



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 09:38 AM EDT

PDB ID : 2FON  
Title : X-ray crystal structure of LeACX1, an acyl-CoA oxidase from *Lycopersicon esculentum* (tomato)  
Authors : Garavito, R.M.; Powers, R.A.  
Deposited on : unknown  
Resolution : 2.74 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.

---

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 : rb-20030345  
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) : rb-20030345

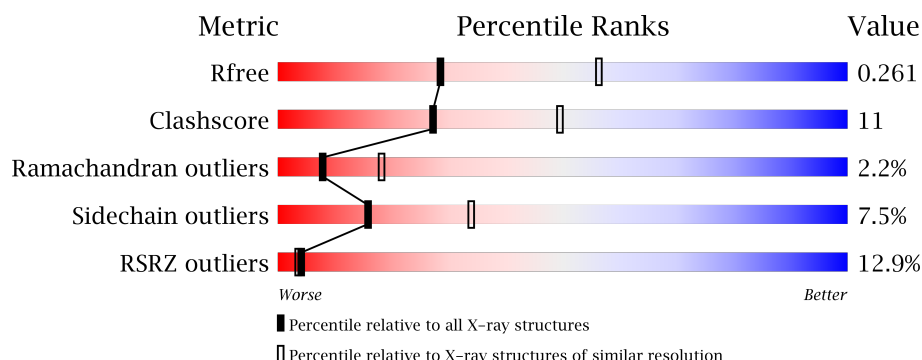
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

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	683	<div> <div>6%</div> <div>69%</div> <div>23%</div> <div>• • •</div> </div>
1	B	683	<div> <div>4%</div> <div>71%</div> <div>21%</div> <div>• •</div> </div>
1	C	683	<div> <div>27%</div> <div>70%</div> <div>22%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14949 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 peroxisomal acyl-CoA oxidase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5010	3180	873	932	25			
1	B	656	Total	C	N	O	S	0	0	0
			5040	3198	878	939	25			
1	C	653	Total	C	N	O	S	0	0	0
			4704	2960	828	892	24			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	CLONING ARTIFACT	UNP Q5D8D3
A	-17	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
A	-16	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
A	-15	SER	-	CLONING ARTIFACT	UNP Q5D8D3
A	-14	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-13	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-12	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-11	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-10	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-9	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-8	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
A	-7	SER	-	CLONING ARTIFACT	UNP Q5D8D3
A	-6	ALA	-	CLONING ARTIFACT	UNP Q5D8D3
A	-5	CYS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-4	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
A	-3	LEU	-	CLONING ARTIFACT	UNP Q5D8D3
A	-2	VAL	-	CLONING ARTIFACT	UNP Q5D8D3
A	-1	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
A	0	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
B	-18	MET	-	CLONING ARTIFACT	UNP Q5D8D3
B	-17	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
B	-16	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
B	-15	SER	-	CLONING ARTIFACT	UNP Q5D8D3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-13	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-12	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-11	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-10	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-9	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-8	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
B	-7	SER	-	CLONING ARTIFACT	UNP Q5D8D3
B	-6	ALA	-	CLONING ARTIFACT	UNP Q5D8D3
B	-5	CYS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-4	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
B	-3	LEU	-	CLONING ARTIFACT	UNP Q5D8D3
B	-2	VAL	-	CLONING ARTIFACT	UNP Q5D8D3
B	-1	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
B	0	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
C	-18	MET	-	CLONING ARTIFACT	UNP Q5D8D3
C	-17	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
C	-16	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
C	-15	SER	-	CLONING ARTIFACT	UNP Q5D8D3
C	-14	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-13	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-12	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-11	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-10	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-9	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-8	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
C	-7	SER	-	CLONING ARTIFACT	UNP Q5D8D3
C	-6	ALA	-	CLONING ARTIFACT	UNP Q5D8D3
C	-5	CYS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-4	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
C	-3	LEU	-	CLONING ARTIFACT	UNP Q5D8D3
C	-2	VAL	-	CLONING ARTIFACT	UNP Q5D8D3
C	-1	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
C	0	GLU	-	CLONING ARTIFACT	UNP Q5D8D3

- 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
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

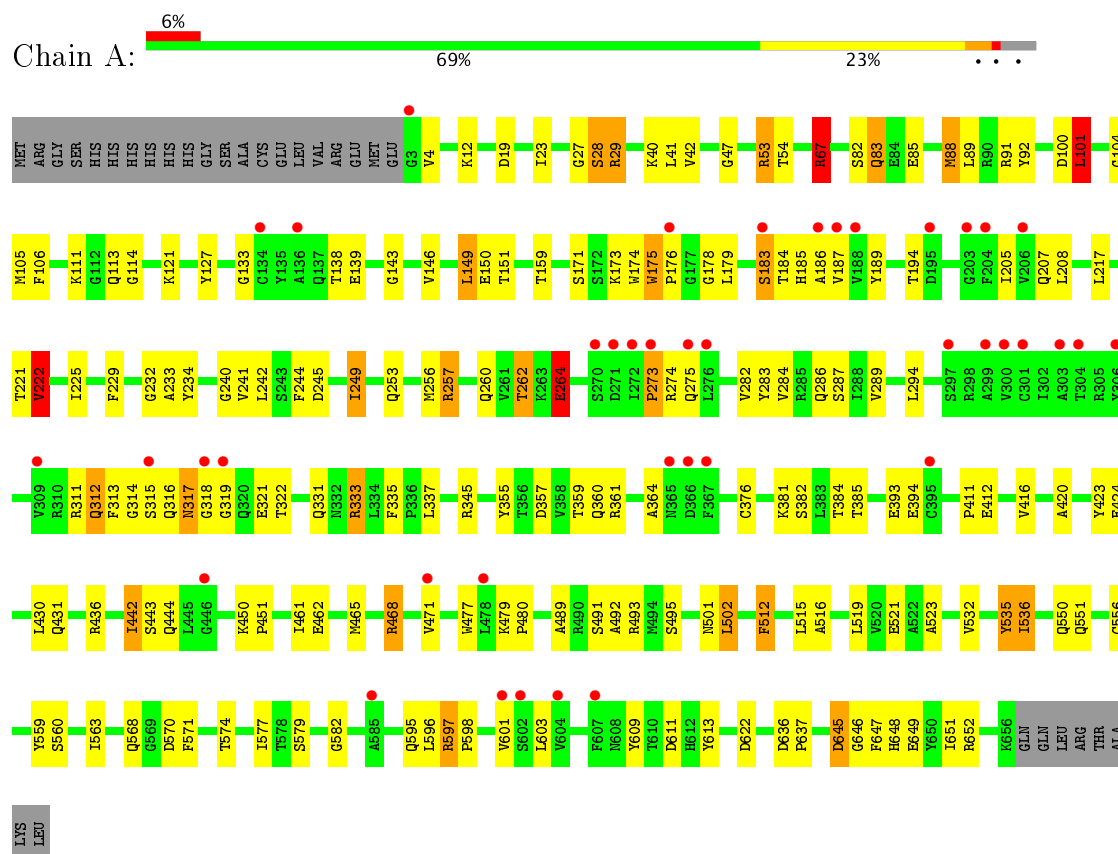
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	14	Total O 14 14	0	0
3	B	22	Total O 22 22	0	0

