



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:50 AM UTC

PDB ID : 2E49 / pdb\_00002e49  
Title : Crystal Structure of Human D-Amino Acid Oxidase in Complex with Imino-Serine  
Authors : Kawazoe, T.; Tsuge, H.; Imagawa, T.; Fukui, K.  
Deposited on : 2006-12-05  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

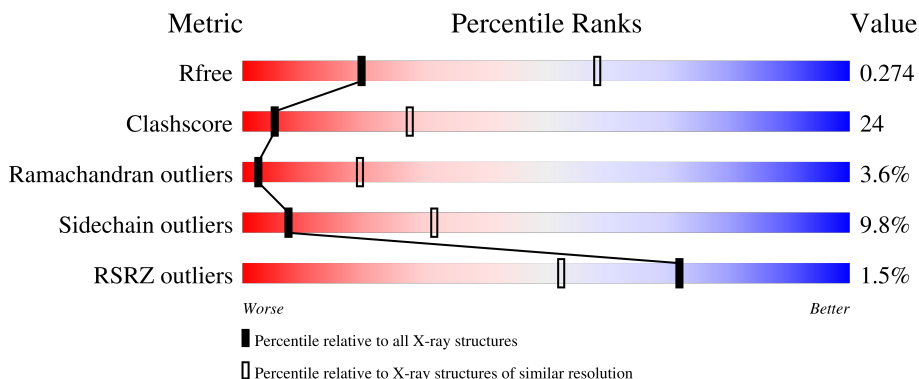
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	347	
1	B	347	
1	C	347	
1	D	347	

## 2 Entry composition [i](#)

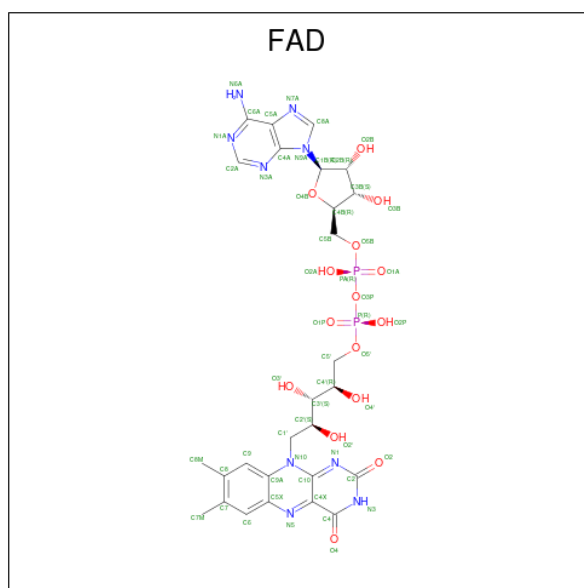
There are 4 unique types of molecules in this entry. The entry contains 11284 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	Total 2733	C 1751	N 479	O 494	S 9	0	0	0
1	B	340	Total 2733	C 1751	N 479	O 494	S 9	0	0	0
1	C	340	Total 2733	C 1751	N 479	O 494	S 9	0	0	0
1	D	340	Total 2733	C 1751	N 479	O 494	S 9	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



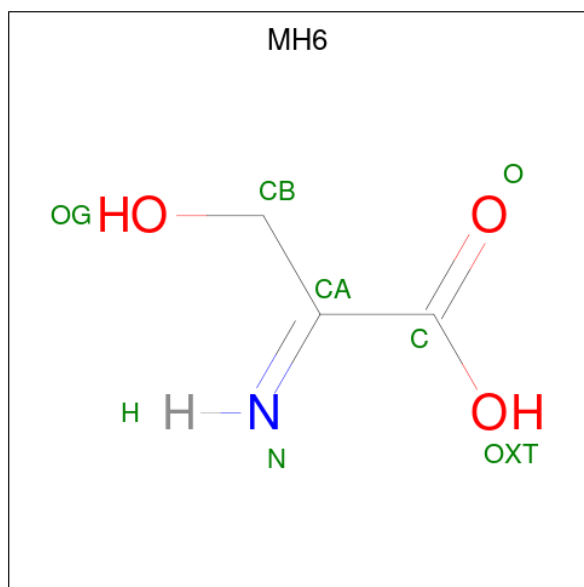
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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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 3-hydroxy-2-iminopropanoic acid (CCD ID: MH6) (formula: C<sub>3</sub>H<sub>5</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	3	1	3		
3	B	1	Total	C	N	O	0	0
			7	3	1	3		
3	C	1	Total	C	N	O	0	0
			7	3	1	3		
3	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	28	Total	O	0	0
			28	28		
4	C	32	Total	O	0	0
			32	32		

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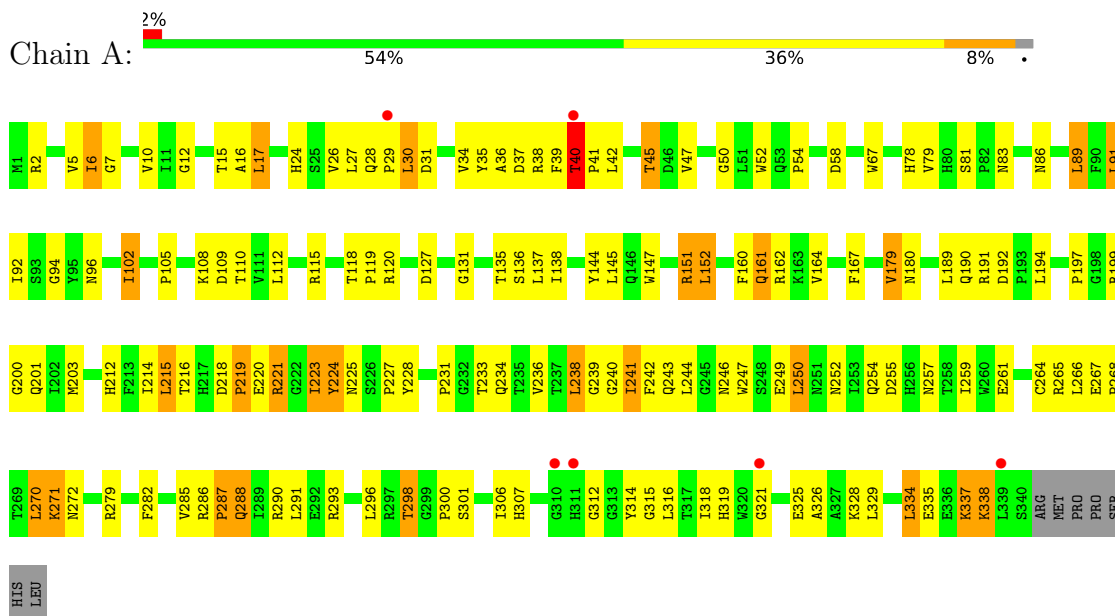
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	D	28	Total	O	0	0
			28	28		

