



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:46 AM GMT

PDB ID : 1V0J  
Title : UDP-GALACTOPYRANOSE MUTASE FROM MYCOBACTERIUM TUBERCULOSIS  
Authors : Beis, K.; Naismith, J.H.  
Deposited on : 2004-03-30  
Resolution : 2.25 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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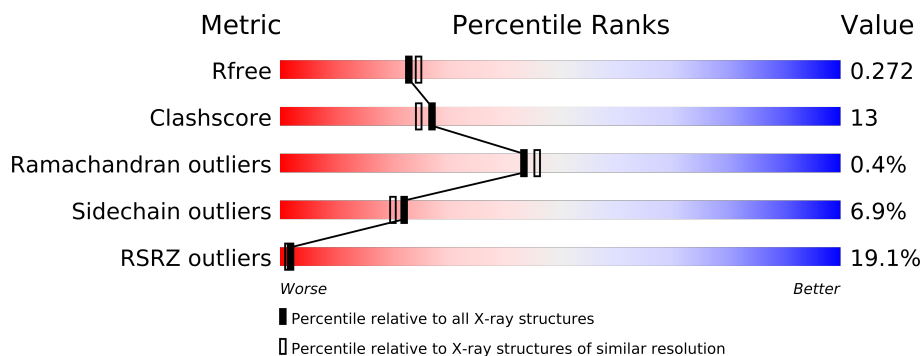
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.25 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))
$R_{free}$	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	399	
1	B	399	
1	C	399	
1	D	399	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	BCN	A	1394	-	X

## 2 Entry composition i

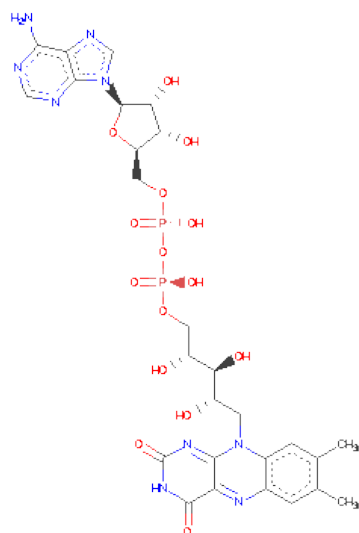
There are 4 unique types of molecules in this entry. The entry contains 13892 atoms, of which 0 are hydrogen and 0 are deuterium.

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 UDP-GALACTOPYRANOSE MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3162	2020	548	585	9			
1	B	388	Total	C	N	O	S	0	0	0
			3162	2020	548	585	9			
1	C	388	Total	C	N	O	S	0	0	0
			3162	2020	548	585	9			
1	D	388	Total	C	N	O	S	0	0	0
			3162	2020	548	585	9			

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



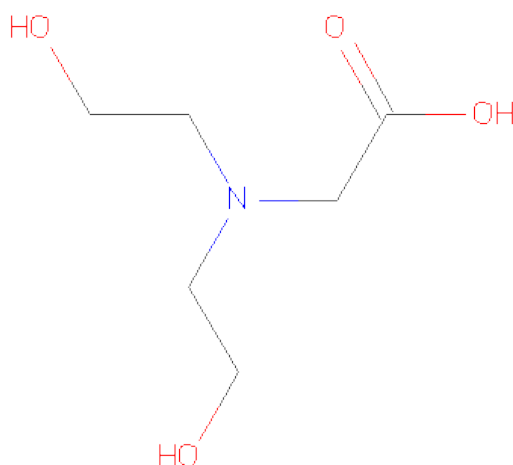
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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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 BICINE (three-letter code: BCN) (formula:  $C_6H_{13}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 4 is water.

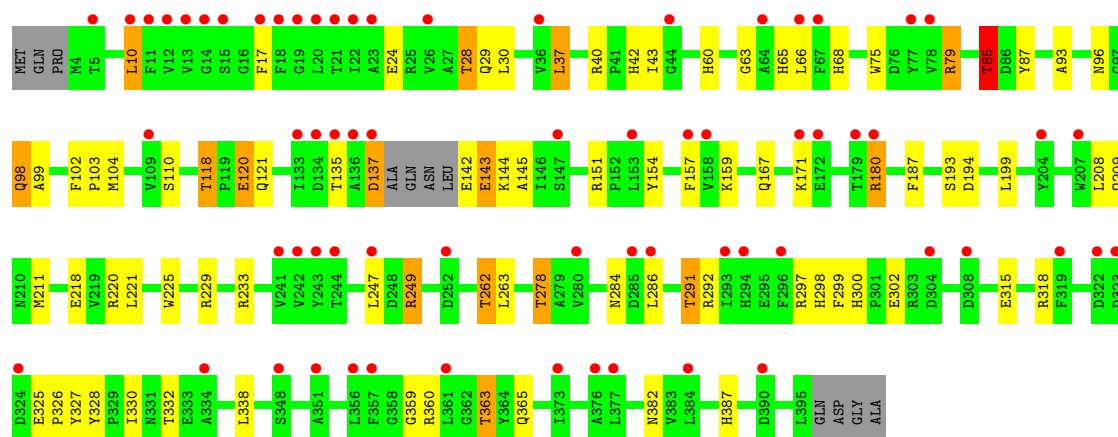
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	334	Total	O	0	0
			334	334		
4	B	238	Total	O	0	0
			238	238		
4	C	267	Total	O	0	0
			267	267		
4	D	182	Total	O	0	0
			182	182		

### 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 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.

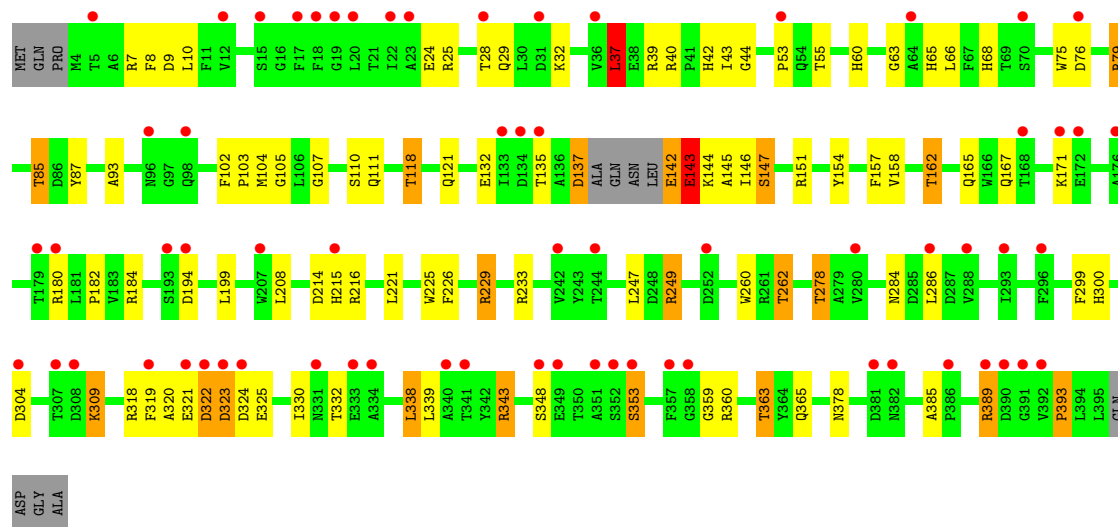
#### • Molecule 1: UDP-GALACTOPYRANOSE MUTASE

Chain A: 