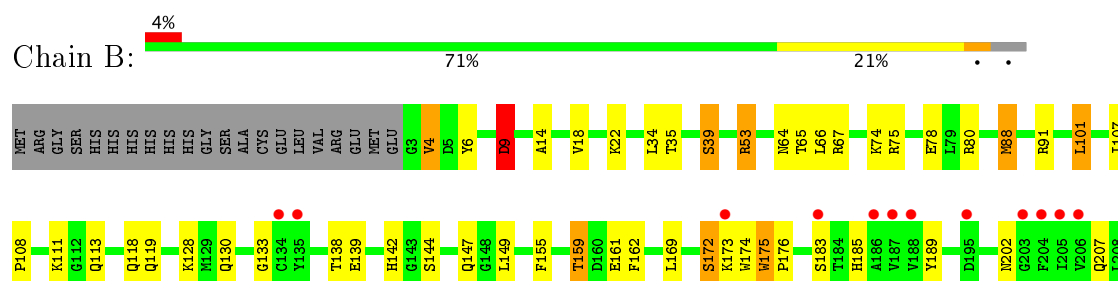
### 3 Residue-property plots

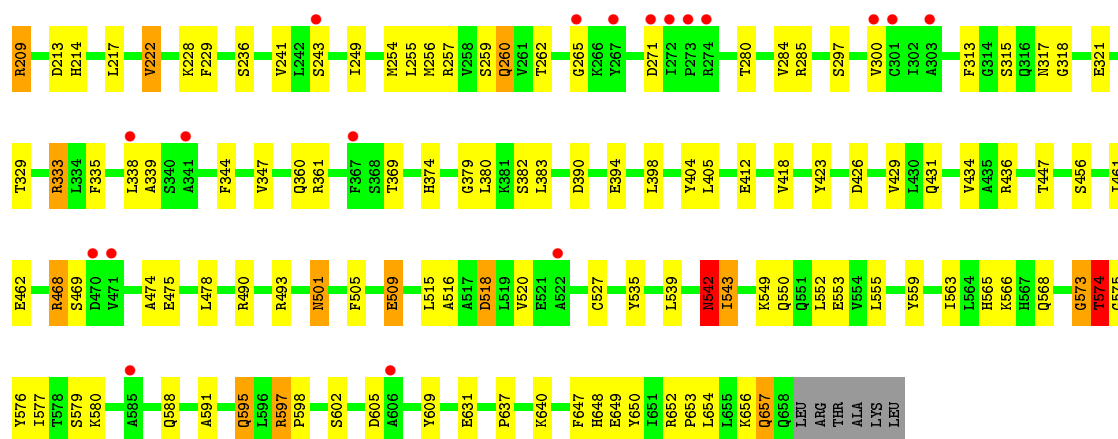
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: peroxisomal acyl-CoA oxidase 1A

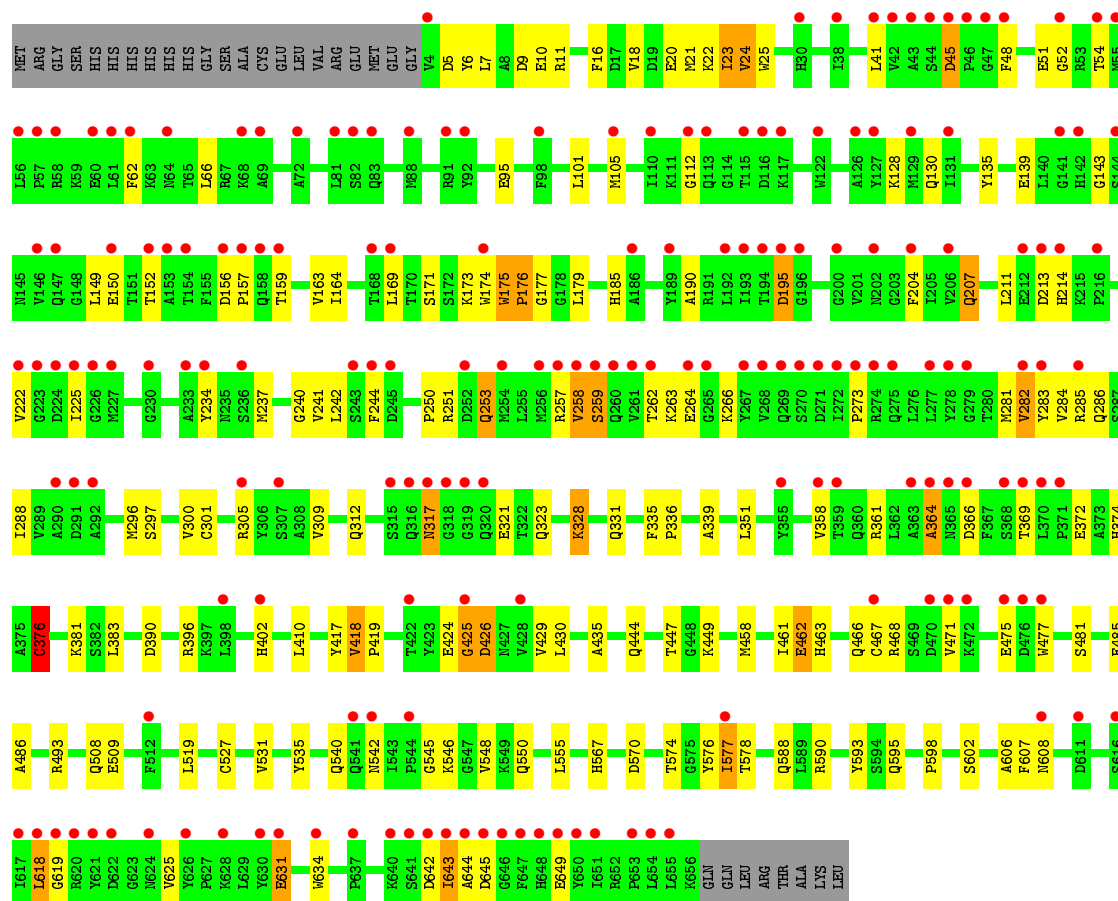


- Molecule 1: peroxisomal acyl-CoA oxidase 1A





• Molecule 1: peroxisomal acyl-CoA oxidase 1A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.20 Å   240.33 Å   89.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.74 29.82 – 2.74	Depositor EDS
% Data completeness (in resolution range)	92.9 (30.00-2.74) 92.8 (29.82-2.74)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.72 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.212   ,   0.267 0.205   ,   0.261	Depositor DCC
$R_{free}$ test set	3221 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 31.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% 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: 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	0.99	2/5120 (0.0%)	1.00	18/6948 (0.3%)
1	B	0.94	4/5150 (0.1%)	0.96	12/6988 (0.2%)
1	C	0.61	1/4803 (0.0%)	0.70	2/6552 (0.0%)
All	All	0.87	7/15073 (0.0%)	0.90	32/20488 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	VAL	CB-CG1	-6.60	1.39	1.52
1	B	243	SER	CA-CB	6.01	1.61	1.52
1	B	404	TYR	CD2-CE2	-5.64	1.30	1.39
1	C	376	CYS	CB-SG	-5.43	1.73	1.81
1	A	100	ASP	CB-CG	5.28	1.62	1.51
1	A	376	CYS	CB-SG	-5.13	1.73	1.81
1	B	631	GLU	CG-CD	5.12	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	NE-CZ-NH2	-10.09	115.26	120.30
1	B	53	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	53	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	B	101	LEU	CA-CB-CG	-7.94	97.04	115.30
1	A	345	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	A	101	LEU	CA-CB-CG	-7.71	97.58	115.30
1	A	100	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	611	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	53	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	333	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	B	390	ASP	CB-CG-OD2	-6.50	112.45	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	LEU	CA-CB-CG	-6.36	100.67	115.30
1	B	222	VAL	CB-CA-C	-5.98	100.03	111.40
1	A	217	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	67	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	213	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	217	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	390	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	333	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	618	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	100	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	B	209	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	41	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	B	605	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	222	VAL	CB-CA-C	-5.31	101.32	111.40
1	A	622	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	80	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	163	VAL	CB-CA-C	5.15	121.19	111.40
1	A	468	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	9	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	611	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	645	ASP	CB-CG-OD1	-5.04	113.77	118.30

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	5010	0	4838	122	0
1	B	5040	0	4884	112	0
1	C	4704	0	4258	98	0
2	A	53	0	31	7	0
2	B	53	0	31	6	0
2	C	53	0	31	5	0
3	A	14	0	0	0	0
3	B	22	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14949	0	14073	329	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 11.

