.71	0.72
1:B:190:ARG:NH1	1:B:191:ARG:HD2	2.04	0.72
1:B:297:LEU:HD12	1:B:304:ILE:HD11	1.71	0.71
1:A:223:ARG:HH11	3:A:1500:MAE:C2	2.03	0.71
4:B:1501:QUM:H173	4:B:1502:QUM:C8	2.20	0.69
1:A:272:GLU:OE2	5:A:2018:HOH:O	2.10	0.69
1:B:139:ARG:HD3	1:B:146:SER:O	1.92	0.69
1:A:63:LEU:HD21	1:B:399:LEU:HG	1.73	0.69
1:A:190:ARG:NH1	1:A:191:ARG:HH11	1.91	0.68
1:B:94:LYS:NZ	1:B:186:PRO:HA	2.09	0.67
1:A:320:SER:O	1:A:321:ASN:HB2	1.95	0.67
1:B:75:ARG:NH2	1:B:406:SER:OG	2.27	0.67
1:A:297:LEU:HD12	1:A:304:ILE:HD11	1.75	0.67
1:A:111:TYR:CE2	4:A:1502:QUM:C8	2.78	0.67
1:B:21:ALA:HB1	1:B:121:LEU:HD11	1.76	0.66
1:A:90:ARG:HD3	1:B:83:GLU:OE2	1.95	0.66
1:B:7:ASP:OD2	1:B:30:LYS:HD3	1.96	0.66
1:A:439:GLN:HE21	1:B:466:GLU:HA	1.62	0.64
1:A:189:PRO:HB2	1:A:192:VAL:HG12	1.80	0.64
1:A:396:PHE:CE1	1:A:467:GLU:HG3	2.33	0.63
1:B:191:ARG:HH21	1:B:278:ASP:HB3	1.63	0.63
4:A:1501:QUM:H173	4:A:1502:QUM:C8	2.26	0.63
1:B:232:ASP:HB3	1:B:235:LEU:CD1	2.13	0.63
1:B:113:GLU:HA	1:B:116:ARG:NE	2.14	0.62
1:A:111:TYR:HE2	4:A:1501:QUM:H173	1.65	0.62
1:A:111:TYR:CE2	4:A:1502:QUM:H8	2.32	0.62
1:A:54:VAL:HG21	1:A:111:TYR:HE1	1.64	0.62
1:B:114:MET:HA	4:B:1501:QUM:H272	1.82	0.61
1:A:21:ALA:HB1	1:A:121:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:NH1	3:A:1500:MAE:C2	2.64	0.61
1:A:111:TYR:HE2	4:A:1502:QUM:C7	2.08	0.61
1:A:18:LEU:HD13	4:A:1501:QUM:H171	1.81	0.61
1:B:113:GLU:HG3	1:B:116:ARG:NH2	2.16	0.60
1:A:52:THR:HG23	1:A:56:VAL:HG23	1.83	0.60
1:A:94:LYS:HZ1	1:A:186:PRO:HA	1.65	0.60
1:B:115:PHE:CD2	1:B:123:PHE:HB2	2.37	0.60
1:B:113:GLU:HA	1:B:116:ARG:HE	1.67	0.60
1:B:297:LEU:HD22	1:B:302:VAL:CG2	2.30	0.59
1:B:131:GLU:HB2	1:B:137:ASN:ND2	2.17	0.59
1:B:214:LYS:HE2	1:B:215:ASP:OD2	2.03	0.59
1:A:114:MET:HA	4:A:1501:QUM:H272	1.84	0.58
1:A:76:GLU:HB3	1:A:404:SER:HB2	1.86	0.58
1:B:214:LYS:HG2	1:B:215:ASP:N	2.19	0.58
1:B:242:GLN:HG3	5:B:2007:HOH:O	2.02	0.57
1:B:42:GLY:HA2	1:B:184:TYR:CZ	2.40	0.57
1:A:19:GLU:HA	4:A:1501:QUM:H4	1.87	0.57
1:A:189:PRO:HG3	1:A:281:LEU:HD22	1.85	0.57
1:A:219:THR:HG23	1:A:251:LEU:HD13	1.87	0.57
1:B:339:ILE:HD11	4:B:1502:QUM:H222	1.87	0.56
1:B:237:GLU:HB3	5:B:2006:HOH:O	2.05	0.56
1:B:440:GLY:HA2	1:B:443:ILE:HD12	1.86	0.56
1:A:7:ASP:OD2	1:A:30:LYS:HD3	2.06	0.56
1:B:255:ASN:HD22	1:B:256:PRO:CD	2.12	0.56
1:A:214:LYS:HG2	1:A:215:ASP:H	1.70	0.56
1:B:396:PHE:CE1	1:B:467:GLU:HG3	2.41	0.56