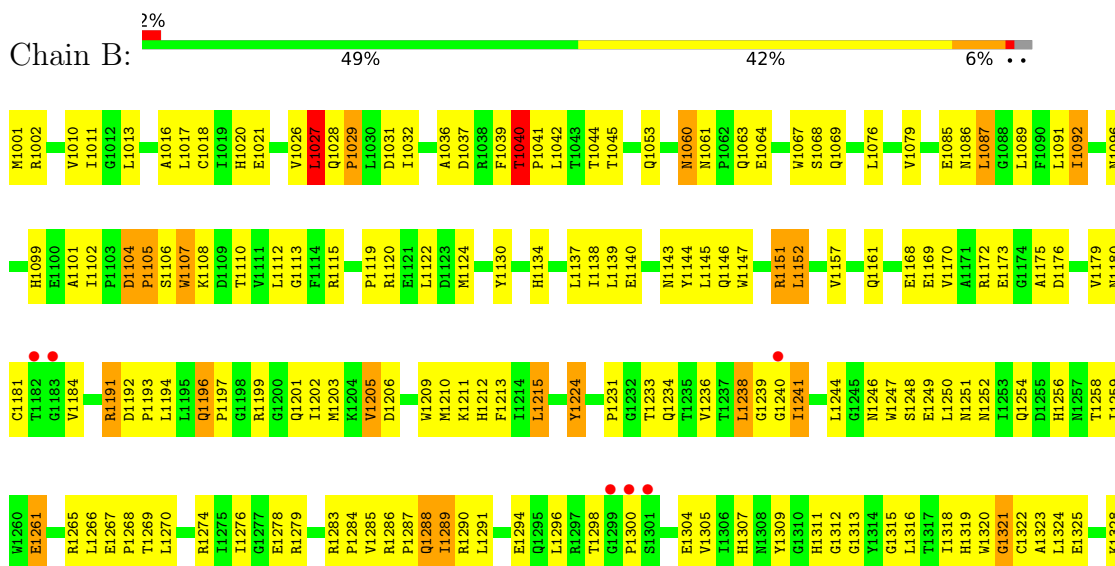
### 3 Residue-property plots [i](#)

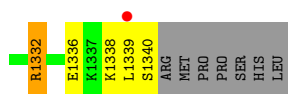
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: D-amino-acid oxidase