All (329) 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:29:ARG:HH11	1:A:29:ARG:HG3	1.15	1.07
1:C:361:ARG:HD2	1:C:369:THR:HG21	1.47	0.97
1:A:29:ARG:HH11	1:A:29:ARG:CG	1.77	0.96
1:B:361:ARG:HD3	1:B:369:THR:HG21	1.45	0.94
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.35	0.90
1:B:516:ALA:O	1:B:520:VAL:HG23	1.72	0.90
1:A:316:GLN:O	1:A:317:ASN:O	1.90	0.88
1:C:475:GLU:HA	1:C:588:GLN:NE2	1.90	0.87
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.40	0.85
1:A:29:ARG:NH1	1:A:29:ARG:HG3	1.92	0.84
1:A:412:GLU:O	1:A:416:VAL:HG12	1.78	0.84
1:B:539:LEU:HD13	1:B:553:GLU:HG3	1.61	0.81
1:A:317:ASN:O	1:A:319:GLY:N	2.13	0.79
1:C:372:GLU:O	1:C:376:CYS:HB2	1.83	0.79
1:C:475:GLU:HA	1:C:588:GLN:HE22	1.48	0.78
1:A:442:ILE:O	1:A:444:GLN:N	2.16	0.78
1:B:490:ARG:HD3	3:B:2013:HOH:O	1.84	0.76
1:A:113:GLN:O	1:A:257:ARG:HB2	1.86	0.75
1:A:333:ARG:HD2	1:A:394:GLU:OE2	1.85	0.75
1:B:595:GLN:O	1:B:598:PRO:HD2	1.85	0.74
1:A:516:ALA:HA	1:A:519:LEU:HD12	1.67	0.74
1:B:637:PRO:O	1:B:640:LYS:HG3	1.87	0.74
1:B:656:LYS:O	1:B:657:GLN:HG2	1.89	0.72
1:C:485:GLU:HG2	1:C:576:TYR:OH	1.89	0.72
1:C:286:GLN:HG2	1:C:351:LEU:HB3	1.70	0.71
1:C:296:MET:O	1:C:300:VAL:HG23	1.91	0.71
1:C:631:GLU:HA	1:C:634:TRP:HD1	1.56	0.71
1:B:333:ARG:HB2	1:B:398:LEU:HD21	1.73	0.70
1:B:34:LEU:HD23	1:B:88:MET:HG2	1.73	0.70
1:B:285:ARG:HG3	1:B:285:ARG:NH1	2.06	0.70
1:C:381:LYS:NZ	1:C:425:GLY:O	2.23	0.70
1:A:143:GLY:HA3	2:A:1000:FAD:O2P	1.92	0.69
1:B:91:ARG:HH11	1:B:91:ARG:HG3	1.58	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:HB3	1:C:240:GLY:HA3	1.75	0.69
1:A:568:GLN:NE2	1:A:582:GLY:HA3	2.08	0.68
1:C:105:MET:HB3	1:C:135:TYR:HB2	1.75	0.68
1:A:185:HIS:NE2	1:A:207:GLN:HG3	2.08	0.68
1:A:442:ILE:HD11	1:A:495:SER:HB3	1.73	0.68
1:C:20:GLU:HA	1:C:23:ILE:HD12	1.75	0.68
1:C:458:MET:HG2	1:C:461:ILE:HD11	1.75	0.68
1:A:101:LEU:HD23	1:A:105:MET:HG3	1.75	0.68
1:A:431:GLN:HG3	1:A:523:ALA:HB1	1.76	0.68
1:A:138:THR:OG1	2:A:1000:FAD:H1'1	1.94	0.67
1:A:502:LEU:HD12	1:A:515:LEU:HD12	1.77	0.67
1:C:284:VAL:HG12	1:C:288:ILE:HD11	1.76	0.67
1:A:502:LEU:HD12	1:A:515:LEU:CD1	2.24	0.66
1:B:118:GLN:NE2	1:B:254:MET:O	2.26	0.66
1:A:91:ARG:NH1	1:A:91:ARG:HG3	2.10	0.66
1:A:316:GLN:C	1:A:317:ASN:O	2.32	0.66
1:B:138:THR:OG1	2:B:2000:FAD:H1'1	1.96	0.66
1:C:339:ALA:HA	1:C:555:LEU:HD22	1.78	0.66
1:A:493:ARG:HD3	1:A:574:THR:HB	1.76	0.66
1:A:105:MET:HA	1:A:105:MET:HE2	1.79	0.65
1:B:174:TRP:C	1:B:176:PRO:HD3	2.17	0.64
1:B:176:PRO:HA	2:B:2000:FAD:C4	2.26	0.64
1:C:493:ARG:HD3	1:C:574:THR:HB	1.80	0.64
1:A:436:ARG:HG2	1:A:512:PHE:CZ	2.33	0.63
1:C:112:GLY:O	1:C:257:ARG:HD3	1.97	0.63
1:C:361:ARG:CD	1:C:369:THR:HG21	2.24	0.63
1:A:570:ASP:O	1:A:574:THR:HG23	1.98	0.63
1:C:174:TRP:O	1:C:175:TRP:HB2	2.00	0.62
1:A:47:GLY:O	1:A:67:ARG:NH2	2.32	0.62
1:C:242:LEU:HD21	1:C:244:PHE:CE1	2.35	0.62
1:B:361:ARG:CD	1:B:369:THR:HG21	2.24	0.62
1:A:283:TYR:HB2	1:A:355:TYR:CE1	2.36	0.61
1:A:88:MET:CE	1:A:91:ARG:HE	2.14	0.61
2:A:1000:FAD:H2'	2:A:1000:FAD:C9	2.30	0.61
1:A:282:VAL:O	1:A:286:GLN:HB2	2.01	0.60
1:A:595:GLN:O	1:A:598:PRO:HD2	2.01	0.60
1:B:209:ARG:HD3	1:B:214:HIS:O	2.01	0.60
1:C:527:CYS:O	1:C:531:VAL:HG23	2.02	0.60
1:C:618:LEU:HA	1:C:625:VAL:HG13	1.84	0.60
1:B:185:HIS:NE2	1:B:207:GLN:HG3	2.16	0.60
1:A:173:LYS:O	1:A:241:VAL:HA	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:HIS:HB3	3:B:2014:HOH:O	2.02	0.59
2:A:1000:FAD:H2'	2:A:1000:FAD:H9	1.84	0.59
1:A:264:GLU:CD	1:A:264:GLU:H	2.06	0.59
1:C:139:GLU:HG3	1:C:149:LEU:HD22	1.83	0.59
1:A:176:PRO:HA	2:A:1000:FAD:C4	2.32	0.59
2:B:2000:FAD:H2'	2:B:2000:FAD:C9	2.33	0.59
1:C:284:VAL:O	1:C:288:ILE:HG13	2.03	0.59
1:B:542:ASN:CG	1:B:543:ILE:H	2.06	0.58
1:B:262:THR:OG1	1:B:265:GLY:O	2.21	0.58
1:A:411:PRO:HB3	1:B:229:PHE:CD2	2.39	0.58
1:C:41:LEU:O	1:C:45:ASP:HB2	2.03	0.58
1:C:361:ARG:HA	1:C:364:ALA:HB3	1.86	0.58
1:C:297:SER:HB2	1:C:607:PHE:CZ	2.38	0.58
1:C:545:GLY:O	1:C:548:VAL:HB	2.05	0.57
1:B:574:THR:OG1	1:B:575:GLY:N	2.37	0.57
1:A:82:SER:OG	1:A:85:GLU:HG3	2.05	0.57
1:A:225:ILE:HD12	1:B:405:LEU:HD21	1.86	0.56
1:A:242:LEU:HD21	1:A:244:PHE:CZ	2.41	0.56
1:B:139:GLU:HG3	1:B:149:LEU:HD22	1.88	0.56
1:B:173:LYS:O	1:B:241:VAL:HA	2.06	0.56
1:C:396:ARG:HA	1:C:410:LEU:HD13	1.86	0.56
1:C:45:ASP:HB3	1:C:48:PHE:HD1	1.70	0.56
1:A:88:MET:HE1	1:A:91:ARG:HE	1.69	0.56
1:B:333:ARG:CZ	1:B:398:LEU:HD23	2.35	0.56
1:B:436:ARG:NH2	1:B:509:GLU:OE2	2.38	0.55
1:A:262:THR:OG1	1:A:264:GLU:OE1	2.19	0.55
1:B:139:GLU:HG2	1:B:173:LYS:HD3	1.87	0.55
1:A:568:GLN:HE22	1:A:582:GLY:HA3	1.72	0.55
1:A:150:GLU:HB2	1:A:171:SER:HB3	1.89	0.55
1:C:590:ARG:HH11	1:C:590:ARG:HG3	1.71	0.55
2:B:2000:FAD:H2'	2:B:2000:FAD:H9	1.89	0.55
1:C:185:HIS:HE2	1:C:207:GLN:HG2	1.71	0.55
1:B:493:ARG:HD3	1:B:574:THR:HB	1.89	0.54
1:C:173:LYS:HB2	1:C:242:LEU:HB3	1.88	0.54
1:C:418:VAL:N	1:C:419:PRO:HD2	2.22	0.54
1:A:636:ASP:CG	1:A:637:PRO:HD2	2.28	0.54