1:A:399:LEU:HD21	1:B:59:VAL:HG13	1.88	0.56
1:A:114:MET:SD	4:A:1501:QUM:H172	2.46	0.56
1:A:297:LEU:HD22	1:A:302:VAL:CG2	2.35	0.56
1:B:131:GLU:HB3	1:B:135:VAL:HB	1.89	0.55
1:A:468:LEU:HA	1:A:471:MET:CE	2.36	0.55
1:A:114:MET:CG	4:A:1501:QUM:H231	2.35	0.55
1:B:113:GLU:HG3	1:B:116:ARG:HH21	1.71	0.55
1:B:255:ASN:O	1:B:272:GLU:HG3	2.06	0.54
1:A:468:LEU:HA	1:A:471:MET:HE3	1.90	0.54
1:B:416:ILE:HD11	5:B:2004:HOH:O	2.07	0.54
1:A:115:PHE:CD2	1:A:123:PHE:HB2	2.43	0.54
1:A:214:LYS:HG2	1:A:215:ASP:N	2.22	0.54
1:B:18:LEU:CD1	1:B:111:TYR:CE1	2.91	0.54
1:A:111:TYR:CE2	4:A:1501:QUM:H173	2.43	0.54
1:A:255:ASN:O	1:A:272:GLU:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:HD22	1:A:256:PRO:HD2	1.73	0.54
1:B:176:CYS:SG	1:B:259:VAL:HG21	2.48	0.54
1:A:479:VAL:HB	1:A:484:MET:HE2	1.90	0.53
1:A:232:ASP:OD1	1:A:414:LYS:HD3	2.09	0.53
1:B:161:SER:O	1:B:291:ARG:HD3	2.08	0.53
1:A:139:ARG:HD3	1:A:146:SER:O	2.09	0.53
1:B:249:GLN:HE21	1:B:251:LEU:HD11	1.72	0.53
1:A:479:VAL:HG21	1:A:484:MET:HE3	1.91	0.53
1:B:375:CYS:SG	1:B:445:LEU:HD12	2.49	0.53
1:B:94:LYS:HZ1	1:B:186:PRO:HA	1.73	0.53
1:A:59:VAL:HG13	1:B:399:LEU:HD21	1.91	0.53
1:A:335:THR:HB	1:A:336:PRO:HD3	1.90	0.53
1:B:26:THR:HG22	1:B:27:LEU:HD12	1.90	0.53
1:B:190:ARG:HA	1:B:213:PRO:HG2	1.89	0.52
1:B:476:TYR:CD2	1:B:483:LYS:HE2	2.44	0.52
1:A:479:VAL:HG23	1:A:484:MET:HG3	1.92	0.52
1:B:255:ASN:ND2	1:B:256:PRO:HD2	2.15	0.52
4:B:1501:QUM:C17	4:B:1502:QUM:C8	2.88	0.52
1:A:214:LYS:HE2	1:A:215:ASP:OD2	2.10	0.52
1:B:114:MET:SD	4:B:1501:QUM:H172	2.50	0.51
1:A:375:CYS:SG	1:A:445:LEU:HD12	2.49	0.51
1:B:41:HIS:HB3	1:B:55:ASN:ND2	2.18	0.51
1:B:41:HIS:CB	1:B:55:ASN:HD22	2.15	0.51
1:A:429:LEU:HD21	1:A:468:LEU:HD21	1.92	0.51
1:B:114:MET:CG	4:B:1501:QUM:H231	2.33	0.51
1:B:314:TYR:O	1:B:315:SER:HB2	2.10	0.51
1:B:298:GLN:HG2	1:B:299:ASN:ND2	2.25	0.51
1:A:198:GLY:O	1:A:202:VAL:HG23	2.10	0.50
1:A:434:ALA:N	1:A:435:PRO:CD	2.74	0.50
1:B:107:ILE:CG2	1:B:111:TYR:HE2	2.24	0.50
1:B:22:TRP:CH2	4:B:1501:QUM:H211	2.45	0.50
1:B:232:ASP:OD1	1:B:414:LYS:HD3	2.11	0.50
1:A:235:LEU:HD11	1:A:428:HIS:CB	2.34	0.50
1:A:297:LEU:HB3	1:A:302:VAL:CG2	2.42	0.50
1:A:235:LEU:CD2	1:A:430:LEU:HB2	2.38	0.50
1:B:127:TRP:O	1:B:138:VAL:HA	2.11	0.50
1:A:190:ARG:NH1	1:A:191:ARG:HD3	2.27	0.50
1:B:191:ARG:NH2	1:B:278:ASP:HB3	2.26	0.49
1:B:344:ALA:HB1	1:B:355:ARG:O	2.12	0.49
1:A:90:ARG:CD	1:B:83:GLU:OE2	2.58	0.49