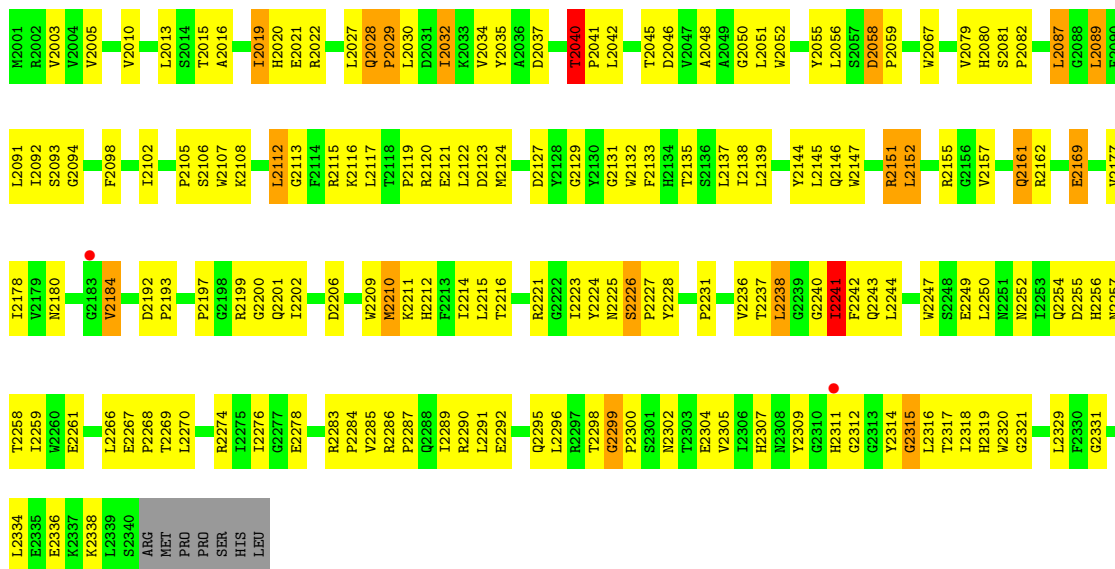


- Molecule 1: D-amino-acid oxidase

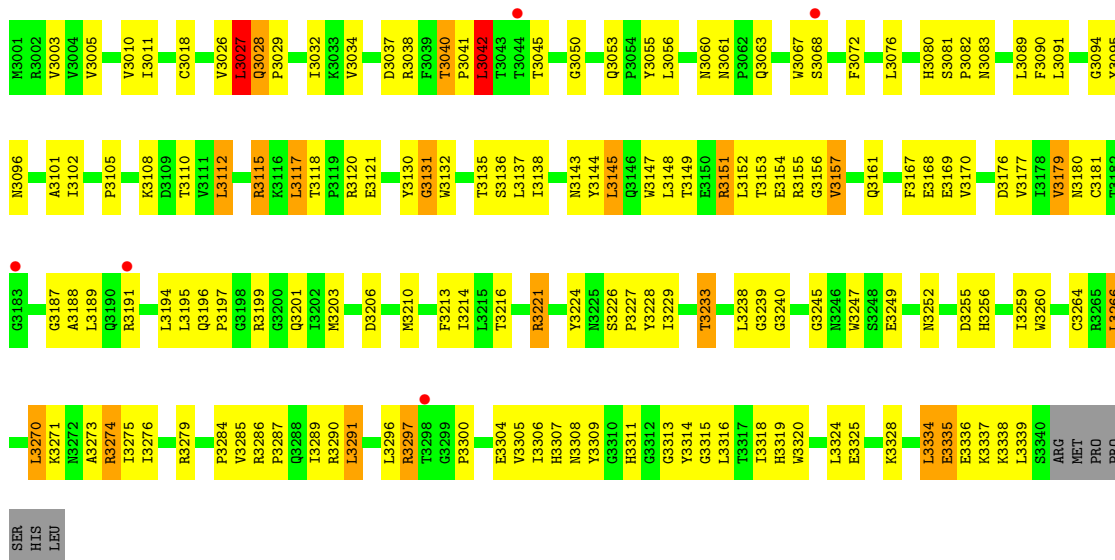




• Molecule 1: D-amino-acid oxidase



• Molecule 1: D-amino-acid oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.66Å 181.75Å 50.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-3.20) 97.4 (50.00-3.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.221 , 0.276 0.219 , 0.274	Depositor DCC
$R_{free}$ test set	1187 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtrriage
Anisotropy	1.057	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 64.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.81 % 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 8.0163e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MH6, 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	0.68	2/2810 (0.1%)	0.94	3/3824 (0.1%)
1	B	0.70	0/2810	0.93	4/3824 (0.1%)
1	C	0.69	0/2810	0.91	3/3824 (0.1%)
1	D	0.67	0/2810	0.94	7/3824 (0.2%)
All	All	0.68	2/11240 (0.0%)	0.93	17/15296 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	LYS	CE-NZ	5.50	1.65	1.49
1	A	223	ILE	CA-CB	5.06	1.59	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	LYS	N-CA-C	-9.20	101.75	113.16
1	D	3094	GLY	N-CA-C	8.20	122.63	110.42
1	B	1040	THR	N-CA-C	6.87	124.99	109.81
1	B	1040	THR	CA-C-N	-6.17	113.42	120.89
1	B	1040	THR	C-N-CA	-6.17	113.42	120.89
1	A	131	GLY	N-CA-C	6.11	120.57	110.55
1	D	3131	GLY	N-CA-C	6.08	120.01	111.19
1	C	2336	GLU	N-CA-C	-6.07	105.78	113.43
1	D	3040	THR	N-CA-C	5.68	122.36	109.81
1	C	2241	ILE	N-CA-C	5.55	115.85	107.75
1	B	1269	THR	N-CA-C	-5.52	106.24	112.87
1	C	2040	THR	N-CA-C	5.46	121.86	109.81
1	D	3040	THR	CA-C-N	-5.39	114.19	119.64
1	D	3040	THR	C-N-CA	-5.39	114.19	119.64
1	A	40	THR	N-CA-C	5.18	121.26	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3042	LEU	N-CA-C	5.18	119.09	109.56
1	D	3275	ILE	N-CA-C	5.10	116.04	108.23

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	2733	0	2680	120	0
1	B	2733	0	2677	143	0
1	C	2733	0	2677	144	0
1	D	2733	0	2677	131	0
2	A	53	0	31	8	0
2	B	53	0	31	11	0
2	C	53	0	31	5	0
2	D	53	0	31	11	0
3	A	7	0	3	0	0
3	B	7	0	3	0	0
3	C	7	0	3	0	0
3	D	7	0	4	2	0
4	A	24	0	0	3	0
4	B	28	0	0	3	0
4	C	32	0	0	4	0
4	D	28	0	0	1	0
All	All	11284	0	10848	536	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 24.