1:C:374:HIS:C	1:C:374:HIS:CD2	2.81	0.54
1:A:139:GLU:OE2	1:A:151:THR:OG1	2.15	0.54
1:B:256:MET:HB3	1:B:260:GLN:HB3	1.89	0.54
1:C:185:HIS:NE2	1:C:207:GLN:HG2	2.23	0.54
1:A:431:GLN:HG3	1:A:523:ALA:CB	2.38	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:VAL:HG22	1:B:6:TYR:CE1	2.43	0.54
1:B:382:SER:HB3	1:B:431:GLN:HE21	1.73	0.54
1:C:435:ALA:HB1	1:C:519:LEU:HB3	1.90	0.54
1:B:4:VAL:HG22	1:B:6:TYR:CZ	2.43	0.53
1:A:29:ARG:NH1	1:A:29:ARG:CG	2.48	0.53
1:B:329:THR:O	1:B:333:ARG:HG3	2.09	0.53
1:B:493:ARG:HH11	1:B:574:THR:HB	1.74	0.53
1:A:174:TRP:O	1:A:175:TRP:HB2	2.08	0.53
1:A:221:THR:O	1:A:242:LEU:HA	2.09	0.52
1:C:297:SER:HB2	1:C:607:PHE:CE2	2.45	0.52
1:C:7:LEU:HD21	1:C:309:VAL:HG22	1.91	0.52
1:C:361:ARG:HB2	1:C:366:ASP:HB3	1.92	0.52
1:A:283:TYR:HB2	1:A:355:TYR:HE1	1.74	0.52
1:A:335:PHE:CG	1:A:596:LEU:HD23	2.45	0.52
1:C:152:THR:O	1:C:164:ILE:HA	2.10	0.52
1:A:331:GLN:HG2	1:A:335:PHE:CE1	2.45	0.52
1:A:382:SER:HB3	1:A:431:GLN:OE1	2.10	0.51
1:B:174:TRP:O	1:B:175:TRP:HB2	2.10	0.51
1:B:256:MET:HA	1:B:259:SER:O	2.10	0.51
1:C:471:VAL:HG11	1:C:477:TRP:NE1	2.25	0.51
1:C:486:ALA:HA	1:C:576:TYR:CE2	2.44	0.51
1:B:475:GLU:O	1:B:478:LEU:HB2	2.11	0.51
1:C:234:TYR:O	1:C:237:MET:HB3	2.11	0.51
1:B:35:THR:OG1	1:B:88:MET:CE	2.58	0.51
1:B:518:ASP:N	1:B:518:ASP:OD2	2.44	0.51
1:C:467:CYS:HG	1:C:576:TYR:HE1	1.58	0.50
1:B:209:ARG:HD2	1:B:214:HIS:CE1	2.46	0.50
1:B:394:GLU:O	1:B:398:LEU:HG	2.12	0.50
1:A:67:ARG:HB2	1:B:650:TYR:CE1	2.46	0.50
1:A:19:ASP:O	1:A:23:ILE:HD13	2.10	0.50
1:B:18:VAL:O	1:B:22:LYS:HG3	2.10	0.50
1:B:53:ARG:HH22	1:B:412:GLU:CD	2.11	0.50
1:A:551:GLN:HE21	1:A:603:LEU:HD11	1.77	0.50
1:B:542:ASN:O	1:B:543:ILE:HB	2.12	0.50
1:A:273:PRO:C	1:A:275:GLN:H	2.15	0.49
1:B:559:TYR:O	1:B:563:ILE:HG12	2.11	0.49
1:C:174:TRP:HD1	1:C:175:TRP:CD1	2.30	0.49
2:C:3000:FAD:O1A	2:C:3000:FAD:H8A	2.12	0.49
1:A:471:VAL:HG21	1:A:477:TRP:CE2	2.46	0.49
1:A:651:ILE:HD13	1:B:66:LEU:HB3	1.94	0.49
1:B:175:TRP:N	1:B:176:PRO:HD3	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ARG:NH1	1:B:575:GLY:O	2.45	0.49
1:A:442:ILE:C	1:A:444:GLN:H	2.15	0.49
1:B:128:LYS:HD2	1:B:130:GLN:NE2	2.27	0.49
1:C:128:LYS:HB2	1:C:130:GLN:NE2	2.27	0.49
1:C:282:VAL:O	1:C:286:GLN:HB2	2.12	0.49
1:B:159:THR:HG21	1:B:161:GLU:OE1	2.12	0.49
1:B:474:ALA:HB1	1:B:588:GLN:HB2	1.94	0.49
1:B:505:PHE:HE1	1:B:515:LEU:HD11	1.77	0.49
1:C:417:TYR:C	1:C:419:PRO:HD2	2.33	0.49
1:A:111:LYS:HZ1	1:A:127:TYR:HH	1.57	0.48
1:C:16:PHE:HZ	1:C:602:SER:O	1.95	0.48
1:A:461:ILE:O	1:A:462:GLU:C	2.50	0.48
1:B:107:ILE:HB	1:B:108:PRO:HD3	1.95	0.48
1:A:88:MET:CE	1:A:91:ARG:NE	2.77	0.48
1:B:159:THR:CG2	1:B:161:GLU:OE1	2.60	0.48
1:A:535:TYR:CE2	1:A:556:CYS:HB2	2.48	0.48
1:B:379:GLY:HA3	1:B:527:CYS:SG	2.53	0.48
1:A:138:THR:HG1	2:A:1000:FAD:H1'1	1.76	0.48
1:A:187:VAL:HG12	1:A:189:TYR:CE1	2.47	0.48
1:A:648:HIS:HD2	1:A:652:ARG:HD2	1.79	0.48
1:C:331:GLN:OE1	1:C:593:TYR:HB3	2.12	0.48
1:C:361:ARG:HD3	1:C:366:ASP:OD2	2.14	0.48
1:B:64:ASN:OD1	1:B:67:ARG:NH1	2.47	0.48
1:C:25:TRP:CD1	1:C:607:PHE:HA	2.49	0.48
1:C:22:LYS:HA	1:C:606:ALA:O	2.12	0.48
1:A:382:SER:CB	1:A:431:GLN:OE1	2.62	0.47
1:B:493:ARG:HH11	1:B:574:THR:CB	2.27	0.47
1:B:133:GLY:HA2	1:B:185:HIS:O	2.13	0.47
1:B:175:TRP:N	1:B:176:PRO:CD	2.77	0.47
1:C:150:GLU:HB2	1:C:171:SER:HB3	1.96	0.47
1:A:106:PHE:CD1	1:A:133:GLY:HA3	2.48	0.47
1:A:420:ALA:HA	1:A:423:TYR:CE2	2.49	0.47
1:A:249:ILE:HG13	1:A:253:GLN:NE2	2.30	0.47
1:B:14:ALA:HB2	1:B:602:SER:OG	2.14	0.47
1:B:647:PHE:C	1:B:647:PHE:CD2	2.88	0.47
1:B:169:LEU:O	1:B:172:SER:HB2	2.15	0.47
1:B:297:SER:OG	1:B:609:TYR:OH	2.17	0.47
1:B:447:THR:HG22	1:B:447:THR:O	2.15	0.47
1:B:542:ASN:CG	1:B:543:ILE:N	2.68	0.47
1:B:426:ASP:HB3	1:B:429:VAL:HB	1.97	0.47
1:A:111:LYS:NZ	1:A:127:TYR:OH	2.35	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PHE:CD1	1:A:596:LEU:HD23	2.49	0.46
2:A:1000:FAD:H2A	1:B:329:THR:OG1	2.16	0.46
1:A:178:GLY:O	1:A:183:SER:HB2	2.15	0.46
1:A:179:LEU:HD23	1:A:240:GLY:HA3	1.98	0.46
1:A:568:GLN:NE2	1:A:582:GLY:CA	2.78	0.46
1:B:111:LYS:O	1:B:119:GLN:NE2	2.48	0.46
1:C:372:GLU:HG2	1:C:372:GLU:O	2.15	0.46
1:B:474:ALA:C	1:B:588:GLN:HE21	2.19	0.46
1:A:284:VAL:O	1:A:287:SER:HB3	2.16	0.46
1:B:573:GLY:O	1:B:575:GLY:N	2.49	0.45
1:B:469:SER:HB2	1:B:576:TYR:CE2	2.51	0.45
1:C:10:GLU:OE2	1:C:323:GLN:NE2	2.49	0.45
1:A:114:GLY:O	1:A:257:ARG:HG3	2.16	0.45
1:C:328:LYS:HA	1:C:328:LYS:HD2	1.59	0.45
1:B:9:ASP:N	1:B:9:ASP:OD1	2.44	0.45
1:C:567:HIS:HB3	1:C:570:ASP:OD2	2.16	0.45
1:B:461:ILE:O	1:B:462:GLU:C	2.54	0.45
1:C:358:VAL:O	1:C:361:ARG:HG2	2.17	0.45
1:A:294:LEU:HD21	1:A:613:TYR:OH	2.16	0.45
1:B:313:PHE:O	1:B:321:GLU:HB3	2.17	0.45
1:C:52:GLY:C	1:C:54:THR:H	2.20	0.45
1:A:88:MET:CE	1:A:88:MET:HA	2.47	0.45
1:B:339:ALA:HA	1:B:555:LEU:HD22	1.99	0.45
1:C:21:MET:HG3	1:C:606:ALA:HB1	1.98	0.45
1:C:101:LEU:HD22	2:C:3000:FAD:O4	2.17	0.45
1:B:280:THR:O	1:B:284:VAL:HG23	2.17	0.44