1:B:191:ARG:HH21	1:B:278:ASP:CB	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LYS:HE3	1:B:319:VAL:HG12	1.95	0.49
1:A:298:GLN:HG2	1:A:299:ASN:N	2.26	0.49
1:A:392:TYR:CZ	1:A:474:PRO:HG3	2.47	0.49
1:B:18:LEU:HD13	4:B:1501:QUM:H171	1.92	0.49
1:B:238:GLU:OE2	5:B:2007:HOH:O	2.19	0.49
1:A:297:LEU:HB3	1:A:302:VAL:HG23	1.95	0.49
1:B:325:ILE:C	1:B:325:ILE:HD12	2.33	0.49
1:A:293:LYS:HG2	1:A:294:ASP:N	2.27	0.49
1:B:198:GLY:O	1:B:202:VAL:HG23	2.11	0.49
1:B:393:LEU:HD12	1:B:394:SER:N	2.27	0.49
1:B:18:LEU:HD13	1:B:111:TYR:CE1	2.48	0.48
1:B:189:PRO:HG3	1:B:281:LEU:HD22	1.94	0.48
1:B:219:THR:HG23	1:B:251:LEU:HD13	1.95	0.48
1:B:299:ASN:HD22	1:B:299:ASN:N	2.09	0.48
1:A:94:LYS:HD3	1:A:94:LYS:HA	1.57	0.48
1:B:7:ASP:N	1:B:7:ASP:OD1	2.46	0.48
1:A:353:THR:HA	1:A:354:PRO:HD3	1.76	0.48
1:A:94:LYS:HZ3	1:A:186:PRO:HA	1.77	0.48
1:B:59:VAL:HB	1:B:60:PRO:HD3	1.95	0.48
1:B:468:LEU:HA	1:B:471:MET:HE3	1.95	0.48
1:B:468:LEU:HA	1:B:471:MET:CE	2.44	0.48
1:A:176:CYS:SG	1:A:259:VAL:HG21	2.54	0.47
1:B:235:LEU:HD11	1:B:428:HIS:CB	2.41	0.47
1:A:235:LEU:CD1	1:A:428:HIS:HB3	2.38	0.47
1:B:113:GLU:CG	1:B:116:ARG:HH21	2.27	0.47
1:B:38:GLN:HG3	1:B:45:PHE:HD2	1.78	0.47
1:A:238:GLU:HG3	1:A:412:VAL:HG21	1.95	0.47
1:B:28:TYR:CD1	1:B:350:PHE:O	2.68	0.47
1:A:113:GLU:HG3	1:A:116:ARG:NH2	2.29	0.47
1:B:107:ILE:HG22	1:B:111:TYR:CE2	2.49	0.47
1:B:28:TYR:CE1	1:B:350:PHE:O	2.67	0.47
1:B:479:VAL:HB	1:B:484:MET:CE	2.41	0.47
1:A:111:TYR:CE2	4:A:1501:QUM:C17	2.98	0.47
1:B:477:TYR:N	1:B:477:TYR:CD1	2.82	0.47
1:A:114:MET:CA	4:A:1501:QUM:H272	2.45	0.47
1:B:293:LYS:HG2	1:B:294:ASP:N	2.30	0.47
1:B:297:LEU:HB3	1:B:302:VAL:CG2	2.45	0.46
1:B:214:LYS:HG2	1:B:215:ASP:H	1.80	0.46
1:B:52:THR:HG23	1:B:56:VAL:HG23	1.96	0.46
1:B:21:ALA:O	1:B:22:TRP:C	2.54	0.46
1:A:4:LYS:CE	1:A:134:ASN:OD1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLY:HA2	1:B:137:ASN:O	2.16	0.46
1:B:317:THR:HB	5:B:2012:HOH:O	2.16	0.46
1:A:189:PRO:HG2	1:A:192:VAL:HG11	1.98	0.46
1:B:388:VAL:HG12	1:B:419:HIS:HB3	1.97	0.46
1:A:83:GLU:OE1	1:B:90:ARG:HD3	2.16	0.45
1:B:38:GLN:NE2	1:B:40:VAL:O	2.49	0.45
1:A:14:GLY:HA2	1:A:51:GLY:HA3	1.97	0.45
1:A:164:TRP:CG	1:A:165:PRO:HD2	2.51	0.45
1:B:19:GLU:HA	4:B:1501:QUM:H4	1.98	0.45
1:B:375:CYS:O	1:B:426:GLY:HA2	2.16	0.45
1:B:446:LYS:HD2	1:B:446:LYS:HA	1.73	0.45
1:A:26:THR:HG22	1:A:27:LEU:HD12	1.98	0.45