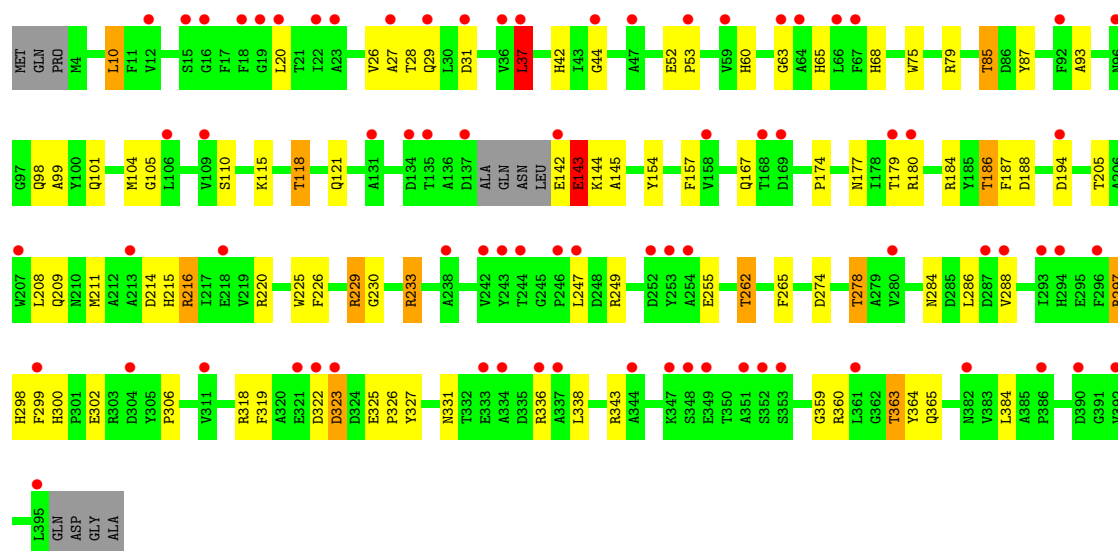
#### • Molecule 1: UDP-GALACTOPYRANOSE MUTASE

Chain B: 



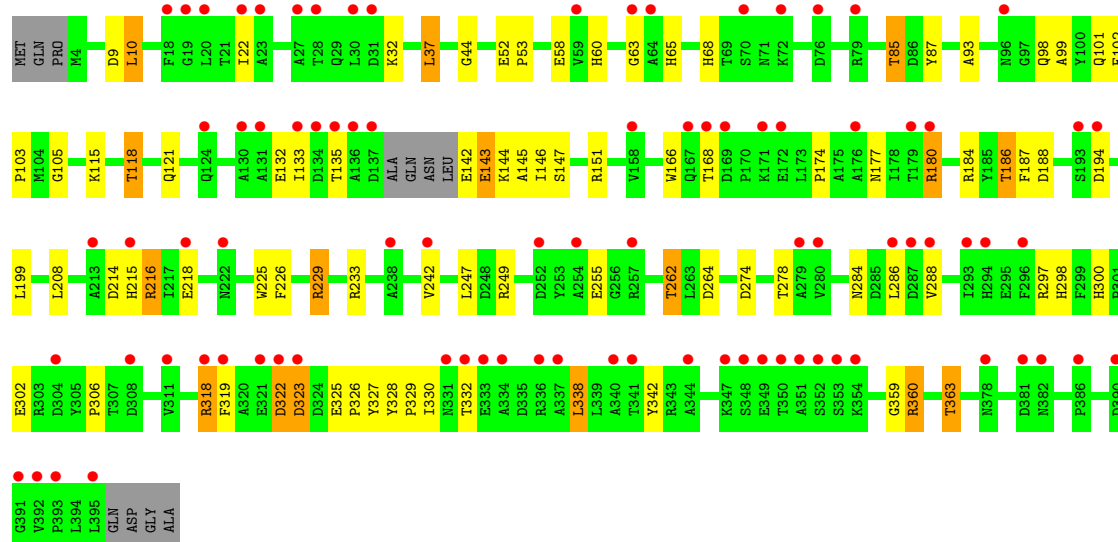
#### • Molecule 1: UDP-GALACTOPYRANOSE MUTASE

Chain C: 