1:A:521:GLU:CD	1:B:565:HIS:HE2	2.21	0.44
1:C:20:GLU:HB2	1:C:548:VAL:HG21	2.00	0.44
1:C:577:ILE:HG23	1:C:578:THR:O	2.16	0.44
1:C:643:ILE:HG12	1:C:644:ALA:N	2.31	0.44
1:A:289:VAL:HG13	1:A:384:THR:HG21	1.99	0.44
1:A:314:GLY:O	1:A:315:SER:C	2.55	0.44
1:A:502:LEU:HD12	1:A:515:LEU:HD13	1.98	0.44
1:C:105:MET:HB3	1:C:135:TYR:CB	2.44	0.44
1:C:176:PRO:HA	2:C:3000:FAD:C4	2.47	0.44
1:C:301:CYS:O	1:C:305:ARG:HG3	2.18	0.44
1:B:597:ARG:HB3	1:B:598:PRO:HD3	1.99	0.44
1:B:75:ARG:HD2	1:B:75:ARG:HA	1.77	0.44
1:C:285:ARG:HA	1:C:288:ILE:HD12	1.99	0.44
1:C:631:GLU:HG2	1:C:631:GLU:O	2.17	0.44
1:A:205:ILE:HB	1:A:253:GLN:HG2	1.99	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:C	1:A:444:GLN:N	2.71	0.44
1:B:447:THR:CG2	1:B:447:THR:O	2.65	0.44
1:A:311:ARG:HA	1:A:322:THR:O	2.17	0.44
1:B:34:LEU:CD2	1:B:88:MET:HG2	2.45	0.44
1:A:479:LYS:HA	1:A:480:PRO:HD2	1.85	0.44
1:B:344:PHE:HA	1:B:347:VAL:HG12	2.00	0.44
1:C:462:GLU:HG3	1:C:463:HIS:H	1.81	0.44
1:A:312:GLN:O	1:A:313:PHE:HB2	2.18	0.44
1:B:74:LYS:O	1:B:78:GLU:HG3	2.18	0.44
1:A:27:GLY:O	1:A:28:SER:HB3	2.17	0.43
1:C:425:GLY:HA3	1:C:430:LEU:HD21	1.99	0.43
1:A:559:TYR:O	1:A:563:ILE:HG12	2.18	0.43
1:B:4:VAL:CG2	1:B:6:TYR:CZ	3.01	0.43
1:C:258:VAL:CG2	1:C:259:SER:N	2.81	0.43
1:C:447:THR:OG1	1:C:449:LYS:HB3	2.18	0.43
1:A:186:ALA:HB2	1:A:208:LEU:HD11	1.99	0.43
1:A:381:LYS:O	1:A:385:THR:HG23	2.18	0.43
1:C:419:PRO:HB3	2:C:3000:FAD:HM71	2.00	0.43
1:A:355:TYR:CD2	1:A:355:TYR:C	2.91	0.43
1:C:101:LEU:HD12	1:C:101:LEU:H	1.82	0.43
1:C:23:ILE:O	1:C:24:VAL:C	2.57	0.43
1:C:281:MET:O	1:C:283:TYR:N	2.52	0.43
1:B:335:PHE:CD2	1:B:335:PHE:N	2.85	0.43
1:A:104:GLY:O	1:A:105:MET:HE3	2.19	0.43
1:A:294:LEU:HD12	1:A:609:TYR:OH	2.19	0.43
1:C:5:ASP:OD1	1:C:11:ARG:NH1	2.52	0.43
1:B:189:TYR:HA	1:B:202:ASN:O	2.19	0.42
1:B:113:GLN:O	1:B:255:LEU:HB3	2.19	0.42
1:C:509:GLU:OE1	1:C:509:GLU:HA	2.19	0.42
1:B:138:THR:HG1	2:B:2000:FAD:H1'1	1.84	0.42
1:B:35:THR:O	1:B:39:SER:HB2	2.18	0.42
1:B:591:ALA:O	1:B:595:GLN:HG2	2.19	0.42
1:A:249:ILE:HG13	1:A:253:GLN:HE21	1.84	0.42
1:C:251:ARG:C	1:C:253:GLN:H	2.23	0.42
1:B:501:ASN:HD22	1:B:501:ASN:HA	1.50	0.42
1:C:101:LEU:HD13	1:C:177:GLY:HA3	2.02	0.42
1:C:426:ASP:OD2	2:C:3000:FAD:H2B	2.19	0.42
1:A:242:LEU:HD21	1:A:244:PHE:HZ	1.84	0.42
1:C:156:ASP:HA	1:C:157:PRO:HD3	1.82	0.42
1:C:190:ALA:HB3	1:C:204:PHE:CE1	2.54	0.42
1:C:262:THR:HG22	1:C:263:LYS:H	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:TYR:O	1:A:286:GLN:HB3	2.20	0.42
1:A:42:VAL:HG11	1:A:92:TYR:C	2.40	0.42
1:B:35:THR:OG1	1:B:88:MET:HE3	2.19	0.42
1:A:646:GLY:HA3	1:B:66:LEU:HD12	2.01	0.42
1:C:95:GLU:HA	1:C:95:GLU:OE1	2.19	0.42
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.60	0.42
1:A:597:ARG:C	1:A:597:ARG:HD2	2.40	0.42
1:B:155:PHE:HB2	1:B:162:PHE:CE2	2.55	0.42
1:C:195:ASP:OD1	1:C:195:ASP:N	2.52	0.42
1:A:222:VAL:HA	1:A:241:VAL:O	2.18	0.41
1:A:83:GLN:HA	1:A:83:GLN:HE21	1.85	0.41
1:B:379:GLY:CA	1:B:434:VAL:HG21	2.50	0.41
1:B:383:LEU:HD12	1:B:383:LEU:HA	1.80	0.41
1:A:381:LYS:HD2	1:A:430:LEU:CD1	2.50	0.41
1:C:176:PRO:HB2	1:C:179:LEU:HB2	2.02	0.41
1:A:184:THR:O	1:A:208:LEU:N	2.43	0.41
1:A:532:VAL:O	1:A:536:ILE:HD12	2.20	0.41
1:B:65:THR:OG1	1:B:236:SER:HB2	2.21	0.41
1:C:435:ALA:CB	1:C:519:LEU:HB3	2.48	0.41
1:C:595:GLN:O	1:C:598:PRO:HD2	2.21	0.41
1:A:273:PRO:C	1:A:275:GLN:N	2.73	0.41
1:A:357:ASP:O	1:A:361:ARG:HG3	2.20	0.41
1:A:450:LYS:HA	1:A:451:PRO:HD3	1.93	0.41
1:A:647:PHE:CE1	1:B:214:HIS:CE1	3.09	0.41
1:A:489:ALA:O	1:A:493:ARG:HD2	2.21	0.41
1:A:491:SER:O	1:A:492:ALA:C	2.58	0.41
1:C:312:GLN:HA	1:C:321:GLU:OE2	2.20	0.41
1:A:83:GLN:CA	1:A:83:GLN:HE21	2.34	0.41
1:B:552:LEU:HD23	1:B:552:LEU:HA	1.94	0.41
1:B:576:TYR:HD2	1:B:577:ILE:HG23	1.86	0.41
1:A:232:GLY:O	1:A:233:ALA:C	2.59	0.40
1:A:571:PHE:HB2	1:A:577:ILE:HD11	2.02	0.40
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.85	0.40
1:A:146:VAL:O	1:A:149:LEU:HG	2.21	0.40
1:B:374:HIS:CD2	1:B:374:HIS:C	2.94	0.40
1:B:652:ARG:O	1:B:653:PRO:C	2.59	0.40
1:C:383:LEU:HD22	1:C:527:CYS:HB2	2.02	0.40
1:A:179:LEU:HD11	1:A:242:LEU:HD22	2.02	0.40
1:A:603:LEU:HD23	1:A:603:LEU:HA	1.84	0.40
1:B:144:SER:HB2	2:B:2000:FAD:O1A	2.22	0.40
1:B:579:SER:O	1:B:580:LYS:C	2.58	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:PHE:N	1:C:336:PRO:CD	2.84	0.40
1:A:245:ASP:OD1	1:A:245:ASP:C	2.60	0.40
1:B:436:ARG:HH22	1:B:509:GLU:CD	2.24	0.40
1:B:539:LEU:O	1:B:549:LYS:HE3	2.21	0.40
1:C:643:ILE:HG12	1:C:645:ASP:H	1.87	0.40
1:A:321:GLU:OE1	1:B:142:HIS:NE2	2.38	0.40
1:A:393:GLU:OE1	1:A:393:GLU:HA	2.21	0.40
1:C:305:ARG:NH1	1:C:619:GLY:O	2.54	0.40
1:C:62:PHE:O	1:C:66:LEU:HG	2.21	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	Percentiles	
1	A	652/683 (96%)	591 (91%)	47 (7%)	14 (2%)	8	19
1	B	654/683 (96%)	617 (94%)	27 (4%)	10 (2%)	12	28
1	C	651/683 (95%)	560 (86%)	71 (11%)	20 (3%)	5	10
All	All	1957/2049 (96%)	1768 (90%)	145 (7%)	44 (2%)	8	18