All (536) 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)
2:B:1351:FAD:C5'	2:B:1351:FAD:C4'	1.79	1.55
2:D:3351:FAD:C5'	2:D:3351:FAD:C4'	1.93	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1351:FAD:C4'	2:B:1351:FAD:O4'	1.65	1.42
3:D:3352:MH6:CB	3:D:3352:MH6:OG	1.72	1.36
1:D:3252:ASN:HB3	1:D:3255:ASP:HB2	1.22	1.10
1:C:2040:THR:OG1	1:C:2041:PRO:HD3	1.66	0.94
1:A:199:ARG:HH22	1:A:201:GLN:HE21	1.17	0.92
1:C:2298:THR:HB	1:C:2302:ASN:HA	1.51	0.92
1:D:3180:ASN:HD22	1:D:3307:HIS:CD2	1.90	0.90
1:B:1040:THR:HG23	1:B:1041:PRO:HD3	1.56	0.86
1:D:3199:ARG:HH22	1:D:3201:GLN:NE2	1.76	0.84
1:D:3010:VAL:HG21	1:D:3316:LEU:HD13	1.60	0.83
1:B:1079:VAL:HG21	1:B:1091:LEU:HD12	1.58	0.82
1:C:2151:ARG:O	1:C:2155:ARG:HG3	1.79	0.82
1:D:3147:TRP:CE2	1:D:3151:ARG:HD3	2.14	0.82
1:C:2112:LEU:HB2	1:C:2135:THR:HB	1.62	0.82
1:D:3037:ASP:HB3	2:D:3351:FAD:O2B	1.81	0.81
1:A:199:ARG:HH22	1:A:201:GLN:NE2	1.79	0.79
1:D:3027:LEU:HD11	1:D:3334:LEU:HG	1.65	0.78
1:B:1079:VAL:HG21	1:B:1091:LEU:CD1	2.14	0.78
2:B:1351:FAD:C5'	2:B:1351:FAD:C3'	2.62	0.78
1:D:3041:PRO:HB2	1:D:3042:LEU:HD23	1.68	0.76
2:D:3351:FAD:C5'	2:D:3351:FAD:C3'	2.64	0.76
1:D:3027:LEU:HD21	1:D:3334:LEU:HD21	1.67	0.76
1:B:1201:GLN:HE22	1:B:1252:ASN:H	1.32	0.76
1:B:1241:ILE:HD13	1:B:1259:ILE:HD11	1.67	0.76
1:C:2199:ARG:HH22	1:C:2201:GLN:HE21	1.30	0.75
1:C:2315:GLY:HA3	2:C:2351:FAD:H4'	1.68	0.74
1:D:3206:ASP:HB2	1:D:3276:ILE:HD11	1.71	0.73
1:B:1028:GLN:HB3	1:B:1029:PRO:HD3	1.70	0.73
1:A:239:GLY:HA2	1:A:259:ILE:HD12	1.70	0.73
1:D:3112:LEU:HB2	1:D:3135:THR:HB	1.72	0.72
1:D:3216:THR:O	1:D:3226:SER:HB2	1.89	0.72
1:B:1010:VAL:HB	1:B:1045:THR:HG21	1.70	0.72
1:B:1144:TYR:OH	1:B:1319:HIS:CE1	2.43	0.71
1:A:199:ARG:NH2	1:A:201:GLN:HE21	1.89	0.71
1:B:1040:THR:HA	1:B:1145:LEU:HD23	1.71	0.71
1:D:3315:GLY:HA3	2:D:3351:FAD:H4'	1.72	0.71
1:A:40:THR:OG1	1:A:41:PRO:HD3	1.91	0.71
1:C:2231:PRO:HA	1:C:2236:VAL:HG13	1.72	0.71
1:B:1087:LEU:HD23	1:B:1089:LEU:HD12	1.74	0.70
1:C:2117:LEU:HB2	1:C:2122:LEU:HD21	1.72	0.70
1:A:255:ASP:O	1:A:259:ILE:HG12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:NE2	1:D:3249:GLU:H	1.89	0.69
1:B:1239:GLY:HA2	1:B:1259:ILE:HD12	1.74	0.69
1:C:2201:GLN:NE2	1:C:2252:ASN:H	1.91	0.69
1:B:1037:ASP:HB3	2:B:1351:FAD:O2B	1.93	0.68
1:B:1233:THR:HG23	1:B:1234:GLN:N	2.09	0.68
1:C:2119:PRO:HA	1:C:2122:LEU:HD12	1.75	0.68
1:D:3252:ASN:CB	1:D:3255:ASP:HB2	2.13	0.68
1:B:1201:GLN:NE2	1:B:1252:ASN:H	1.90	0.68
1:C:2115:ARG:NH2	1:C:2121:GLU:OE2	2.26	0.68
1:D:3196:GLN:O	1:D:3285:VAL:HB	1.94	0.68
1:B:1180:ASN:HB3	1:B:1307:HIS:HD2	1.58	0.67
1:C:2127:ASP:HA	4:C:83:HOH:O	1.93	0.67
1:B:1119:PRO:HA	1:B:1122:LEU:HD12	1.75	0.67
1:D:3003:VAL:HB	1:D:3032:ILE:HG12	1.77	0.67
1:C:2199:ARG:HH22	1:C:2201:GLN:NE2	1.92	0.67
1:D:3152:LEU:HD12	1:D:3157:VAL:HG21	1.76	0.67
1:A:200:GLY:HA2	1:A:241:ILE:HG22	1.76	0.67
1:A:201:GLN:HE22	1:A:252:ASN:H	1.40	0.67
1:C:2252:ASN:HD21	1:C:2254:GLN:HB3	1.60	0.66
1:B:1199:ARG:HH22	1:B:1201:GLN:HE21	1.41	0.66
1:C:2201:GLN:HE22	1:C:2252:ASN:H	1.44	0.66
1:A:67:TRP:HB2	1:A:318:ILE:HD11	1.76	0.66
1:C:2120:ARG:HH22	1:D:3110:THR:C	2.04	0.65
1:B:1001:MET:HE2	1:B:1176:ASP:HB3	1.78	0.65
1:B:1092:ILE:HG21	1:B:1138:ILE:HG13	1.77	0.65
1:A:223:ILE:O	1:A:225:ASN:N	2.30	0.65
1:B:1315:GLY:HA3	2:B:1351:FAD:H4'	1.78	0.65
1:A:197:PRO:HG3	1:A:247:TRP:CE2	2.31	0.65
1:B:1096:ASN:HD22	1:B:1134:HIS:HE1	1.43	0.65
1:A:17:LEU:HB2	1:A:152:LEU:HD11	1.79	0.64
1:B:1199:ARG:HH22	1:B:1201:GLN:NE2	1.96	0.64
1:B:1224:TYR:CE2	1:B:1313:GLY:HA3	2.33	0.64
1:C:2291:LEU:HA	1:C:2307:HIS:O	1.98	0.64
1:D:3028:GLN:NE2	1:D:3029:PRO:HD3	2.12	0.64
1:D:3180:ASN:HD22	1:D:3307:HIS:HD2	1.45	0.64
1:C:2010:VAL:HG21	1:C:2316:LEU:HD13	1.80	0.63
1:C:2045:THR:HG23	1:C:2316:LEU:HD21	1.80	0.63