• Molecule 1: UDP-GALACTOPYRANOSE MUTASE

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.60Å 153.73Å 137.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.25 25.46 – 2.25	Depositor EDS
% Data completeness (in resolution range)	88.4 (15.00-2.25) 88.4 (25.46-2.25)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, $R_{free}$	0.225 , 0.266 0.241 , 0.272	Depositor DCC
$R_{free}$ test set	6218 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 42.0	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 122411 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.64 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2839e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCN, 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	0.69	0/3251	0.79	7/4417 (0.2%)
1	B	0.63	0/3251	0.73	2/4417 (0.0%)
1	C	0.77	3/3251 (0.1%)	0.79	3/4417 (0.1%)
1	D	0.67	1/3251 (0.0%)	0.70	1/4417 (0.0%)
All	All	0.69	4/13004 (0.0%)	0.75	13/17668 (0.1%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	255	GLU	C-N	11.39	1.53	1.33
1	C	143	GLU	CD-OE2	5.86	1.32	1.25
1	C	255	GLU	C-N	5.76	1.43	1.33
1	C	364	TYR	CE1-CZ	5.40	1.45	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ARG	NE-CZ-NH2	-7.95	116.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	297	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	37	LEU	CA-CB-CG	-5.74	102.09	115.30
1	C	233	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	297	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	37	LEU	CA-CB-CG	-5.49	102.67	115.30
1	A	10	LEU	CA-CB-CG	5.45	127.83	115.30
1	C	37	LEU	CA-CB-CG	-5.41	102.86	115.30
1	A	85	THR	N-CA-CB	-5.32	100.20	110.30
1	A	79	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	79	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	10	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLU	Peptide
1	B	143	GLU	Peptide
1	C	143	GLU	Peptide
1	D	143	GLU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3162	0	3019	87	0
1	B	3162	0	3019	87	0
1	C	3162	0	3019	83	0
1	D	3162	0	3019	68	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
2	C	53	0	31	4	0
2	D	53	0	31	4	0
3	A	11	0	12	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	334	0	0	34	0
4	B	238	0	0	15	0
4	C	267	0	0	25	0
4	D	182	0	0	16	0
All	All	13892	0	12212	326	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (326) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1394:BCN:C4	4:A:2330:HOH:O	2.05	1.01
3:A:1394:BCN:O21	4:A:2329:HOH:O	1.77	1.01
1:A:28:THR:CG2	1:A:29:GLN:HE21	1.74	0.99
1:A:142:GLU:N	1:A:154:TYR:HH	1.61	0.98
1:C:93:ALA:HB1	1:C:284:ASN:HD21	1.29	0.98
1:C:142:GLU:O	1:C:143:GLU:HG2	1.63	0.97
1:A:262:THR:HG23	1:A:325:GLU:O	1.65	0.96
1:B:142:GLU:HB2	1:B:154:TYR:OH	1.66	0.95
1:B:300:HIS:HE1	4:B:2203:HOH:O	1.53	0.92
1:B:142:GLU:O	1:B:143:GLU:HG2	1.69	0.92
1:A:42:HIS:CD2	4:A:2034:HOH:O	2.21	0.91
3:A:1394:BCN:O4	4:A:2330:HOH:O	1.87	0.91
1:C:363:THR:HG21	4:C:2255:HOH:O	1.70	0.91
1:A:291:THR:HG22	1:A:292:ARG:HG3	1.52	0.90
1:C:85:THR:HG21	4:C:2223:HOH:O	1.69	0.90
1:A:142:GLU:O	1:A:143:GLU:HG2	1.71	0.90
1:D:60:HIS:HD2	1:D:65:HIS:H	1.15	0.90
1:B:262:THR:HG23	1:B:325:GLU:O	1.72	0.89
1:A:382:ASN:HD21	3:A:1394:BCN:H11	1.40	0.87
1:D:93:ALA:HB1	1:D:284:ASN:HD21	1.38	0.86
1:D:60:HIS:CD2	1:D:65:HIS:H	1.94	0.86
3:A:1394:BCN:H41	4:A:2330:HOH:O	1.67	0.86
1:A:363:THR:HG21	4:A:2135:HOH:O	1.74	0.86
1:C:322:ASP:O	1:C:323:ASP:HB3	1.74	0.85
1:A:28:THR:HG22	1:A:29:GLN:HE21	1.41	0.85
3:A:1394:BCN:O22	4:A:2331:HOH:O	1.95	0.84
3:A:1394:BCN:H32	4:A:2334:HOH:O	1.78	0.84
1:B:118:THR:HG22	1:B:121:GLN:H	1.42	0.84
1:B:339:LEU:O	1:B:343:ARG:HG3	1.79	0.83
1:A:93:ALA:HB1	1:A:284:ASN:HD21	1.42	0.82
1:B:42:HIS:CD2	4:B:2013:HOH:O	2.32	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:262:THR:HG23	1:C:325:GLU:O	1.77	0.82
1:D:327:TYR:HD2	2:D:1388:FAD:HM82	1.44	0.81
1:B:85:THR:HG21	4:B:2202:HOH:O	1.78	0.81
1:D:132:GLU:OE2	1:D:151:ARG:NH1	2.12	0.81
1:B:158:VAL:O	1:B:162:THR:HG22	1.81	0.81
1:A:382:ASN:HD21	3:A:1394:BCN:C1	1.94	0.81
1:A:382:ASN:ND2	3:A:1394:BCN:H11	1.94	0.80
1:B:143:GLU:N	4:B:2105:HOH:O	2.13	0.80
1:B:68:HIS:HD2	1:B:194:ASP:OD2	1.65	0.80
1:A:60:HIS:HD2	1:A:65:HIS:H	1.26	0.78
1:B:214:ASP:OD2	1:B:216:ARG:HD3	1.82	0.78
1:C:115:LYS:NZ	4:C:2101:HOH:O	2.14	0.78
1:D:118:THR:HG21	4:D:2015:HOH:O	1.84	0.78
1:C:60:HIS:HD2	1:C:65:HIS:H	1.33	0.77
1:D:142:GLU:O	1:D:143:GLU:HG2	1.85	0.77
1:A:120:GLU:HG2	4:A:2121:HOH:O	1.85	0.76
1:C:142:GLU:O	1:C:143:GLU:CG	2.33	0.76
1:C:322:ASP:O	1:C:323:ASP:CB	2.34	0.76
1:C:118:THR:HG21	4:C:2025:HOH:O	1.86	0.76
1:A:137:ASP:HB3	4:A:2144:HOH:O	1.84	0.76
1:A:85:THR:HG21	4:A:2267:HOH:O	1.84	0.75
1:B:37:LEU:HD13	1:B:225:TRP:CE3	2.21	0.75
1:C:60:HIS:CD2	1:C:65:HIS:H	2.05	0.74
1:C:143:GLU:N	4:C:2125:HOH:O	2.20	0.74
1:B:319:PHE:HB2	4:B:2209:HOH:O	1.86	0.74
1:B:93:ALA:HB1	1:B:284:ASN:HD21	1.51	0.74
1:B:262:THR:CG2	1:B:325:GLU:O	2.35	0.74
1:B:158:VAL:O	1:B:162:THR:CG2	2.36	0.74
1:B:76:ASP:HB2	4:B:2044:HOH:O	1.87	0.74
1:A:60:HIS:CD2	1:A:65:HIS:H	2.04	0.73
1:D:363:THR:HG21	4:D:2173:HOH:O	1.88	0.73
1:C:359:GLY:O	1:C:363:THR:HB	1.89	0.73
1:C:118:THR:HG22	1:C:121:GLN:H	1.54	0.73
1:A:98:GLN:HE21	1:A:99:ALA:H	1.36	0.73
1:B:60:HIS:CD2	1:B:65:HIS:H	2.07	0.72
1:A:382:ASN:HD21	3:A:1394:BCN:C2	2.02	0.72
1:C:327:TYR:CZ	4:C:2244:HOH:O	2.41	0.72
1:B:142:GLU:O	1:B:143:GLU:CG	2.39	0.71
1:A:68:HIS:HD2	1:A:194:ASP:OD2	1.73	0.71
1:A:300:HIS:HE1	4:A:2268:HOH:O	1.73	0.71
1:A:298:HIS:HD2	4:A:2266:HOH:O	1.73	0.70
1:A:142:GLU:O	1:A:143:GLU:CG	2.40	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:42:HIS:NE2	4:B:2013:HOH:O	2.24	0.70