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	175	TRP
1	A	317	ASN
1	A	318	GLY
1	B	175	TRP
1	B	271	ASP
1	B	574	THR
1	C	23	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	175	TRP
1	C	266	LYS
1	C	273	PRO
1	C	282	VAL
1	C	546	LYS
1	A	12	LYS
1	A	53	ARG
1	A	273	PRO
1	A	442	ILE
1	A	443	SER
1	B	318	GLY
1	B	573	GLY
1	C	24	VAL
1	C	51	GLU
1	C	159	THR
1	C	214	HIS
1	C	468	ARG
1	B	317	ASN
1	B	542	ASN
1	C	317	ASN
1	C	364	ALA
1	C	424	GLU
1	A	28	SER
1	A	264	GLU
1	A	274	ARG
1	A	364	ALA
1	A	424	GLU
1	C	608	ASN
1	B	543	ILE
1	B	597	ARG
1	B	657	GLN
1	C	176	PRO
1	C	6	TYR
1	C	143	GLY
1	C	425	GLY
1	C	250	PRO

### 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	509/571 (89%)	470 (92%)	39 (8%)	15	32
1	B	516/571 (90%)	482 (93%)	34 (7%)	19	41
1	C	434/571 (76%)	397 (92%)	37 (8%)	12	27
All	All	1459/1713 (85%)	1349 (92%)	110 (8%)	16	34