1:B:1268:PRO:C	1:B:1270:LEU:H	2.07	0.63
1:D:3197:PRO:HG3	1:D:3247:TRP:CE2	2.34	0.63
1:A:115:ARG:HD3	4:A:373:HOH:O	1.98	0.63
1:A:189:LEU:HD11	2:A:351:FAD:H61A	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3284:PRO:HG2	1:D:3311:HIS:H	1.64	0.63
1:A:41:PRO:HG2	1:D:3279:ARG:HD3	1.80	0.62
1:C:2124:MET:SD	1:D:3091:LEU:HD11	2.39	0.62
1:A:201:GLN:NE2	1:A:252:ASN:H	1.96	0.62
1:B:1147:TRP:CE2	1:B:1151:ARG:HD3	2.34	0.62
1:D:3274:ARG:HE	1:D:3274:ARG:HA	1.63	0.62
1:B:1196:GLN:NE2	1:B:1244:LEU:HD13	2.15	0.62
1:A:5:VAL:HA	1:A:179:VAL:HG23	1.81	0.61
1:C:2206:ASP:HB2	1:C:2276:ILE:HD11	1.82	0.61
1:C:2037:ASP:HB3	2:C:2351:FAD:O2B	2.00	0.61
1:A:298:THR:HG23	1:A:301:SER:O	1.99	0.61
1:C:2199:ARG:HH11	1:C:2243:GLN:HE22	1.46	0.61
1:C:2021:GLU:HG3	1:C:2022:ARG:H	1.66	0.61
1:A:147:TRP:NE1	1:A:151:ARG:HD3	2.16	0.61
1:C:2199:ARG:NH2	1:C:2201:GLN:HE21	1.98	0.60
1:B:1179:VAL:HG12	1:B:1181:CYS:SG	2.42	0.60
1:A:179:VAL:HG12	1:A:306:ILE:HB	1.83	0.60
1:B:1279:ARG:HG3	1:B:1279:ARG:HH11	1.66	0.60
1:C:2177:VAL:HG22	1:C:2304:GLU:HB2	1.84	0.60
1:B:1053:GLN:HE22	1:B:1096:ASN:HD21	1.48	0.60
2:B:1351:FAD:C4'	2:B:1351:FAD:O5'	2.50	0.60
1:A:216:THR:HG23	1:A:266:LEU:HD11	1.84	0.60
1:B:1018:CYS:SG	1:B:1324:LEU:HD12	2.42	0.60
1:B:1233:THR:HG23	1:B:1234:GLN:H	1.66	0.60
1:A:6:ILE:HG21	1:A:164:VAL:HG21	1.84	0.59
1:D:3274:ARG:HA	1:D:3274:ARG:NE	2.16	0.59
1:B:1339:LEU:O	1:B:1340:SER:HB2	2.02	0.59
1:B:1168:GLU:HG3	1:B:1298:THR:HG22	1.84	0.59
1:B:1250:LEU:HD12	1:B:1251:ASN:N	2.18	0.59
1:C:2028:GLN:HG3	1:C:2029:PRO:HD3	1.84	0.59
1:A:215:LEU:HD22	1:A:228:TYR:HB2	1.85	0.59
1:B:1274:ARG:HA	1:B:1274:ARG:NE	2.18	0.59
1:C:2027:LEU:HD11	1:C:2334:LEU:HD13	1.83	0.59
1:B:1105:PRO:HD2	1:B:1108:LYS:HB2	1.86	0.58
1:B:1184:VAL:HG22	1:B:1247:TRP:CH2	2.38	0.58
1:A:38:ARG:O	2:A:351:FAD:O3B	2.21	0.58
1:A:120:ARG:NH1	1:B:1110:THR:O	2.36	0.58
1:B:1256:HIS:HD1	1:B:1278:GLU:CD	2.12	0.58
2:B:1351:FAD:C4'	2:B:1351:FAD:HO4'	2.09	0.58
1:A:167:PHE:HB3	1:A:296:LEU:HD21	1.86	0.57
1:A:199:ARG:HH11	1:A:243:GLN:HE22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2210:MET:SD	1:C:2267:GLU:HG2	2.44	0.57
1:A:270:LEU:C	1:A:272:ASN:H	2.12	0.57
1:C:2144:TYR:HE2	1:C:2319:HIS:CE1	2.22	0.57
1:D:3005:VAL:HG13	1:D:3179:VAL:HB	1.87	0.57
1:D:3194:LEU:HB3	1:D:3287:PRO:HD2	1.86	0.57
1:C:2040:THR:O	1:C:2046:ASP:OD2	2.23	0.57
1:C:2079:VAL:HA	1:C:2089:LEU:CD1	2.34	0.57
1:B:1336:GLU:C	1:B:1338:LYS:H	2.13	0.56
1:A:221:ARG:O	1:A:225:ASN:HB3	2.05	0.56
1:B:1061:ASN:O	1:B:1064:GLU:HB2	2.05	0.56
1:B:1241:ILE:HD13	1:B:1259:ILE:CD1	2.34	0.56
1:C:2079:VAL:HA	1:C:2089:LEU:HD11	1.87	0.56
1:C:2092:ILE:HG21	1:C:2138:ILE:HG13	1.86	0.56
1:D:3117:LEU:HD23	1:D:3121:GLU:HG3	1.88	0.56
1:B:1144:TYR:OH	1:B:1319:HIS:HE1	1.87	0.56
1:D:3028:GLN:CD	1:D:3028:GLN:H	2.14	0.56
1:A:96:ASN:HA	1:A:215:LEU:O	2.05	0.56
1:B:1203:MET:HB3	1:B:1238:LEU:HB2	1.88	0.56
1:C:2035:TYR:CE2	1:C:2162:ARG:HD3	2.40	0.56
1:D:3255:ASP:O	1:D:3259:ILE:HG12	2.06	0.56
1:B:1028:GLN:CB	1:B:1029:PRO:HD3	2.36	0.56
1:A:110:THR:C	1:B:1120:ARG:HH22	2.14	0.56
1:A:221:ARG:HB2	1:A:221:ARG:NH2	2.20	0.56
1:B:1325:GLU:O	1:B:1328:LYS:HB3	2.05	0.56
1:D:3203:MET:HB3	1:D:3238:LEU:HB2	1.88	0.56
1:A:37:ASP:HB3	2:A:351:FAD:O2B	2.06	0.55
1:B:1104:ASP:HB3	1:B:1105:PRO:CD	2.36	0.55
1:C:2032:ILE:HB	1:C:2157:VAL:HG22	1.88	0.55
1:D:3040:THR:HA	1:D:3145:LEU:HD23	1.87	0.55
1:D:3199:ARG:HH22	1:D:3201:GLN:HE21	1.52	0.55
1:B:1201:GLN:HE22	1:B:1252:ASN:N	2.00	0.55
1:D:3038:ARG:O	2:D:3351:FAD:O3B	2.23	0.55
1:A:167:PHE:HB3	1:A:296:LEU:CD2	2.37	0.55
1:C:2139:LEU:HD21	1:C:2144:TYR:CD2	2.42	0.55
1:A:216:THR:OG1	1:A:227:PRO:O	2.23	0.55
1:C:2121:GLU:HA	1:C:2124:MET:HE2	1.89	0.55
1:A:115:ARG:HH12	1:B:1113:GLY:HA3	1.70	0.55