1:D:214:ASP:OD2	1:D:216:ARG:HD3	1.92	0.70
1:B:363:THR:HG21	4:B:2099:HOH:O	1.92	0.70
1:D:300:HIS:HE1	4:D:2157:HOH:O	1.73	0.70
1:A:209:GLN:HG3	4:A:2203:HOH:O	1.90	0.69
1:D:300:HIS:HD2	1:D:302:GLU:OE1	1.75	0.69
1:A:359:GLY:O	1:A:363:THR:HB	1.92	0.69
1:A:291:THR:HG21	4:A:2276:HOH:O	1.91	0.69
1:B:28:THR:HG22	1:B:29:GLN:NE2	2.07	0.69
1:C:265:PHE:HE1	4:C:2244:HOH:O	1.75	0.68
1:D:68:HIS:HD2	1:D:194:ASP:OD2	1.76	0.68
1:A:98:GLN:HE22	1:C:110:SER:HB2	1.59	0.68
1:A:118:THR:HG22	1:A:121:GLN:H	1.58	0.67
1:C:68:HIS:HD2	1:C:194:ASP:OD2	1.76	0.67
1:A:24:GLU:O	1:A:28:THR:HB	1.94	0.67
1:B:60:HIS:HD2	1:B:65:HIS:H	1.41	0.67
3:A:1394:BCN:H61	4:A:2333:HOH:O	1.95	0.66
1:B:215:HIS:CE1	1:B:216:ARG:HD2	2.29	0.66
1:C:214:ASP:OD2	1:C:216:ARG:HD3	1.94	0.66
1:C:233:ARG:HD2	4:C:2182:HOH:O	1.94	0.65
1:C:186:THR:HG23	1:C:188:ASP:H	1.62	0.64
1:D:85:THR:HG21	4:D:2155:HOH:O	1.97	0.64
1:A:98:GLN:HE21	1:A:99:ALA:N	1.96	0.63
1:A:85:THR:HG23	1:A:87:TYR:H	1.62	0.63
1:B:233:ARG:HD2	4:B:2170:HOH:O	1.97	0.63
1:B:110:SER:HB2	1:D:98:GLN:HE22	1.63	0.63
1:A:233:ARG:HD2	4:A:2235:HOH:O	1.99	0.63
1:A:65:HIS:HE1	2:A:1393:FAD:O2'	1.82	0.63
1:A:135:THR:HG23	1:A:144:LYS:HD2	1.80	0.63
1:D:322:ASP:O	1:D:323:ASP:HB3	1.98	0.62
1:C:65:HIS:HE1	2:C:1388:FAD:O2'	1.80	0.62
1:A:360:ARG:HD2	4:A:2323:HOH:O	1.99	0.62
1:C:327:TYR:CE2	4:C:2244:HOH:O	2.53	0.62
1:A:17:PHE:CD2	1:A:211:MET:HE1	2.35	0.61
1:C:265:PHE:CE1	4:C:2244:HOH:O	2.51	0.61
1:D:288:VAL:HG13	4:D:2151:HOH:O	1.99	0.61
1:C:300:HIS:HE1	4:C:2039:HOH:O	1.82	0.61
1:B:322:ASP:O	1:B:323:ASP:HB2	1.99	0.61
1:C:98:GLN:HE21	1:C:99:ALA:H	1.48	0.61
1:A:28:THR:HG23	1:A:29:GLN:HE21	1.62	0.61
1:D:135:THR:HG23	1:D:144:LYS:HD2	1.81	0.61
1:C:143:GLU:CA	4:C:2125:HOH:O	2.49	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:360:ARG:HD2	2:D:1388:FAD:O4'	2.01	0.60
1:A:387:HIS:HE1	4:A:2234:HOH:O	1.84	0.60
1:A:315:GLU:OE1	4:A:2275:HOH:O	2.15	0.60
1:A:42:HIS:HD2	4:A:2034:HOH:O	1.72	0.60
1:B:28:THR:HG22	1:B:29:GLN:HE21	1.67	0.59
1:B:143:GLU:CA	4:B:2105:HOH:O	2.47	0.59
1:A:66:LEU:HD11	1:A:299:PHE:CE2	2.38	0.58
1:B:37:LEU:HD13	1:B:225:TRP:HE3	1.64	0.58
1:C:319:PHE:HA	4:C:2239:HOH:O	2.03	0.58
1:A:300:HIS:HD2	1:A:302:GLU:OE1	1.87	0.58
1:A:382:ASN:ND2	3:A:1394:BCN:C1	2.61	0.57
1:D:85:THR:HG22	1:D:199:LEU:H	1.69	0.57
1:C:42:HIS:CD2	4:C:2023:HOH:O	2.56	0.57
1:B:63:GLY:O	1:B:65:HIS:HD2	1.87	0.57
1:C:93:ALA:HB1	1:C:284:ASN:ND2	2.11	0.57
1:D:215:HIS:CE1	1:D:216:ARG:HD2	2.38	0.57
1:D:330:ILE:HG22	1:D:332:THR:HG23	1.87	0.57
1:B:142:GLU:N	1:B:146:ILE:HD12	2.19	0.57
1:A:110:SER:HB2	1:C:98:GLN:HE22	1.68	0.57
1:D:359:GLY:O	1:D:363:THR:HB	2.05	0.57
1:A:17:PHE:CE2	1:A:211:MET:HE2	2.40	0.56
1:D:186:THR:HG22	1:D:188:ASP:H	1.70	0.56
1:D:186:THR:CG2	1:D:188:ASP:H	2.19	0.56
1:C:298:HIS:HD2	4:C:2097:HOH:O	1.89	0.56
1:A:142:GLU:HG2	1:A:171:LYS:HG2	1.87	0.56
1:B:142:GLU:HB2	1:B:154:TYR:CZ	2.39	0.56
1:C:262:THR:CG2	1:C:325:GLU:O	2.52	0.56
1:B:28:THR:CG2	1:B:29:GLN:HE21	2.18	0.55
1:A:249:ARG:HG3	4:A:2095:HOH:O	2.06	0.55
1:C:319:PHE:HB2	4:C:2237:HOH:O	2.06	0.55
1:B:65:HIS:HE1	2:B:1390:FAD:O2'	1.89	0.55
1:C:262:THR:HA	1:C:327:TYR:HD1	1.72	0.55
1:A:118:THR:HG21	4:A:2124:HOH:O	2.06	0.55
1:D:133:ILE:HD12	1:D:146:ILE:HG21	1.89	0.55
1:B:66:LEU:HD11	1:B:299:PHE:CE1	2.41	0.55
1:C:142:GLU:HB3	1:C:154:TYR:CE2	2.42	0.55
1:D:37:LEU:HD13	1:D:225:TRP:CE3	2.41	0.55
1:A:291:THR:HG22	1:A:292:ARG:CG	2.32	0.55
1:D:37:LEU:HD13	1:D:225:TRP:HE3	1.72	0.55
1:C:63:GLY:O	1:C:65:HIS:HD2	1.90	0.54
1:A:167:GLN:HG3	1:A:318:ARG:HA	1.89	0.54
1:B:359:GLY:O	1:B:363:THR:HB	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:THR:HG23	4:C:2203:HOH:O	2.09	0.53
1:C:363:THR:HG22	1:C:365:GLN:HB2	1.90	0.53
1:D:65:HIS:HE1	2:D:1388:FAD:O2'	1.91	0.53
1:B:85:THR:HB	1:B:199:LEU:O	2.09	0.53
1:A:360:ARG:HD2	2:A:1393:FAD:O4'	2.07	0.53
1:C:143:GLU:HB3	1:C:145:ALA:H	1.74	0.53
1:C:174:PRO:O	1:C:177:ASN:HB2	2.09	0.53
1:A:63:GLY:O	1:A:65:HIS:HD2	1.92	0.53
1:B:233:ARG:CD	4:B:2170:HOH:O	2.56	0.53
1:A:40:ARG:NH2	4:A:2030:HOH:O	2.41	0.53
1:D:133:ILE:HD12	1:D:146:ILE:CG2	2.39	0.53
1:C:10:LEU:HD12	1:C:26:VAL:HG11	1.91	0.52
1:B:278:THR:CG2	4:D:2027:HOH:O	2.57	0.52
1:A:330:ILE:HG22	1:A:332:THR:HG23	1.91	0.52
1:B:360:ARG:HB2	1:B:365:GLN:O	2.09	0.52
1:C:326:PRO:O	1:C:360:ARG:NH2	2.42	0.52
1:C:299:PHE:CG	4:C:2073:HOH:O	2.63	0.52
1:D:180:ARG:HD3	4:D:2092:HOH:O	2.09	0.52
1:B:85:THR:CG2	1:B:87:TYR:H	2.22	0.52
1:A:365:GLN:HG3	4:A:2302:HOH:O	2.08	0.52
1:D:44:GLY:HA2	1:D:208:LEU:HD22	1.90	0.52
1:A:37:LEU:HD13	1:A:225:TRP:CE3	2.44	0.51
1:C:288:VAL:HG22	4:C:2218:HOH:O	2.10	0.51
1:B:102:PHE:CG	1:B:103:PRO:HA	2.45	0.51
1:B:118:THR:HG23	4:D:2141:HOH:O	2.10	0.51
1:D:142:GLU:O	1:D:143:GLU:CG	2.58	0.51
1:A:278:THR:HG22	4:C:2051:HOH:O	2.11	0.51
1:B:43:ILE:HG23	1:B:221:LEU:HD21	1.93	0.51
1:A:28:THR:CG2	1:A:29:GLN:NE2	2.59	0.51
1:C:143:GLU:HB2	4:C:2125:HOH:O	2.11	0.50
1:D:93:ALA:HB1	1:D:284:ASN:ND2	2.16	0.50
1:B:28:THR:CG2	1:B:29:GLN:NE2	2.74	0.50
1:D:322:ASP:O	1:D:323:ASP:CB	2.59	0.50
1:C:274:ASP:OD1	1:C:298:HIS:HE1	1.94	0.50
1:D:133:ILE:HG22	1:D:147:SER:HB3	1.94	0.50
1:D:300:HIS:CD2	1:D:302:GLU:OE1	2.61	0.50
1:A:278:THR:CG2	4:C:2051:HOH:O	2.58	0.50
1:C:101:GLN:NE2	4:C:2092:HOH:O	2.45	0.50
1:C:205:THR:O	1:C:209:GLN:HG2	2.11	0.50
1:A:159:LYS:HD3	4:A:2156:HOH:O	2.11	0.50
1:A:365:GLN:CG	4:A:2302:HOH:O	2.59	0.50
1:B:142:GLU:HG3	1:B:171:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:17:PHE:CE2	1:A:211:MET:CE	2.94	0.50
1:A:85:THR:CG2	1:A:87:TYR:H	2.23	0.50
1:B:278:THR:HG23	1:D:187:PHE:HB2	1.94	0.50
1:D:226:PHE:HA	1:D:229:ARG:HD2	1.94	0.50
1:D:338:LEU:HD22	1:D:342:TYR:CE1	2.47	0.49
1:B:107:GLY:O	1:B:111:GLN:HG3	2.13	0.49