1:B:291:ARG:NH1	2:B:1492:FAD:H2B	2.30	0.45
2:B:1492:FAD:H1'1	2:B:1492:FAD:H9	1.77	0.45
1:B:296:GLN:O	1:B:297:LEU:C	2.54	0.45
1:A:22:TRP:CH2	4:A:1501:QUM:H211	2.52	0.45
1:B:355:ARG:HD3	1:B:355:ARG:HH11	1.58	0.45
1:A:74:LEU:HD23	1:B:74:LEU:HD23	1.99	0.45
1:A:214:LYS:HG2	5:A:2014:HOH:O	2.16	0.44
1:A:446:LYS:HA	1:A:446:LYS:HD2	1.69	0.44
1:B:319:VAL:O	1:B:320:SER:C	2.55	0.44
1:B:9:VAL:HG23	1:B:154:THR:HG21	2.00	0.44
1:A:91:ALA:HB1	1:A:211:TYR:CD2	2.53	0.44
4:A:1501:QUM:C17	4:A:1502:QUM:C8	2.95	0.44
1:A:4:LYS:HE2	1:A:134:ASN:OD1	2.18	0.44
1:B:94:LYS:HD3	1:B:94:LYS:HA	1.58	0.44
1:A:59:VAL:HB	1:A:60:PRO:HD3	1.99	0.44
1:B:21:ALA:O	1:B:24:ALA:N	2.51	0.44
1:B:177:ILE:HB	1:B:181:GLU:HB2	2.00	0.43
1:A:195:VAL:HG21	1:A:284:MET:CE	2.48	0.43
1:A:375:CYS:O	1:A:426:GLY:HA2	2.18	0.43
1:B:392:TYR:HB2	1:B:415:ILE:HB	2.00	0.43
1:A:320:SER:HA	5:A:2021:HOH:O	2.19	0.43
4:B:1502:QUM:H221	4:B:1502:QUM:H202	1.62	0.43
1:B:297:LEU:HB3	1:B:302:VAL:HG23	2.00	0.43
1:A:94:LYS:HE2	1:A:186:PRO:O	2.19	0.43
1:B:298:GLN:HG2	1:B:299:ASN:N	2.33	0.43
1:B:353:THR:HA	1:B:354:PRO:HD3	1.75	0.43
1:B:361:ARG:NH2	1:B:446:LYS:HA	2.34	0.43
1:B:387:GLU:CD	1:B:480:LYS:HD2	2.39	0.43
4:A:1502:QUM:H221	4:A:1502:QUM:H202	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HE3	1:A:319:VAL:HG12	2.01	0.42
1:B:190:ARG:NH1	1:B:191:ARG:CD	2.80	0.42
1:A:93:TRP:O	1:A:97:ILE:HG12	2.19	0.42
1:A:228:LEU:CD1	1:A:239:LEU:HD23	2.49	0.42
1:A:433:ASN:O	1:A:437:ILE:HG13	2.20	0.42
1:B:143:ASP:OD2	1:B:145:ALA:HB3	2.19	0.42
1:B:412:VAL:O	1:B:429:LEU:HA	2.20	0.42
1:A:434:ALA:HB3	1:A:435:PRO:HD3	2.01	0.42
1:A:220:LEU:C	1:A:220:LEU:CD1	2.88	0.42
1:B:228:LEU:HD12	1:B:239:LEU:HD23	2.01	0.42
1:A:232:ASP:HA	5:A:2016:HOH:O	2.19	0.42
1:B:164:TRP:CG	1:B:165:PRO:HD2	2.55	0.42
1:A:114:MET:SD	4:A:1501:QUM:C17	3.08	0.42
1:A:39:MET:HE3	1:A:39:MET:HB3	1.95	0.41
1:B:434:ALA:N	1:B:435:PRO:CD	2.82	0.41
1:B:94:LYS:HZ3	1:B:186:PRO:HA	1.82	0.41
1:A:18:LEU:HD13	4:A:1501:QUM:C17	2.48	0.41
1:A:116:ARG:HB2	1:A:116:ARG:HE	1.48	0.41
1:A:190:ARG:HH11	1:A:191:ARG:HH11	1.64	0.41
1:B:107:ILE:CG2	1:B:111:TYR:CE2	3.03	0.41
1:A:388:VAL:HG12	1:A:419:HIS:HB3	2.02	0.41
1:A:38:GLN:HG3	1:A:45:PHE:HD2	1.84	0.41
1:B:429:LEU:HD21	1:B:468:LEU:HD21	2.03	0.41
1:A:143:ASP:OD1	1:A:144:PRO:HD2	2.20	0.41
1:B:238:GLU:HG3	1:B:412:VAL:HG21	2.02	0.41
1:A:143:ASP:OD2	1:A:145:ALA:HB3	2.20	0.41