1:D:3216:THR:O	1:D:3226:SER:CB	2.55	0.55
1:A:5:VAL:O	1:A:34:VAL:HA	2.07	0.55
1:D:3011:ILE:HG12	2:D:3351:FAD:O5'	2.06	0.55
1:D:3067:TRP:CZ2	1:D:3325:GLU:HG2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2081:SER:HB2	1:C:2082:PRO:HD2	1.89	0.54
1:D:3199:ARG:HH22	1:D:3201:GLN:HE22	1.53	0.54
1:B:1196:GLN:O	1:B:1285:VAL:HB	2.08	0.54
1:A:5:VAL:HG21	1:A:16:ALA:HB2	1.90	0.54
1:A:286:ARG:CZ	1:A:290:ARG:HB2	2.38	0.54
1:B:1107:TRP:CD1	1:B:1107:TRP:H	2.24	0.54
1:D:3105:PRO:HD3	1:D:3132:TRP:CZ2	2.42	0.54
1:B:1286:ARG:HH12	1:B:1290:ARG:HD2	1.72	0.54
1:A:293:ARG:HB2	1:A:329:LEU:HD22	1.88	0.54
1:C:2255:ASP:O	1:C:2259:ILE:HG12	2.08	0.54
1:A:108:LYS:HG3	1:A:109:ASP:OD1	2.08	0.54
1:A:267:GLU:O	1:A:270:LEU:HB2	2.08	0.54
2:B:1351:FAD:C5'	2:B:1351:FAD:O4'	2.55	0.54
1:A:233:THR:HG23	1:A:234:GLN:HG2	1.90	0.54
2:B:1351:FAD:O4'	2:B:1351:FAD:C3'	2.51	0.54
1:C:2005:VAL:HB	1:C:2034:VAL:HG22	1.89	0.53
1:D:3018:CYS:SG	1:D:3324:LEU:HD23	2.47	0.53
1:C:2290:ARG:HD3	1:C:2309:TYR:CE2	2.43	0.53
1:C:2319:HIS:CG	1:C:2320:TRP:N	2.76	0.53
1:D:3216:THR:HG23	1:D:3266:LEU:HD11	1.91	0.53
1:C:2268:PRO:HG2	1:D:3080:HIS:HB3	1.88	0.53
1:D:3101:ALA:HA	1:D:3130:TYR:CD2	2.43	0.53
1:D:3147:TRP:NE1	1:D:3151:ARG:HD3	2.22	0.53
1:B:1180:ASN:HB3	1:B:1307:HIS:CD2	2.41	0.53
1:C:2112:LEU:HG	1:D:3121:GLU:HB3	1.91	0.53
1:C:2298:THR:HG22	1:C:2299:GLY:N	2.23	0.53
1:D:3214:ILE:HG21	1:D:3266:LEU:CD2	2.39	0.53
1:A:325:GLU:O	1:A:328:LYS:HB3	2.09	0.53
1:B:1060:ASN:ND2	1:B:1288:GLN:HB3	2.24	0.53
1:C:2231:PRO:CA	1:C:2236:VAL:HG13	2.39	0.53
1:A:41:PRO:HG2	1:D:3279:ARG:CD	2.39	0.52
1:A:250:LEU:O	1:A:250:LEU:HD23	2.08	0.52
1:B:1250:LEU:HD12	1:B:1251:ASN:H	1.74	0.52
1:B:1332:ARG:HG3	4:B:32:HOH:O	2.08	0.52
1:A:27:LEU:HD11	1:A:334:LEU:HD11	1.91	0.52
1:D:3227:PRO:HA	1:D:3239:GLY:O	2.09	0.52
1:B:1267:GLU:O	1:B:1270:LEU:HB2	2.09	0.52
1:D:3286:ARG:NH1	1:D:3290:ARG:HB2	2.23	0.52
1:B:1061:ASN:OD1	1:B:1063:GLN:HB2	2.09	0.52
1:B:1184:VAL:HG21	1:B:1197:PRO:HB3	1.91	0.52
1:D:3147:TRP:O	1:D:3151:ARG:HD2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2242:PHE:CZ	1:C:2285:VAL:HG21	2.45	0.52
1:A:7:GLY:O	1:A:12:GLY:HA3	2.09	0.52
1:B:1261:GLU:HB3	1:B:1265:ARG:NH1	2.25	0.52
1:C:2144:TYR:CE2	1:C:2319:HIS:CE1	2.98	0.52
1:D:3050:GLY:O	1:D:3138:ILE:HA	2.10	0.52
1:D:3224:TYR:HE2	1:D:3313:GLY:HA3	1.75	0.52
1:B:1319:HIS:CG	1:B:1320:TRP:N	2.77	0.52
1:C:2087:LEU:HD23	1:C:2139:LEU:HD11	1.91	0.52
1:D:3290:ARG:HD3	1:D:3309:TYR:CE2	2.45	0.52
1:B:1233:THR:HG23	1:B:1234:GLN:HG2	1.92	0.52
1:B:1086:ASN:O	1:B:1143:ASN:HB3	2.09	0.52
1:B:1244:LEU:HD21	1:B:1285:VAL:HG11	1.92	0.51
1:D:3076:LEU:HD13	1:D:3112:LEU:HD21	1.93	0.51
1:A:201:GLN:HE22	1:A:252:ASN:N	2.06	0.51
1:D:3319:HIS:CG	1:D:3320:TRP:N	2.78	0.51
1:A:50:GLY:O	1:A:138:ILE:HA	2.10	0.51
1:C:2091:LEU:HD12	1:C:2137:LEU:HD23	1.92	0.51
1:A:231:PRO:HA	1:A:236:VAL:HG22	1.92	0.51
1:C:2151:ARG:O	1:C:2155:ARG:CG	2.56	0.51
1:D:3199:ARG:NH2	1:D:3201:GLN:NE2	2.53	0.51
1:A:112:LEU:HB2	1:A:135:THR:HB	1.93	0.51
1:A:120:ARG:NH1	1:B:1112:LEU:HD12	2.25	0.51
1:A:203:MET:HB3	1:A:238:LEU:HB2	1.93	0.50
1:C:2289:ILE:HD13	1:C:2311:HIS:CD2	2.46	0.50
1:B:1233:THR:CG2	1:B:1234:GLN:N	2.74	0.50
1:A:10:VAL:HB	1:A:45:THR:HG21	1.93	0.50
1:A:17:LEU:HD12	1:A:152:LEU:HD13	1.92	0.50
1:A:24:HIS:HA	1:A:30:LEU:HD22	1.94	0.50
1:A:91:LEU:HD11	1:B:1124:MET:SD	2.52	0.50
1:D:3053:GLN:HE22	1:D:3096:ASN:HD21	1.57	0.50
1:D:3147:TRP:HZ3	4:D:1:HOH:O	1.93	0.50
1:C:2177:VAL:HA	1:C:2304:GLU:O	2.12	0.50
1:D:3315:GLY:O	1:D:3319:HIS:N	2.43	0.50
1:D:3296:LEU:HD13	1:D:3305:VAL:HG21	1.94	0.50
1:A:271:LYS:HE2	4:A:355:HOH:O	2.12	0.50
1:B:1294:GLU:HB3	1:B:1305:VAL:HB	1.93	0.50
1:C:2040:THR:CB	1:C:2041:PRO:HD3	2.42	0.50
1:B:1106:SER:C	1:B:1108:LYS:H	2.17	0.50