1:A:298:HIS:CD2	4:A:2266:HOH:O	2.58	0.49
1:A:365:GLN:CB	4:A:2302:HOH:O	2.61	0.49
1:C:142:GLU:O	1:C:143:GLU:CB	2.61	0.49
1:B:249:ARG:C	1:B:249:ARG:HD3	2.33	0.49
1:D:166:TRP:O	1:D:168:THR:HG23	2.11	0.49
1:B:137:ASP:HB2	4:B:2101:HOH:O	2.12	0.49
1:D:60:HIS:HD2	1:D:65:HIS:N	1.98	0.49
1:B:167:GLN:HG3	1:B:318:ARG:HA	1.95	0.49
1:A:93:ALA:HB1	1:A:284:ASN:ND2	2.21	0.48
1:C:68:HIS:HE1	4:C:2257:HOH:O	1.96	0.48
1:B:233:ARG:HH22	1:B:353:SER:HB2	1.78	0.48
1:C:297:ARG:NH2	1:C:306:PRO:O	2.40	0.48
1:C:104:MET:CE	1:C:157:PHE:HB2	2.43	0.48
1:D:102:PHE:CG	1:D:103:PRO:HA	2.48	0.48
1:D:143:GLU:CB	1:D:145:ALA:H	2.27	0.48
1:D:174:PRO:O	1:D:177:ASN:HB2	2.14	0.48
1:B:104:MET:CE	1:B:157:PHE:HB2	2.43	0.48
1:B:9:ASP:HB2	1:B:32:LYS:HB3	1.94	0.48
1:D:118:THR:HG22	1:D:121:GLN:H	1.79	0.48
1:B:182:PRO:HD2	4:B:2127:HOH:O	2.14	0.48
1:D:63:GLY:O	1:D:65:HIS:HD2	1.97	0.48
1:B:55:THR:HG22	1:B:309:LYS:HG2	1.96	0.48
1:A:43:ILE:HG23	1:A:221:LEU:HD21	1.95	0.48
1:D:166:TRP:HZ3	1:D:330:ILE:HG23	1.77	0.47
1:C:37:LEU:HD13	1:C:225:TRP:CE3	2.48	0.47
1:B:142:GLU:O	1:B:143:GLU:CB	2.62	0.47
1:B:322:ASP:O	1:B:323:ASP:CB	2.62	0.47
1:B:110:SER:HB2	1:D:98:GLN:NE2	2.27	0.47
1:B:142:GLU:N	1:B:146:ILE:CD1	2.78	0.47
1:B:330:ILE:HG22	1:B:332:THR:HG23	1.96	0.47
1:D:319:PHE:HD2	4:D:2088:HOH:O	1.97	0.47
1:D:233:ARG:HD2	4:D:2133:HOH:O	2.15	0.47
1:D:101:GLN:NE2	4:D:2055:HOH:O	2.47	0.47
4:A:2254:HOH:O	1:C:118:THR:HG23	2.14	0.47
1:A:327:TYR:HA	1:A:360:ARG:NH2	2.28	0.47
1:C:360:ARG:HD3	2:C:1388:FAD:O4'	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:208:LEU:HD23	1:A:211:MET:HE3	1.97	0.46
1:A:199:LEU:HD12	1:A:299:PHE:O	2.15	0.46
1:D:85:THR:HG23	1:D:87:TYR:H	1.81	0.46
1:C:226:PHE:HA	1:C:229:ARG:HD2	1.97	0.46
1:D:262:THR:HG23	1:D:325:GLU:O	2.16	0.46
1:C:208:LEU:HD23	1:C:211:MET:CE	2.46	0.46
1:D:98:GLN:HE21	1:D:99:ALA:H	1.63	0.46
1:A:278:THR:HG23	1:C:187:PHE:HB2	1.98	0.46
1:B:75:TRP:O	1:B:79:ARG:HD3	2.16	0.46
1:D:297:ARG:NH2	1:D:306:PRO:O	2.42	0.46
1:D:22:ILE:HG21	1:D:242:VAL:HG21	1.98	0.46
1:C:262:THR:HG22	1:C:327:TYR:HE1	1.81	0.46
1:B:338:LEU:HA	1:B:338:LEU:HD23	1.84	0.46
1:B:249:ARG:O	1:B:249:ARG:HD3	2.16	0.45
1:B:143:GLU:HB3	1:B:145:ALA:H	1.80	0.45
1:A:143:GLU:HB3	1:A:145:ALA:H	1.82	0.45
1:D:262:THR:CG2	1:D:325:GLU:O	2.65	0.45
1:C:44:GLY:HA3	1:C:208:LEU:HD13	1.99	0.45
1:B:44:GLY:HA3	1:B:208:LEU:HD13	1.98	0.45
1:C:143:GLU:CB	1:C:145:ALA:H	2.30	0.45
1:B:135:THR:HG23	1:B:144:LYS:HD2	1.99	0.45
1:C:215:HIS:CE1	1:C:216:ARG:HD2	2.52	0.45
1:A:387:HIS:CE1	4:A:2234:HOH:O	2.64	0.45
1:B:158:VAL:O	1:B:162:THR:HG23	2.15	0.44
1:A:102:PHE:CG	1:A:103:PRO:HA	2.52	0.44
1:B:40:ARG:NH2	4:B:2009:HOH:O	2.50	0.44
1:C:85:THR:CG2	1:C:87:TYR:H	2.31	0.44
1:C:28:THR:HG22	1:C:29:GLN:HE21	1.82	0.44
1:A:17:PHE:HE2	1:A:211:MET:HE2	1.82	0.44
1:B:142:GLU:N	1:B:142:GLU:CD	2.70	0.44
1:A:208:LEU:HD23	1:A:211:MET:CE	2.47	0.44
1:C:229:ARG:HG2	1:C:230:GLY:N	2.33	0.44
1:B:24:GLU:CD	1:B:25:ARG:HH11	2.20	0.44
1:A:187:PHE:HB2	1:C:278:THR:HG23	2.00	0.44
1:C:105:GLY:HA2	1:C:184:ARG:O	2.18	0.44
1:C:360:ARG:NH1	2:C:1388:FAD:O2A	2.51	0.44
1:D:274:ASP:OD1	1:D:298:HIS:HE1	2.00	0.44
1:C:98:GLN:HE21	1:C:99:ALA:N	2.13	0.43
1:B:226:PHE:HA	1:B:229:ARG:HD2	2.00	0.43
1:B:85:THR:HG22	1:B:87:TYR:H	1.82	0.43
1:C:27:ALA:O	1:C:31:ASP:HA	2.18	0.43
1:A:365:GLN:HB3	4:A:2302:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:52:GLU:HA	1:D:53:PRO:HD3	1.87	0.43
1:A:104:MET:CE	1:A:157:PHE:HB2	2.48	0.43
1:D:105:GLY:HA2	1:D:184:ARG:O	2.18	0.43
1:D:264:ASP:OD2	1:D:318:ARG:HD3	2.19	0.43
1:B:385:ALA:O	1:B:389:ARG:HB2	2.18	0.43
1:C:20:LEU:HD23	1:C:20:LEU:HA	1.89	0.43
1:C:300:HIS:HD2	1:C:302:GLU:OE1	2.02	0.43
1:C:262:THR:HG22	1:C:327:TYR:CE1	2.54	0.43
1:D:319:PHE:HA	4:D:2164:HOH:O	2.18	0.43
1:A:28:THR:HG22	1:A:29:GLN:HG2	2.00	0.42
1:B:278:THR:HG22	4:D:2027:HOH:O	2.19	0.42
1:D:327:TYR:CD2	2:D:1388:FAD:HM82	2.36	0.42
1:B:7:ARG:HG2	1:B:8:PHE:CE1	2.54	0.42
1:B:105:GLY:HA2	1:B:184:ARG:O	2.20	0.42
1:D:326:PRO:O	1:D:360:ARG:NH2	2.47	0.42
1:C:75:TRP:O	1:C:79:ARG:HD3	2.19	0.42
1:A:326:PRO:O	1:A:360:ARG:NH2	2.48	0.42
1:C:331:ASN:O	1:C:336:ARG:NH1	2.53	0.42
1:C:360:ARG:CD	2:C:1388:FAD:O4'	2.68	0.42
1:D:9:ASP:HB2	1:D:32:LYS:HB3	2.02	0.42
1:B:118:THR:HG21	4:D:2050:HOH:O	2.19	0.42
1:A:328:TYR:OH	2:A:1393:FAD:HM73	2.19	0.42
1:B:321:GLU:O	1:B:324:ASP:HB2	2.19	0.42
1:D:218:GLU:HG2	4:D:2116:HOH:O	2.19	0.42
1:C:104:MET:HG3	4:C:2096:HOH:O	2.20	0.42
1:B:135:THR:HG1	1:B:147:SER:HG	1.49	0.42
1:B:93:ALA:HB1	1:B:284:ASN:ND2	2.27	0.42
1:C:186:THR:CG2	1:C:188:ASP:H	2.30	0.42
1:C:208:LEU:HD23	1:C:211:MET:HE2	2.02	0.42
1:B:165:GLN:NE2	4:B:2115:HOH:O	2.52	0.42
1:C:37:LEU:HD13	1:C:225:TRP:HE3	1.86	0.41
1:A:180:ARG:HD3	4:A:2166:HOH:O	2.19	0.41
1:A:75:TRP:O	1:A:79:ARG:HD3	2.20	0.41
1:C:52:GLU:HA	1:C:53:PRO:HD3	1.96	0.41
1:D:58:GLU:CD	4:D:2021:HOH:O	2.59	0.41
2:B:1390:FAD:H9	2:B:1390:FAD:H1'1	1.83	0.41
1:B:260:TRP:O	1:B:320:ALA:HB3	2.21	0.41
1:B:132:GLU:OE2	1:B:151:ARG:NH1	2.54	0.41
1:C:167:GLN:HG3	1:C:318:ARG:HA	2.03	0.41
1:A:263:LEU:HD12	4:A:2052:HOH:O	2.22	0.40
1:A:143:GLU:CB	1:A:145:ALA:H	2.34	0.40
1:B:135:THR:OG1	1:B:147:SER:OG	2.23	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:328:TYR:HA	1:D:329:PRO:HD3	1.98	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	384/399 (96%)	372 (97%)	12 (3%)	0	100	100
1	B	384/399 (96%)	372 (97%)	8 (2%)	4 (1%)	22	17
1	C	384/399 (96%)	370 (96%)	12 (3%)	2 (0%)	38	38
1	D	384/399 (96%)	377 (98%)	7 (2%)	0	100	100
All	All	1536/1596 (96%)	1491 (97%)	39 (2%)	6 (0%)	43	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	323	ASP
1	B	393	PRO
1	C	143	GLU
1	B	143	GLU
1	B	53	PRO
1	B	323	ASP