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	29	ARG
1	A	40	LYS
1	A	67	ARG
1	A	83	GLN
1	A	88	MET
1	A	89	LEU
1	A	101	LEU
1	A	121	LYS
1	A	149	LEU
1	A	159	THR
1	A	183	SER
1	A	194	THR
1	A	222	VAL
1	A	229	PHE
1	A	234	TYR
1	A	249	ILE
1	A	256	MET
1	A	257	ARG
1	A	260	GLN
1	A	262	THR
1	A	264	GLU
1	A	312	GLN
1	A	359	THR
1	A	360	GLN
1	A	465	MET
1	A	468	ARG
1	A	501	ASN
1	A	502	LEU
1	A	512	PHE
1	A	535	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	536	ILE
1	A	550	GLN
1	A	560	SER
1	A	579	SER
1	A	597	ARG
1	A	601	VAL
1	A	645	ASP
1	A	649	GLU
1	B	4	VAL
1	B	9	ASP
1	B	39	SER
1	B	88	MET
1	B	101	LEU
1	B	147	GLN
1	B	159	THR
1	B	172	SER
1	B	183	SER
1	B	222	VAL
1	B	228	LYS
1	B	249	ILE
1	B	257	ARG
1	B	260	GLN
1	B	315	SER
1	B	333	ARG
1	B	338	LEU
1	B	360	GLN
1	B	418	VAL
1	B	423	TYR
1	B	456	SER
1	B	468	ARG
1	B	501	ASN
1	B	509	GLU
1	B	518	ASP
1	B	535	TYR
1	B	542	ASN
1	B	550	GLN
1	B	566	LYS
1	B	568	GLN
1	B	574	THR
1	B	595	GLN
1	B	649	GLU
1	B	654	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	9	ASP
1	C	18	VAL
1	C	45	ASP
1	C	169	LEU
1	C	195	ASP
1	C	207	GLN
1	C	211	LEU
1	C	213	ASP
1	C	222	VAL
1	C	225	ILE
1	C	241	VAL
1	C	253	GLN
1	C	258	VAL
1	C	259	SER
1	C	264	GLU
1	C	317	ASN
1	C	328	LYS
1	C	376	CYS
1	C	390	ASP
1	C	402	HIS
1	C	418	VAL
1	C	426	ASP
1	C	429	VAL
1	C	444	GLN
1	C	462	GLU
1	C	466	GLN
1	C	481	SER
1	C	508	GLN
1	C	535	TYR
1	C	540	GLN
1	C	542	ASN
1	C	550	GLN
1	C	577	ILE
1	C	631	GLU
1	C	642	ASP
1	C	643	ILE
1	C	649	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	83	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	202	ASN
1	A	253	GLN
1	A	444	GLN
1	A	473	GLN
1	A	501	ASN
1	A	567	HIS
1	A	568	GLN
1	A	588	GLN
1	A	648	HIS
1	B	130	GLN
1	B	202	ASN
1	B	260	GLN
1	B	374	HIS
1	B	444	GLN
1	B	501	ASN
1	B	542	ASN
1	B	588	GLN
1	C	202	ASN
1	C	360	GLN
1	C	374	HIS
1	C	466	GLN
1	C	501	ASN
1	C	541	GLN
1	C	550	GLN
1	C	588	GLN