1:D:3325:GLU:OE1	1:D:3328:LYS:HD2	2.12	0.50
2:D:3351:FAD:C4'	2:D:3351:FAD:O5'	2.57	0.50
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2139:LEU:HD21	1:C:2144:TYR:CE2	2.47	0.49
1:C:2216:THR:O	1:C:2226:SER:HB3	2.12	0.49
1:A:5:VAL:HG21	1:A:16:ALA:CB	2.42	0.49
1:B:1013:LEU:HD22	1:B:1152:LEU:HD23	1.94	0.49
1:C:2112:LEU:CB	1:C:2135:THR:HB	2.39	0.49
1:C:2197:PRO:HG3	1:C:2247:TRP:CE2	2.47	0.49
1:A:162:ARG:O	2:A:351:FAD:H2A	2.12	0.49
1:C:2267:GLU:HG3	1:C:2269:THR:OG1	2.12	0.49
1:A:40:THR:CB	1:A:41:PRO:HD3	2.42	0.49
1:A:337:LYS:HD2	1:A:337:LYS:N	2.27	0.49
1:B:1101:ALA:HA	1:B:1130:TYR:CD2	2.48	0.49
1:B:1206:ASP:HB2	1:B:1276:ILE:HD11	1.94	0.49
1:C:2045:THR:HG21	1:C:2145:LEU:HD11	1.94	0.49
1:C:2051:LEU:HA	1:C:2138:ILE:HG12	1.94	0.49
1:D:3089:LEU:O	1:D:3090:PHE:HB3	2.13	0.49
1:D:3177:VAL:HA	1:D:3304:GLU:O	2.13	0.49
1:D:3289:ILE:HD11	1:D:3314:TYR:HE2	1.76	0.49
1:B:1289:ILE:CD1	1:B:1318:ILE:HD13	2.43	0.49
1:C:2040:THR:HG21	1:C:2146:GLN:OE1	2.12	0.49
1:C:2199:ARG:HH11	1:C:2243:GLN:NE2	2.10	0.49
1:D:3067:TRP:HZ2	1:D:3325:GLU:HG2	1.78	0.49
1:D:3197:PRO:HD2	1:D:3245:GLY:HA2	1.94	0.49
1:C:2200:GLY:HA2	1:C:2241:ILE:HG22	1.94	0.49
1:C:2228:TYR:CD1	1:C:2228:TYR:C	2.91	0.49
1:A:252:ASN:HB3	1:A:255:ASP:HB2	1.95	0.49
1:B:1290:ARG:HD3	1:B:1309:TYR:CZ	2.48	0.49
1:C:2147:TRP:CD1	1:C:2151:ARG:HH21	2.30	0.49
1:D:3213:PHE:HA	1:D:3229:ILE:O	2.13	0.49
1:A:83:ASN:HA	1:A:86:ASN:ND2	2.28	0.48
1:B:1147:TRP:NE1	1:B:1151:ARG:HD3	2.28	0.48
1:C:2162:ARG:NH2	1:C:2169:GLU:OE2	2.45	0.48
1:D:3081:SER:OG	1:D:3082:PRO:HD2	2.13	0.48
1:D:3181:CYS:SG	1:D:3308:ASN:HB3	2.53	0.48
1:B:1036:ALA:O	1:B:1161:GLN:HA	2.13	0.48
1:C:2298:THR:CB	1:C:2302:ASN:HA	2.35	0.48
3:D:3352:MH6:OG	3:D:3352:MH6:CA	2.55	0.48
1:A:115:ARG:NH1	1:B:1113:GLY:HA3	2.29	0.48
1:B:1139:LEU:HD21	1:B:1144:TYR:CE2	2.48	0.48
1:B:1202:ILE:HG22	1:B:1239:GLY:HA3	1.96	0.48
1:C:2210:MET:HA	1:C:2210:MET:CE	2.43	0.48
1:C:2045:THR:HG21	1:C:2145:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3214:ILE:HG21	1:D:3266:LEU:HD22	1.95	0.48
1:A:279:ARG:HD2	1:D:3041:PRO:CB	2.44	0.48
1:A:127:ASP:OD1	1:A:265:ARG:HD2	2.14	0.48
1:D:3187:GLY:O	1:D:3189:LEU:N	2.47	0.48
1:A:135:THR:HG23	1:B:1212:HIS:HE1	1.78	0.48
1:C:2027:LEU:HB2	1:C:2030:LEU:HB2	1.95	0.48
1:C:2035:TYR:CD2	1:C:2162:ARG:HD3	2.49	0.48
1:D:3147:TRP:CD2	1:D:3151:ARG:HD3	2.49	0.48
1:D:3199:ARG:NH2	1:D:3201:GLN:HE21	2.12	0.48
1:C:2015:THR:HG22	1:C:2019:ILE:HD12	1.96	0.47
1:C:2055:TYR:CE1	1:C:2314:TYR:HD1	2.32	0.47
1:C:2093:SER:OG	1:C:2135:THR:HG23	2.14	0.47
1:D:3228:TYR:CZ	1:D:3239:GLY:HA3	2.49	0.47
1:C:2021:GLU:HG3	1:C:2022:ARG:N	2.28	0.47
1:C:2209:TRP:O	1:C:2211:LYS:HG2	2.13	0.47
1:C:2010:VAL:HG11	1:C:2316:LEU:HD22	1.95	0.47
1:C:2242:PHE:HA	1:C:2283:ARG:HH12	1.79	0.47
1:A:28:GLN:HB3	1:A:29:PRO:HD3	1.97	0.47
1:A:78:HIS:HA	1:A:81:SER:OG	2.13	0.47
1:A:286:ARG:O	1:A:288:GLN:N	2.48	0.47
1:B:1209:TRP:O	1:B:1211:LYS:HG2	2.14	0.47
1:C:2201:GLN:HE22	1:C:2252:ASN:N	2.11	0.47
1:D:3203:MET:HE2	1:D:3256:HIS:ND1	2.29	0.47
1:A:94:GLY:HA2	1:A:212:HIS:HB3	1.97	0.47
1:B:1233:THR:CG2	1:B:1234:GLN:H	2.26	0.47
1:A:264:CYS:HB3	1:A:271:LYS:HG3	1.97	0.47
1:B:1002:ARG:O	1:B:1176:ASP:HB2	2.15	0.47
1:D:3151:ARG:NH1	1:D:3154:GLU:OE2	2.48	0.47
1:D:3316:LEU:HD22	1:D:3316:LEU:H	1.80	0.47
1:C:2028:GLN:HG3	1:C:2029:PRO:CD	2.44	0.47
1:A:242:PHE:HE1	1:A:244:LEU:HG	1.80	0.47
1:B:1042:LEU:CD2	1:C:2042:LEU:HD22	2.45	0.47
1:D:3297:ARG:HH21	1:D:3297:ARG:HB2	1.80	0.47
1:D:3307:HIS:CD2	1:D:3309:TYR:HE2	2.33	0.47
1:C:2120:ARG:HA	1:C:2123:ASP:OD2	2.14	0.47
1:C:2286:ARG:O	1:C:2287:PRO:C	2.57	0.47
1:A:291:LEU:HA	1:A:307:HIS:O	2.14	0.46
1:B:1039:PHE:O	1:B:1041:PRO:HD2	2.15	0.46
1:D:3335:GLU:HG3	1:D:3336:GLU:N	2.30	0.46