### 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	326/334 (98%)	303 (93%)	23 (7%)	21	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	326/334 (98%)	299 (92%)	27 (8%)	16	13
1	C	326/334 (98%)	306 (94%)	20 (6%)	26	25
1	D	326/334 (98%)	306 (94%)	20 (6%)	26	25
All	All	1304/1336 (98%)	1214 (93%)	90 (7%)	22	20

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	28	THR
1	A	30	LEU
1	A	85	THR
1	A	96	ASN
1	A	98	GLN
1	A	118	THR
1	A	120	GLU
1	A	137	ASP
1	A	151	ARG
1	A	180	ARG
1	A	193	SER
1	A	218	GLU
1	A	220	ARG
1	A	229	ARG
1	A	247	LEU
1	A	249	ARG
1	A	262	THR
1	A	278	THR
1	A	286	LEU
1	A	291	THR
1	A	338	LEU
1	A	363	THR
1	B	10	LEU
1	B	37	LEU
1	B	39	ARG
1	B	85	THR
1	B	118	THR
1	B	137	ASP
1	B	142	GLU
1	B	147	SER
1	B	162	THR
1	B	180	ARG

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Mol	Chain	Res	Type
1	B	229	ARG
1	B	247	LEU
1	B	249	ARG
1	B	262	THR
1	B	278	THR
1	B	286	LEU
1	B	304	ASP
1	B	309	LYS
1	B	322	ASP
1	B	338	LEU
1	B	343	ARG
1	B	348	SER
1	B	353	SER
1	B	363	THR
1	B	378	ASN
1	B	389	ARG
1	B	393	PRO
1	C	10	LEU
1	C	37	LEU
1	C	85	THR
1	C	118	THR
1	C	144	LYS
1	C	179	THR
1	C	180	ARG
1	C	186	THR
1	C	216	ARG
1	C	220	ARG
1	C	229	ARG
1	C	247	LEU
1	C	249	ARG
1	C	262	THR
1	C	278	THR
1	C	286	LEU
1	C	338	LEU
1	C	343	ARG
1	C	363	THR
1	C	384	LEU
1	D	10	LEU
1	D	37	LEU
1	D	85	THR
1	D	115	LYS
1	D	118	THR

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Mol	Chain	Res	Type
1	D	180	ARG
1	D	186	THR
1	D	216	ARG
1	D	229	ARG
1	D	247	LEU
1	D	249	ARG
1	D	262	THR
1	D	278	THR
1	D	286	LEU
1	D	318	ARG
1	D	322	ASP
1	D	323	ASP
1	D	338	LEU
1	D	360	ARG
1	D	363	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	60	HIS
1	A	65	HIS
1	A	68	HIS
1	A	80	GLN
1	A	98	GLN
1	A	165	GLN
1	A	284	ASN
1	A	298	HIS
1	A	300	HIS
1	A	382	ASN
1	A	387	HIS
1	B	29	GLN
1	B	60	HIS
1	B	65	HIS
1	B	68	HIS
1	B	101	GLN
1	B	165	GLN
1	B	215	HIS
1	B	284	ASN
1	B	298	HIS
1	B	300	HIS
1	B	387	HIS

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Mol	Chain	Res	Type
1	C	29	GLN
1	C	60	HIS
1	C	65	HIS
1	C	68	HIS
1	C	80	GLN
1	C	98	GLN
1	C	101	GLN
1	C	165	GLN
1	C	215	HIS
1	C	284	ASN
1	C	298	HIS
1	C	300	HIS
1	C	331	ASN
1	D	60	HIS
1	D	65	HIS
1	D	68	HIS
1	D	80	GLN
1	D	98	GLN
1	D	101	GLN
1	D	124	GLN
1	D	165	GLN
1	D	215	HIS
1	D	284	ASN
1	D	298	HIS
1	D	300	HIS
1	D	387	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

5 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	1393	-	58,58,58	1.19	4 (6%)	85,89,89	1.93	13 (15%)
3	BCN	A	1394	-	10,10,10	0.69	0	11,11,11	1.66	2 (18%)
2	FAD	B	1390	-	58,58,58	1.20	7 (12%)	85,89,89	1.84	15 (17%)
2	FAD	C	1388	-	58,58,58	1.27	5 (8%)	85,89,89	1.96	15 (17%)
2	FAD	D	1388	-	58,58,58	1.27	5 (8%)	85,89,89	1.81	13 (15%)

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	1393	-	-	0/34/50/50	0/1/6/6
3	BCN	A	1394	-	-	0/10/10/10	0/0/0/0
2	FAD	B	1390	-	-	0/34/50/50	0/1/6/6
2	FAD	C	1388	-	-	0/34/50/50	0/1/6/6
2	FAD	D	1388	-	-	0/34/50/50	0/1/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1388	FAD	C1'-N10	4.37	1.53	1.48
2	C	1388	FAD	C2A-N3A	4.27	1.40	1.32
2	A	1393	FAD	C2A-N3A	4.19	1.40	1.32
2	B	1390	FAD	C2A-N3A	4.10	1.40	1.32
2	C	1388	FAD	C1'-N10	4.06	1.52	1.48
2	B	1390	FAD	C1'-N10	3.88	1.52	1.48
2	D	1388	FAD	C2A-N3A	3.88	1.39	1.32
2	A	1393	FAD	C1'-N10	3.86	1.52	1.48
2	D	1388	FAD	C1'-C2'	3.20	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1388	FAD	C1'-C2'	3.11	1.54	1.51
2	D	1388	FAD	C2A-N1A	2.99	1.39	1.33
2	C	1388	FAD	C2A-N1A	2.88	1.39	1.33
2	A	1393	FAD	C1'-C2'	2.87	1.54	1.51
2	D	1388	FAD	C5X-N5	2.56	1.39	1.35
2	A	1393	FAD	C2A-N1A	2.51	1.38	1.33
2	B	1390	FAD	C2A-N1A	2.45	1.38	1.33
2	B	1390	FAD	C1'-C2'	2.43	1.53	1.51
2	C	1388	FAD	C5X-N5	2.42	1.39	1.35
2	B	1390	FAD	P-O3P	2.37	1.64	1.59
2	B	1390	FAD	C5X-N5	2.37	1.38	1.35
2	B	1390	FAD	PA-O3P	2.04	1.63	1.59