1:A:220:LEU:HD13	1:A:221:CYS:N	2.36	0.41
1:A:345:LEU:HD13	1:A:345:LEU:C	2.41	0.41
1:A:387:GLU:OE2	1:A:480:LYS:HD2	2.20	0.41
1:B:131:GLU:OE1	1:B:137:ASN:ND2	2.47	0.41
1:B:158:LEU:HD13	1:B:323:TYR:HB2	2.03	0.41
1:A:114:MET:CB	4:A:1501:QUM:H231	2.51	0.41
1:A:61:LYS:NZ	2:A:1492:FAD:O4	2.54	0.41
1:A:162:GLY:HA2	1:A:327:ASP:HB2	2.01	0.41
1:B:114:MET:CA	4:B:1501:QUM:H272	2.49	0.41
1:B:349:VAL:HG12	1:B:350:PHE:CD1	2.56	0.41
1:A:228:LEU:HD12	1:A:239:LEU:HD23	2.03	0.40
1:A:400:MET:O	1:A:404:SER:N	2.52	0.40
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.91	0.40
1:A:251:LEU:HD12	1:A:251:LEU:N	2.36	0.40
1:A:42:GLY:HA2	1:A:184:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:VAL:CG2	1:A:484:MET:HG3	2.52	0.40
1:B:292:THR:O	1:B:293:LYS:C	2.59	0.40
1:A:100:LYS:HE3	1:A:100:LYS:HB3	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:ND2	1:B:407:LYS:NZ[3_554]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	483/492 (98%)	450 (93%)	30 (6%)	3 (1%)	28	56
1	B	482/492 (98%)	442 (92%)	36 (8%)	4 (1%)	22	49
All	All	965/984 (98%)	892 (92%)	66 (7%)	7 (1%)	25	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	LYS
1	B	299	ASN
1	A	41	HIS
1	B	320	SER
1	B	21	ALA
1	B	146	SER
1	A	227	ILE

### 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	405/412 (98%)	369 (91%)	36 (9%)	11	26
1	B	404/412 (98%)	366 (91%)	38 (9%)	10	23
All	All	809/824 (98%)	735 (91%)	74 (9%)	11	25

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	53	CYS
1	A	61	LYS
1	A	83	GLU
1	A	90	ARG
1	A	92	GLU
1	A	100	LYS
1	A	102	GLU
1	A	106	ASN
1	A	113	GLU
1	A	117	ASP
1	A	125	LEU
1	A	134	ASN
1	A	139	ARG
1	A	140	GLU
1	A	150	GLU
1	A	190	ARG
1	A	192	VAL
1	A	214	LYS
1	A	215	ASP
1	A	220	LEU
1	A	223	ARG
1	A	229	ARG
1	A	244	THR
1	A	293	LYS
1	A	306	ASN
1	A	323	TYR

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Mol	Chain	Res	Type
1	A	328	VAL
1	A	330	ASN
1	A	383	SER
1	A	384	LYS
1	A	395	SER
1	A	446	LYS
1	A	450	LYS
1	A	480	LYS
1	A	484	MET
1	B	7	ASP
1	B	47	SER
1	B	53	CYS
1	B	61	LYS
1	B	83	GLU
1	B	90	ARG
1	B	92	GLU
1	B	100	LYS
1	B	102	GLU
1	B	113	GLU
1	B	117	ASP
1	B	119	GLU
1	B	125	LEU
1	B	129	SER
1	B	134	ASN
1	B	139	ARG
1	B	140	GLU
1	B	153	GLU
1	B	215	ASP
1	B	220	LEU
1	B	223	ARG
1	B	229	ARG
1	B	237	GLU
1	B	244	THR
1	B	255	ASN
1	B	293	LYS
1	B	306	ASN
1	B	316	ARG
1	B	323	TYR
1	B	328	VAL
1	B	331	ARG
1	B	383	SER
1	B	395	SER