### 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 ⓘ

3 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	1000	-	51,58,58	1.60	10 (19%)	54,89,89	2.50	12 (22%)
2	FAD	B	2000	-	51,58,58	1.49	8 (15%)	54,89,89	2.14	11 (20%)
2	FAD	C	3000	-	51,58,58	1.46	6 (11%)	54,89,89	1.84	6 (11%)

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	1000	-	-	0/28/50/50	0/6/6/6
2	FAD	B	2000	-	-	0/28/50/50	0/6/6/6
2	FAD	C	3000	-	-	0/28/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	FAD	C6-C5X	-3.35	1.36	1.41
2	B	2000	FAD	C6-C5X	-3.05	1.37	1.41
2	A	1000	FAD	O2'-C2'	-2.34	1.38	1.43
2	B	2000	FAD	O3B-C3B	-2.18	1.37	1.43
2	B	2000	FAD	O2'-C2'	-2.04	1.38	1.43
2	A	1000	FAD	O3B-C3B	-2.02	1.38	1.43
2	C	3000	FAD	C5X-N5	2.19	1.38	1.35
2	A	1000	FAD	C4-N3	2.22	1.37	1.33
2	A	1000	FAD	C2A-N1A	2.24	1.38	1.33
2	B	2000	FAD	C1'-N10	2.27	1.50	1.48
2	A	1000	FAD	C1'-N10	3.15	1.51	1.48
2	B	2000	FAD	C4-N3	3.16	1.38	1.33
2	C	3000	FAD	C2A-N1A	3.27	1.40	1.33
2	A	1000	FAD	C2A-N3A	3.36	1.37	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	FAD	C10-N1	3.49	1.38	1.33
2	A	1000	FAD	C9A-N10	3.51	1.43	1.38
2	B	2000	FAD	C10-N1	3.54	1.38	1.33
2	B	2000	FAD	C2A-N3A	3.57	1.38	1.32
2	C	3000	FAD	C4-N3	3.57	1.39	1.33
2	C	3000	FAD	C10-N1	3.68	1.38	1.33
2	C	3000	FAD	C4X-N5	4.24	1.39	1.33
2	A	1000	FAD	C4X-N5	4.52	1.39	1.33
2	B	2000	FAD	C4X-N5	4.59	1.39	1.33
2	C	3000	FAD	C2A-N3A	5.19	1.40	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	FAD	N3A-C2A-N1A	-11.56	118.79	128.86
2	B	2000	FAD	N3A-C2A-N1A	-10.26	119.92	128.86
2	C	3000	FAD	N3A-C2A-N1A	-9.03	120.99	128.86
2	A	1000	FAD	O2'-C2'-C3'	-3.88	99.46	109.09
2	B	2000	FAD	O5'-C5'-C4'	-3.80	99.22	109.36
2	B	2000	FAD	C7M-C7-C6	-2.54	113.97	120.34
2	C	3000	FAD	C4X-C4-N3	-2.43	120.03	123.48
2	B	2000	FAD	O2'-C2'-C3'	-2.32	103.34	109.09
2	A	1000	FAD	O5B-C5B-C4B	-2.24	101.04	109.00
2	A	1000	FAD	O3B-C3B-C2B	-2.07	105.19	111.83
2	A	1000	FAD	C9A-C5X-N5	-2.04	119.21	122.24
2	B	2000	FAD	C4X-C4-N3	-2.03	120.59	123.48
2	A	1000	FAD	C4X-C4-N3	-2.02	120.61	123.48
2	B	2000	FAD	O3B-C3B-C4B	-2.02	105.19	111.09
2	A	1000	FAD	O3B-C3B-C4B	-2.01	105.22	111.09
2	B	2000	FAD	C4X-N5-C5X	2.33	119.22	116.76
2	C	3000	FAD	C4X-N5-C5X	2.59	119.50	116.76
2	B	2000	FAD	C4-C4X-N5	2.73	121.67	118.68
2	B	2000	FAD	C1'-C2'-C3'	3.02	118.46	109.82
2	C	3000	FAD	C5X-C9A-N10	3.06	119.93	117.66
2	A	1000	FAD	C1'-C2'-C3'	3.39	119.52	109.82
2	C	3000	FAD	C1'-N10-C9A	3.46	121.52	118.35
2	A	1000	FAD	C6-C5X-C9A	3.49	123.54	119.00
2	B	2000	FAD	C4-N3-C2	4.42	119.03	115.16
2	B	2000	FAD	C1'-N10-C9A	4.50	122.47	118.35
2	A	1000	FAD	C1'-N10-C9A	4.95	122.88	118.35
2	A	1000	FAD	C4X-N5-C5X	5.50	122.57	116.76
2	C	3000	FAD	C4-N3-C2	5.65	120.10	115.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	1000	FAD	C4-N3-C2	6.69	121.01	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	FAD	7	0
2	B	2000	FAD	6	0
2	C	3000	FAD	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	654/683 (95%)	0.44	41 (6%) 21 20	49, 67, 78, 91	0
1	B	656/683 (96%)	0.42	30 (4%) 33 33	53, 67, 78, 85	0
1	C	653/683 (95%)	1.33	183 (28%) 1 0	55, 70, 89, 112	0
All	All	1963/2049 (95%)	0.73	254 (12%) 4 3	49, 68, 81, 112	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	GLY	8.3
1	C	646	GLY	8.3
1	C	617	ILE	7.1
1	C	272	ILE	7.0
1	C	245	ASP	6.8
1	C	644	ALA	6.5
1	C	158	GLN	6.4
1	C	48	PHE	6.2
1	C	55	MET	5.9
1	C	650	TYR	5.7
1	C	645	ASP	5.7
1	C	471	VAL	5.7
1	C	273	PRO	5.6
1	C	194	THR	5.6
1	C	62	PHE	5.6
1	C	648	HIS	5.6
1	C	318	GLY	5.4
1	C	42	VAL	5.3
1	C	470	ASP	5.3
1	C	92	TYR	5.1
1	C	642	ASP	5.1
1	C	30	HIS	5.0
1	C	98	PHE	5.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	616	SER	4.8
1	C	157	PRO	4.8
1	C	363	ALA	4.8
1	C	159	THR	4.7
1	C	223	GLY	4.6
1	C	261	VAL	4.6
1	C	643	ILE	4.6
1	C	57	PRO	4.6
1	C	195	ASP	4.6
1	C	127	TYR	4.6
1	C	112	GLY	4.5
1	C	88	MET	4.4
1	C	56	LEU	4.4
1	C	268	VAL	4.3
1	A	271	ASP	4.3
1	C	64	ASN	4.3
1	C	47	GLY	4.3
1	C	649	GLU	4.3
1	C	154	THR	4.2
1	C	117	LYS	4.2
1	C	365	ASN	4.2
1	C	271	ASP	4.2
1	C	214	HIS	4.1
1	C	619	GLY	4.1
1	C	233	ALA	4.1
1	A	365	ASN	4.1
1	C	655	LEU	4.1
1	C	193	ILE	4.1
1	A	272	ILE	4.0
1	C	81	LEU	4.0
1	C	192	LEU	4.0
1	C	113	GLN	4.0
1	C	156	ASP	4.0
1	A	273	PRO	4.0
1	C	122	TRP	3.9
1	C	647	PHE	3.9
1	C	69	ALA	3.9
1	A	276	LEU	3.9
1	C	110	ILE	3.9
1	A	301	CYS	3.8
1	C	624	ASN	3.7
1	A	366	ASP	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	470	ASP	3.7
1	C	216	PRO	3.7
1	C	630	TYR	3.7
1	C	43	ALA	3.6
1	C	317	ASN	3.6
1	C	477	TRP	3.6
1	C	269	GLN	3.6
1	C	54	THR	3.6
1	C	52	GLY	3.6
1	C	227	MET	3.5
1	A	446	GLY	3.5
1	A	187	VAL	3.5
1	C	359	THR	3.5
1	A	195	ASP	3.4
1	C	169	LEU	3.4
1	C	259	SER	3.4
1	A	604	VAL	3.4
1	C	126	ALA	3.4
1	C	61	LEU	3.4
1	C	368	SER	3.4
1	B	272	ILE	3.4
1	C	291	ASP	3.4
1	C	654	LEU	3.3
1	C	116	ASP	3.3
1	C	252	ASP	3.3
1	C	146	VAL	3.3
1	C	651	ILE	3.3
1	C	355	TYR	3.3
1	C	641	SER	3.3
1	B	301	CYS	3.3
1	C	41	LEU	3.3
1	C	44	SER	3.2
1	A	367	PHE	3.2
1	C	213	ASP	3.2
1	C	637	PRO	3.2
1	C	626	TYR	3.2
1	C	234	TYR	3.2
1	C	467	CYS	3.2
1	C	204	PHE	3.2
1	C	316	GLN	3.2
1	B	271	ASP	3.1
1	C	131	ILE	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	83	GLN	3.1
1	B	187	VAL	3.1
1	C	283	TYR	3.1
1	C	319	GLY	3.1
1	C	512	PHE	3.0
1	C	370	LEU	3.0
1	A	304	THR	3.0
1	C	422	THR	3.0
1	A	270	SER	3.0
1	C	244	PHE	3.0
1	C	174	TRP	3.0
1	C	254	MET	3.0
1	C	144	SER	2.9
1	C	243	SER	2.9
1	B	273	PRO	2.9
1	C	264	GLU	2.9
1	C	369	THR	2.9
1	C	628	LYS	2.9
1	B	265	GLY	2.9
1	C	189	TYR	2.9
1	C	274	ARG	2.8
1	A	297	SER	2.8
1	A	186	ALA	2.8
1	A	471	VAL	2.8
1	C	262	THR	2.8
1	A	134	CYS	2.8
1	C	224	ASP	2.8
1	C	222	VAL	2.8
1	C	472	LYS	2.8
1	B	471	VAL	2.8
1	C	290	ALA	2.8
1	B	606	ALA	2.8
1	C	265	GLY	2.8
1	C	611	ASP	2.7
1	A	203	GLY	2.7
1	C	142	HIS	2.7
1	C	267	TYR	2.7
1	A	601	VAL	2.7
1	A	607	PHE	2.7
1	C	285	ARG	2.7
1	C	292	ALA	2.7
1	C	275	GLN	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	256	MET	2.7
1	C	46	PRO	2.6
1	C	68	LYS	2.6
1	B	267	TYR	2.6
1	C	82	SER	2.6
1	B	205	ILE	2.6
1	C	631	GLU	2.6
1	A	299	ALA	2.6
1	C	196	GLY	2.6
1	C	152	THR	2.6
1	A	300	VAL	2.6
1	C	577	ILE	2.6
1	C	282	VAL	2.6
1	C	270	SER	2.6
1	C	147	GLN	2.5
1	A	478	LEU	2.5
1	C	236	SER	2.5
1	B	303	ALA	2.5
1	B	204	PHE	2.5
1	C	105	MET	2.5
1	C	634	TRP	2.5
1	C	225	ILE	2.5
1	C	150	GLU	2.5
1	C	258	VAL	2.5
1	A	318	GLY	2.5
1	C	230	GLY	2.5
1	C	398	LEU	2.5
1	C	618	LEU	2.5
1	B	206	VAL	2.5
1	C	115	THR	2.5
1	C	320	GLN	2.5
1	C	72	ALA	2.4
1	C	544	PRO	2.4
1	C	620	ARG	2.4
1	B	203	GLY	2.4
1	B	341	ALA	2.4
1	C	622	ASP	2.4
1	B	188	VAL	2.4
1	C	206	VAL	2.4
1	C	279	GLY	2.4
1	C	129	MET	2.4
1	C	402	HIS	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	45	ASP	2.4
1	B	135	TYR	2.4
1	B	300	VAL	2.4
1	C	91	ARG	2.4
1	A	204	PHE	2.3
1	A	306	TYR	2.3
1	B	186	ALA	2.3
1	B	243	SER	2.3
1	C	200	GLY	2.3
1	B	367	PHE	2.3
1	C	278	TYR	2.3
1	C	168	THR	2.3
1	B	195	ASP	2.3
1	C	58	ARG	2.3
1	A	315	SER	2.3
1	C	653	PRO	2.3
1	B	585	ALA	2.3
1	C	153	ALA	2.3
1	C	4	VAL	2.3
1	C	315	SER	2.3
1	C	38	ILE	2.3
1	C	186	ALA	2.3
1	C	358	VAL	2.3
1	A	395	CYS	2.2
1	A	183	SER	2.2
1	C	608	ASN	2.2
1	A	176	PRO	2.2
1	C	425	GLY	2.2
1	B	183	SER	2.2
1	B	274	ARG	2.2
1	A	585	ALA	2.2
1	C	366	ASP	2.2
1	C	428	VAL	2.2
1	C	305	ARG	2.2
1	C	141	GLY	2.2
1	C	257	ARG	2.2
1	C	307	SER	2.2
1	C	364	ALA	2.2
1	A	206	VAL	2.1
1	A	275	GLN	2.1
1	A	3	GLY	2.1
1	B	134	CYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	202	ASN	2.1
1	C	475	GLU	2.1
1	A	319	GLY	2.1
1	C	260	GLN	2.1
1	C	542	ASN	2.1
1	C	60	GLU	2.1
1	B	522	ALA	2.1
1	C	277	LEU	2.1
1	A	602	SER	2.1
1	B	338	LEU	2.1
1	C	541	GLN	2.1
1	B	173	LYS	2.1
1	A	303	ALA	2.1
1	C	476	ASP	2.1
1	A	188	VAL	2.0
1	A	309	VAL	2.0
1	C	621	TYR	2.0
1	A	136	ALA	2.0
1	C	640	LYS	2.0
1	C	212	GLU	2.0
1	C	371	PRO	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
2	FAD	C	3000	53/53	0.78	0.30	0.74	87,99,107,107	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	1000	53/53	0.93	0.18	-1.00	43,55,59,63	0
2	FAD	B	2000	53/53	0.94	0.18	-1.04	45,49,55,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.