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1388	FAD	N3A-C2A-N1A	-11.09	119.44	128.71
2	D	1388	FAD	N3A-C2A-N1A	-10.05	120.31	128.71
2	A	1393	FAD	N3A-C2A-N1A	-9.92	120.41	128.71
2	B	1390	FAD	N3A-C2A-N1A	-9.06	121.13	128.71
2	A	1393	FAD	C2-N1-C10	6.40	121.43	114.98
2	C	1388	FAD	C2-N1-C10	5.39	120.41	114.98
2	B	1390	FAD	C2-N1-C10	5.27	120.29	114.98
2	D	1388	FAD	C2-N1-C10	5.10	120.11	114.98
2	B	1390	FAD	O4B-C1B-N9A	4.50	112.63	108.44
2	B	1390	FAD	C5X-C9A-N10	4.46	121.19	116.80
2	D	1388	FAD	C5X-C9A-N10	4.43	121.17	116.80
2	C	1388	FAD	N3A-C4A-N9A	4.13	132.89	125.43
3	A	1394	BCN	C1-N1-C3	-4.11	102.04	112.34
2	A	1393	FAD	N3A-C4A-N9A	3.99	132.63	125.43
2	A	1393	FAD	C9A-N10-C10	-3.94	117.90	121.77
2	A	1393	FAD	C5X-C9A-N10	3.90	120.64	116.80
2	A	1393	FAD	C4X-N5-C5X	3.85	121.02	116.69
2	B	1390	FAD	N3A-C4A-N9A	3.85	132.38	125.43
2	A	1393	FAD	C4X-C10-N1	-3.78	118.95	122.73
2	D	1388	FAD	N3A-C4A-N9A	3.64	132.00	125.43
2	C	1388	FAD	C5X-C9A-N10	3.61	120.36	116.80
2	C	1388	FAD	C4X-N5-C5X	3.43	120.55	116.69
2	C	1388	FAD	C4X-C10-N1	-3.24	119.50	122.73
2	C	1388	FAD	O4'-C4'-C5'	-3.21	103.53	110.12
2	C	1388	FAD	O4B-C1B-N9A	3.16	111.38	108.44
2	C	1388	FAD	C8A-N9A-C4A	3.05	109.22	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1393	FAD	O4'-C4'-C5'	-3.03	103.90	110.12
2	D	1388	FAD	C4X-N5-C5X	2.95	120.00	116.69
2	A	1393	FAD	C4-N3-C2	-2.92	119.41	125.39
3	A	1394	BCN	C5-N1-C3	-2.91	104.33	111.45
2	D	1388	FAD	C4X-C10-N1	-2.81	119.92	122.73
2	D	1388	FAD	O4B-C1B-N9A	2.81	111.05	108.44
2	B	1390	FAD	C9A-N10-C10	-2.80	119.02	121.77
2	B	1390	FAD	C4X-N5-C5X	2.79	119.82	116.69
2	C	1388	FAD	C9A-N10-C10	-2.75	119.07	121.77
2	B	1390	FAD	C2'-C1'-N10	2.72	116.06	112.45
2	A	1393	FAD	C5A-C4A-N3A	-2.68	119.86	125.70
2	C	1388	FAD	C4B-O4B-C1B	-2.59	106.94	109.75
2	D	1388	FAD	C9A-N10-C10	-2.52	119.29	121.77
2	B	1390	FAD	O4'-C4'-C5'	-2.41	105.16	110.12
2	C	1388	FAD	N7A-C8A-N9A	-2.38	107.61	114.36
2	A	1393	FAD	C2A-N3A-C4A	2.36	120.74	114.01
2	D	1388	FAD	O4'-C4'-C5'	-2.36	105.28	110.12
2	B	1390	FAD	C4X-C10-N1	-2.31	120.42	122.73
2	B	1390	FAD	C5A-C4A-N3A	-2.26	120.78	125.70
2	B	1390	FAD	C8M-C8-C9	-2.26	114.93	120.38
2	B	1390	FAD	C4-N3-C2	-2.25	120.76	125.39
2	C	1388	FAD	C2A-N3A-C4A	2.24	120.39	114.01
2	C	1388	FAD	C5A-C4A-N3A	-2.24	120.83	125.70
2	B	1390	FAD	C4A-C5A-N7A	-2.17	107.66	109.52
2	B	1390	FAD	C9A-C5X-N5	-2.15	119.07	122.37
2	D	1388	FAD	C5A-C4A-N3A	-2.13	121.05	125.70
2	D	1388	FAD	C2'-C1'-N10	2.13	115.28	112.45
2	D	1388	FAD	N7A-C8A-N9A	-2.12	108.37	114.36
2	A	1393	FAD	C4-C4X-C10	2.12	120.37	116.95
2	C	1388	FAD	C1B-N9A-C4A	-2.07	123.05	126.64
2	D	1388	FAD	C4-N3-C2	-2.04	121.20	125.39
2	A	1393	FAD	C1'-N10-C9A	2.00	120.82	118.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	388/399 (97%)	0.92	67 (17%) 2 2	29, 39, 55, 64	0
1	B	388/399 (97%)	0.86	66 (17%) 2 2	30, 40, 56, 64	0
1	C	388/399 (97%)	0.95	77 (19%) 2 1	30, 40, 55, 64	0
1	D	388/399 (97%)	1.05	87 (22%) 1 1	31, 40, 55, 64	0
All	All	1552/1596 (97%)	0.94	297 (19%) 2 1	29, 40, 55, 64	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	76	ASP	7.3
1	B	351	ALA	6.8
1	B	390	ASP	6.5
1	A	135	THR	6.1
1	D	347	LYS	6.0
1	D	390	ASP	5.8
1	A	179	THR	5.7
1	D	344	ALA	5.6
1	D	341	THR	5.3
1	D	352	SER	5.3
1	B	20	LEU	5.2
1	D	22	ILE	5.2
1	D	134	ASP	5.2
1	D	238	ALA	5.1
1	D	322	ASP	5.1
1	D	135	THR	5.1
1	D	348	SER	5.0
1	C	337	ALA	5.0
1	C	20	LEU	4.9
1	A	134	ASP	4.9
1	B	304	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	322	ASP	4.8
1	D	254	ALA	4.8
1	A	334	ALA	4.8
1	C	323	ASP	4.7
1	A	286	LEU	4.6
1	C	322	ASP	4.6
1	D	323	ASP	4.6
1	B	386	PRO	4.5
1	B	252	ASP	4.5
1	A	351	ALA	4.4
1	A	20	LEU	4.3
1	D	136	ALA	4.3
1	B	319	PHE	4.3
1	D	392	VAL	4.3
1	C	252	ASP	4.2
1	D	133	ILE	4.2
1	B	28	THR	4.2
1	A	180	ARG	4.2
1	C	137	ASP	4.2
1	C	347	LYS	4.2
1	D	252	ASP	4.1
1	D	337	ALA	4.1
1	C	180	ARG	4.1
1	A	19	GLY	4.1
1	C	304	ASP	4.0
1	D	20	LEU	4.0
1	D	288	VAL	4.0
1	D	179	THR	4.0
1	A	22	ILE	4.0
1	B	179	THR	4.0
1	C	19	GLY	3.9
1	C	131	ALA	3.9
1	C	334	ALA	3.9
1	D	194	ASP	3.9
1	B	333	GLU	3.9
1	B	392	VAL	3.8
1	C	22	ILE	3.8
1	D	172	GLU	3.8
1	A	242	VAL	3.8
1	C	135	THR	3.8
1	C	168	THR	3.8
1	B	135	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	321	GLU	3.7
1	B	22	ILE	3.7
1	A	319	PHE	3.7
1	D	395	LEU	3.7