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Mol	Chain	Res	Type
1	B	403	VAL
1	B	446	LYS
1	B	450	LYS
1	B	480	LYS
1	B	484	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	180	ASN
1	A	255	ASN
1	A	306	ASN
1	A	433	ASN
1	A	439	GLN
1	B	55	ASN
1	B	69	GLN
1	B	106	ASN
1	B	166	HIS
1	B	180	ASN
1	B	249	GLN
1	B	255	ASN
1	B	299	ASN
1	B	306	ASN
1	B	433	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

7 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	1492	-	51,58,58	1.40	6 (11%)	54,89,89	1.83	6 (11%)
3	MAE	A	1500	-	1,7,7	0.51	0	0,8,8	0.00	-
4	QUM	A	1501	1	26,30,32	0.93	1 (3%)	35,41,43	1.55	4 (11%)
4	QUM	A	1502	1	27,31,32	1.09	2 (7%)	36,42,43	1.97	6 (16%)
2	FAD	B	1492	-	51,58,58	1.39	5 (9%)	54,89,89	1.83	8 (14%)
4	QUM	B	1501	1	26,30,32	0.93	1 (3%)	35,41,43	1.61	4 (11%)
4	QUM	B	1502	1	27,31,32	1.11	2 (7%)	36,42,43	1.79	5 (13%)

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	1492	-	-	0/28/50/50	0/6/6/6
3	MAE	A	1500	-	-	0/0/5/5	0/0/0/0
4	QUM	A	1501	1	-	0/14/16/18	0/3/3/3
4	QUM	A	1502	1	-	1/15/17/18	0/3/3/3
2	FAD	B	1492	-	-	0/28/50/50	0/6/6/6
4	QUM	B	1501	1	-	0/14/16/18	0/3/3/3
4	QUM	B	1502	1	-	0/15/17/18	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1502	QUM	C19-N18	-4.12	1.42	1.47
4	B	1502	QUM	C19-N18	-4.07	1.42	1.47
2	A	1492	FAD	C2B-C1B	-3.66	1.47	1.53
4	A	1501	QUM	C19-N18	-3.48	1.43	1.47
4	B	1501	QUM	C19-N18	-3.39	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1492	FAD	C2B-C1B	-2.79	1.49	1.53
2	A	1492	FAD	C8A-N7A	-2.06	1.30	1.34
2	A	1492	FAD	O4B-C4B	-2.06	1.40	1.45
2	B	1492	FAD	C4-N3	2.03	1.36	1.33
4	B	1502	QUM	C27-N24	2.28	1.52	1.47
4	A	1502	QUM	C27-N24	2.41	1.53	1.47
2	A	1492	FAD	O4B-C1B	2.86	1.45	1.41
2	B	1492	FAD	O4B-C1B	3.15	1.45	1.41
2	A	1492	FAD	C1'-N10	3.73	1.52	1.48
2	B	1492	FAD	C1'-N10	4.10	1.52	1.48
2	A	1492	FAD	C4-C4X	4.94	1.50	1.41
2	B	1492	FAD	C4-C4X	4.99	1.50	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1502	QUM	C13-C14-N10	-8.88	118.61	123.67
4	B	1502	QUM	C13-C14-N10	-7.14	119.60	123.67
4	A	1501	QUM	C12-C11-N10	-6.08	120.20	123.67
4	B	1501	QUM	C12-C11-N10	-5.77	120.38	123.67
4	B	1501	QUM	C13-C14-N10	-5.32	120.64	123.67
2	A	1492	FAD	C4X-C4-N3	-5.07	116.26	123.48
2	B	1492	FAD	C4X-C4-N3	-4.80	116.65	123.48
4	A	1501	QUM	C13-C14-N10	-4.10	121.33	123.67
4	B	1502	QUM	C12-C11-N10	-3.96	121.41	123.67
2	B	1492	FAD	O4'-C4'-C5'	-3.55	102.09	110.00