1	D	31	ASP	3.7
1	A	323	ASP	3.7
1	D	137	ASP	3.7
1	D	353	SER	3.7
1	B	172	GLU	3.7
1	D	382	ASN	3.6
1	B	323	ASP	3.6
1	C	386	PRO	3.6
1	C	390	ASP	3.6
1	A	136	ALA	3.6
1	C	238	ALA	3.5
1	B	171	LYS	3.5
1	C	179	THR	3.5
1	D	304	ASP	3.5
1	D	351	ALA	3.5
1	A	322	ASP	3.5
1	A	348	SER	3.5
1	D	28	THR	3.5
1	B	134	ASP	3.4
1	D	19	GLY	3.5
1	A	17	PHE	3.4
1	B	334	ALA	3.4
1	A	5	THR	3.4
1	C	280	VAL	3.4
1	D	76	ASP	3.4
1	D	218	GLU	3.4
1	C	348	SER	3.4
1	A	252	ASP	3.4
1	C	134	ASP	3.4
1	A	78	VAL	3.3
1	D	193	SER	3.3
1	B	358	GLY	3.3
1	B	215	HIS	3.3
1	C	254	ALA	3.3
1	B	193	SER	3.3
1	D	131	ALA	3.3
1	C	12	VAL	3.2
1	A	21	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	109	VAL	3.2
1	D	386	PRO	3.2
1	A	207	TRP	3.2
1	A	304	ASP	3.2
1	B	19	GLY	3.2
1	C	64	ALA	3.2
1	C	31	ASP	3.2
1	A	10	LEU	3.2
1	D	213	ALA	3.2
1	A	12	VAL	3.2
1	B	242	VAL	3.1
1	A	23	ALA	3.1
1	C	299	PHE	3.1
1	A	172	GLU	3.1
1	A	13	VAL	3.1
1	A	66	LEU	3.1
1	D	319	PHE	3.1
1	B	12	VAL	3.1
1	B	382	ASN	3.1
1	D	215	HIS	3.1
1	C	36	VAL	3.0
1	D	391	GLY	3.0
1	D	96	ASN	3.0
1	C	242	VAL	3.0
1	A	296	PHE	3.0
1	D	287	ASP	3.0
1	A	36	VAL	3.0
1	A	137	ASP	3.0
1	C	194	ASP	3.0
1	A	14	GLY	3.0
1	C	288	VAL	3.0
1	D	124	GLN	3.0
1	B	348	SER	2.9
1	B	352	SER	2.9
1	A	157	PHE	2.9
1	B	353	SER	2.9
1	B	18	PHE	2.9
1	C	351	ALA	2.9
1	B	5	THR	2.9
1	A	280	VAL	2.9
1	A	171	LYS	2.8
1	D	286	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	207	TRP	2.8
1	B	349	GLU	2.8
1	D	393	PRO	2.8
1	C	96	ASN	2.8
1	A	390	ASP	2.8
1	B	180	ARG	2.8
1	D	336	ARG	2.8
1	D	381	ASP	2.7
1	D	331	ASN	2.7
1	C	287	ASP	2.7
1	D	334	ALA	2.7
1	A	44	GLY	2.7
1	D	180	ARG	2.7
1	B	36	VAL	2.7
1	A	153	LEU	2.7
1	D	30	LEU	2.7
1	D	378	ASN	2.7
1	B	31	ASP	2.7
1	C	23	ALA	2.7
1	C	392	VAL	2.7
1	A	356	LEU	2.7
1	C	27	ALA	2.7
1	C	333	GLU	2.7
1	A	373	ILE	2.6
1	D	222	ASN	2.6
1	D	72	LYS	2.6
1	A	244	THR	2.6
1	D	280	VAL	2.6
1	B	340	ALA	2.6
1	C	296	PHE	2.6
1	B	194	ASP	2.6
1	B	286	LEU	2.6
1	C	352	SER	2.6
1	D	59	VAL	2.6
1	C	67	PHE	2.6
1	C	244	THR	2.6
1	B	64	ALA	2.6
1	C	344	ALA	2.6
1	D	340	ALA	2.6
1	B	17	PHE	2.6
1	C	29	GLN	2.6
1	C	349	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	23	ALA	2.5
1	C	353	SER	2.5
1	B	280	VAL	2.5
1	D	242	VAL	2.5
1	D	64	ALA	2.5
1	B	168	THR	2.5
1	B	207	TRP	2.5
1	B	321	GLU	2.5
1	A	26	VAL	2.5
1	C	63	GLY	2.5
1	B	133	ILE	2.5
1	B	176	ALA	2.5
1	D	349	GLU	2.5
1	D	167	GLN	2.5
1	A	64	ALA	2.5
1	C	18	PHE	2.4
1	B	53	PRO	2.4
1	A	294	HIS	2.4
1	C	66	LEU	2.4
1	A	133	ILE	2.4
1	A	384	LEU	2.4
1	D	354	LYS	2.4
1	C	321	GLU	2.4
1	D	332	THR	2.4
1	D	308	ASP	2.4
1	A	377	LEU	2.4
1	D	333	GLU	2.4
1	D	350	THR	2.4
1	A	67	PHE	2.4
1	A	357	PHE	2.4
1	D	18	PHE	2.4
1	D	296	PHE	2.4
1	A	77	TYR	2.3
1	C	106	LEU	2.3
1	D	169	ASP	2.3
1	C	47	ALA	2.3
1	C	218	GLU	2.3
1	A	18	PHE	2.3
1	C	395	LEU	2.3
1	D	158	VAL	2.3
1	A	147	SER	2.3
1	D	171	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	318	ARG	2.3
1	C	293	ILE	2.3
1	B	308	ASP	2.3
1	B	331	ASN	2.3
1	D	130	ALA	2.3
1	D	294	HIS	2.3
1	C	336	ARG	2.3
1	A	361	LEU	2.3
1	C	294	HIS	2.3
1	B	288	VAL	2.3
1	C	382	ASN	2.3
1	B	324	ASP	2.3
1	C	243	TYR	2.3
1	B	381	ASP	2.3
1	A	241	VAL	2.2
1	D	311	VAL	2.2
1	D	79	ARG	2.2
1	C	44	GLY	2.2
1	D	168	THR	2.2
1	C	142	GLU	2.2
1	D	70	SER	2.2
1	D	293	ILE	2.2
1	A	11	PHE	2.2
1	C	53	PRO	2.2
1	B	23	ALA	2.2
1	A	204	TYR	2.2
1	D	63	GLY	2.1
1	B	244	THR	2.1
1	C	213	ALA	2.1
1	A	247	LEU	2.1
1	D	257	ARG	2.1
1	C	246	PRO	2.1
1	D	27	ALA	2.1
1	B	96	ASN	2.1
1	C	37	LEU	2.1
1	C	253	TYR	2.1
1	A	293	ILE	2.1
1	B	296	PHE	2.1
1	A	324	ASP	2.1
1	C	109	VAL	2.1
1	B	389	ARG	2.1
1	A	15	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	98	GLN	2.1
1	B	293	ILE	2.1
1	B	307	THR	2.1
1	B	357	PHE	2.1
1	C	92	PHE	2.1
1	C	169	ASP	2.1
1	B	391	GLY	2.1
1	C	361	LEU	2.1
1	A	243	TYR	2.1
1	B	341	THR	2.1
1	D	176	ALA	2.1
1	C	247	LEU	2.0
1	A	158	VAL	2.0
1	C	158	VAL	2.0
1	C	311	VAL	2.0
1	A	308	ASP	2.0
1	B	15	SER	2.0
1	A	376	ALA	2.0
1	C	16	GLY	2.0
1	A	285	ASP	2.0
1	C	59	VAL	2.0
1	D	279	ALA	2.0
1	B	70	SER	2.0
1	C	15	SER	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BCN	A	1394	11/11	0.35	3.89	48,58,65,66	0
2	FAD	D	1388	53/53	0.14	-0.70	45,50,54,56	0
2	FAD	C	1388	53/53	0.15	-0.77	43,51,56,56	0
2	FAD	B	1390	53/53	0.13	-0.86	36,44,48,49	0
2	FAD	A	1393	53/53	0.14	-0.91	40,46,53,55	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.