2	A	1492	FAD	C4X-C10-N10	-3.34	118.20	120.52
2	A	1492	FAD	O4'-C4'-C5'	-3.20	102.86	110.00
4	A	1502	QUM	C12-C11-N10	-2.65	122.16	123.67
2	B	1492	FAD	O5'-C5'-C4'	-2.13	103.67	109.36
4	B	1501	QUM	C9-C12-C11	2.05	120.27	118.51
4	A	1502	QUM	C5-C14-C13	2.14	122.09	119.63
4	A	1501	QUM	C9-C12-C11	2.25	120.44	118.51
4	A	1502	QUM	C8-C7-C6	2.26	121.94	119.21
2	A	1492	FAD	C4B-O4B-C1B	2.43	112.36	109.77
4	B	1502	QUM	C1-C12-C9	2.55	124.19	120.74
2	B	1492	FAD	C1'-N10-C10	2.69	121.26	118.50
2	B	1492	FAD	C4-C4X-N5	2.77	121.72	118.68
2	B	1492	FAD	C4A-C5A-N7A	2.85	112.16	109.41
4	A	1501	QUM	C14-N10-C11	2.95	121.63	117.84
4	B	1501	QUM	C14-N10-C11	3.09	121.81	117.84
4	A	1502	QUM	C14-N10-C11	3.12	121.86	117.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1502	QUM	C22-C23-N24	3.45	122.52	113.90
4	B	1502	QUM	C14-N10-C11	3.72	122.62	117.84
4	A	1502	QUM	C9-C13-C14	4.17	122.08	118.51
2	A	1492	FAD	C4X-N5-C5X	4.69	121.71	116.76
2	B	1492	FAD	C4X-N5-C5X	4.87	121.91	116.76
2	B	1492	FAD	C4-N3-C2	8.23	122.36	115.16
2	A	1492	FAD	C4-N3-C2	8.27	122.39	115.16

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1502	QUM	C20-C19-N18-C9

There are no ring outliers.

7 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1492	FAD	1	0
3	A	1500	MAE	3	0
4	A	1501	QUM	18	0
4	A	1502	QUM	18	0
2	B	1492	FAD	3	0
4	B	1501	QUM	12	0
4	B	1502	QUM	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	485/492 (98%)	-0.39	4 (0%) 86 86	19, 42, 73, 90	0
1	B	484/492 (98%)	-0.40	13 (2%) 55 55	19, 42, 73, 90	0
All	All	969/984 (98%)	-0.40	17 (1%) 69 70	19, 42, 73, 90	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	THR	4.0
1	B	263	ALA	3.7
1	B	354	PRO	3.3
1	B	488	SER	3.1
1	B	352	THR	3.1
1	A	4	LYS	3.0
1	B	145	ALA	2.8
1	A	488	SER	2.7
1	B	487	PRO	2.4
1	B	355	ARG	2.4
1	B	143	ASP	2.3
1	A	352	THR	2.3
1	B	147	ALA	2.3
1	B	119	GLU	2.1
1	B	146	SER	2.1
1	B	144	PRO	2.1
1	A	90	ARG	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
4	QUM	A	1502	29/30	0.72	0.41	9.18	47,55,57,58	29
4	QUM	B	1502	29/30	0.74	0.40	5.61	47,55,57,58	29
4	QUM	B	1501	28/30	0.58	0.53	5.45	53,55,68,71	28
4	QUM	A	1501	28/30	0.75	0.41	4.46	53,56,68,71	28
3	MAE	A	1500	8/8	0.94	0.20	2.30	29,31,33,35	0
2	FAD	B	1492	53/53	0.97	0.12	-0.12	17,33,49,50	0
2	FAD	A	1492	53/53	0.97	0.14	-0.25	16,33,49,50	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.