1:A:315:GLY:HA3	2:A:351:FAD:H4'	1.97	0.46
1:B:1010:VAL:HG13	1:B:1011:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2105:PRO:HG3	1:C:2132:TRP:CH2	2.50	0.46
1:B:1194:LEU:O	1:B:1286:ARG:HG3	2.16	0.46
1:B:1197:PRO:HG3	1:B:1247:TRP:CE2	2.50	0.46
1:B:1291:LEU:HA	1:B:1307:HIS:O	2.15	0.46
1:D:3270:LEU:O	1:D:3273:ALA:HB3	2.15	0.46
1:B:1205:VAL:HA	1:B:1274:ARG:O	2.16	0.46
1:D:3286:ARG:O	1:D:3287:PRO:C	2.57	0.46
1:B:1016:ALA:HB3	1:B:1152:LEU:HD21	1.98	0.46
1:B:1040:THR:HG23	1:B:1041:PRO:CD	2.35	0.46
1:C:2105:PRO:HB3	1:C:2107:TRP:CE2	2.51	0.46
1:C:2199:ARG:NH1	1:C:2255:ASP:OD2	2.49	0.46
1:C:2013:LEU:HD22	1:C:2152:LEU:HD23	1.97	0.46
1:C:2214:ILE:O	1:C:2214:ILE:HG22	2.14	0.46
2:C:2351:FAD:H9	2:C:2351:FAD:H1'1	1.58	0.46
1:D:3239:GLY:HA2	1:D:3259:ILE:HD12	1.97	0.46
2:D:3351:FAD:C5'	2:D:3351:FAD:O4'	2.60	0.46
1:C:2215:LEU:HD22	1:C:2228:TYR:HB2	1.97	0.46
1:B:1191:ARG:HH22	1:B:1193:PRO:HB3	1.81	0.46
1:C:2202:ILE:HG23	2:C:2351:FAD:HM71	1.98	0.46
1:C:2267:GLU:HG3	1:C:2269:THR:HG1	1.81	0.46
1:D:3179:VAL:HG13	1:D:3306:ILE:HB	1.98	0.46
1:C:2050:GLY:O	1:C:2138:ILE:HA	2.16	0.46
1:D:3118:THR:OG1	1:D:3121:GLU:HG2	2.15	0.46
2:D:3351:FAD:H9	2:D:3351:FAD:H1'1	1.66	0.46
1:B:1238:LEU:HD11	1:B:1270:LEU:HD21	1.98	0.45
1:B:1286:ARG:HG2	1:B:1287:PRO:HD2	1.98	0.45
1:D:3027:LEU:HD11	1:D:3334:LEU:CG	2.41	0.45
1:D:3045:THR:HG21	1:D:3145:LEU:HD13	1.98	0.45
1:A:325:GLU:OE2	1:A:328:LYS:HD3	2.15	0.45
1:B:1224:TYR:HE2	1:B:1313:GLY:HA3	1.79	0.45
1:B:1231:PRO:HA	1:B:1236:VAL:HA	1.97	0.45
1:C:2115:ARG:HD2	1:C:2116:LYS:O	2.17	0.45
1:C:2161:GLN:HE21	1:C:2161:GLN:HB3	1.63	0.45
1:C:2199:ARG:HB3	1:C:2243:GLN:HB2	1.99	0.45
1:D:3072:PHE:HZ	1:D:3112:LEU:HD22	1.81	0.45
1:B:1170:VAL:HG12	1:B:1175:ALA:HB2	1.98	0.45
1:D:3005:VAL:HB	1:D:3034:VAL:HG22	1.98	0.45
1:A:199:ARG:NH2	1:A:250:LEU:O	2.50	0.45
1:A:214:ILE:O	1:A:228:TYR:HA	2.17	0.45
1:A:270:LEU:C	1:A:272:ASN:N	2.74	0.45
1:C:2290:ARG:N	1:C:2309:TYR:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3040:THR:HG23	1:D:3041:PRO:HD3	1.99	0.45
1:D:3095:TYR:CD2	1:D:3117:LEU:HD21	2.52	0.45
1:B:1092:ILE:HG13	1:B:1213:PHE:HD2	1.82	0.45
1:B:1170:VAL:HA	1:B:1173:GLU:HG2	1.99	0.45
1:D:3115:ARG:NH2	1:D:3121:GLU:OE2	2.50	0.45
1:B:1011:ILE:HG12	2:B:1351:FAD:O5'	2.17	0.45
1:B:1296:LEU:HD23	1:B:1305:VAL:HG21	1.98	0.45
1:A:67:TRP:HB3	1:A:321:GLY:HA3	1.99	0.45
1:A:79:VAL:HA	1:A:89:LEU:HD13	1.99	0.45
1:A:194:LEU:HD22	1:A:287:PRO:HG2	1.99	0.45
1:C:2283:ARG:O	1:C:2285:VAL:N	2.50	0.45
1:A:45:THR:HG21	1:A:145:LEU:HD11	1.98	0.45
1:A:223:ILE:C	1:A:225:ASN:H	2.24	0.45
1:B:1325:GLU:O	1:B:1328:LYS:CB	2.65	0.45
1:C:2016:ALA:HB3	1:C:2152:LEU:HD21	1.99	0.45
1:C:2216:THR:HG23	1:C:2227:PRO:O	2.16	0.45
1:A:167:PHE:CB	1:A:296:LEU:HD21	2.46	0.44
1:B:1041:PRO:HG2	1:B:1042:LEU:HG	1.99	0.44
1:B:1104:ASP:HB3	1:B:1105:PRO:HD3	1.99	0.44
1:B:1268:PRO:C	1:B:1270:LEU:N	2.65	0.44
1:B:1283:ARG:O	1:B:1285:VAL:N	2.49	0.44
1:D:3090:PHE:CE1	1:D:3233:THR:HG22	2.52	0.44
2:D:3351:FAD:N1	2:D:3351:FAD:H2'	2.32	0.44
1:A:270:LEU:O	1:A:272:ASN:N	2.50	0.44
1:C:2221:ARG:HH11	1:C:2225:ASN:ND2	2.16	0.44
1:C:2242:PHE:HZ	1:C:2285:VAL:HG21	1.82	0.44
1:C:2256:HIS:ND1	1:C:2278:GLU:OE1	2.48	0.44
1:C:2252:ASN:ND2	1:C:2255:ASP:H	2.16	0.44
1:D:3076:LEU:O	1:D:3076:LEU:HG	2.17	0.44
1:D:3153:THR:C	1:D:3155:ARG:H	2.26	0.44
1:B:1010:VAL:HG21	1:B:1316:LEU:HD13	1.98	0.44
1:C:2117:LEU:CD2	1:C:2133:PHE:HB2	2.47	0.44
1:C:2120:ARG:NH2	1:D:3110:THR:O	2.48	0.44
1:D:3168:GLU:O	1:D:3170:VAL:N	2.50	0.44
1:B:1320:TRP:O	1:B:1321:GLY:C	2.60	0.44
1:A:36:ALA:HB3	1:A:39:PHE:CZ	2.52	0.44
1:B:1053:GLN:NE2	1:B:1215:LEU:HD12	2.32	0.44
1:D:3055:TYR:CE2	1:D:3314:TYR:HE1	2.35	0.44
1:D:3177:VAL:HG22	1:D:3304:GLU:HB2	2.00	0.44
1:D:3228:TYR:CE1	1:D:3239:GLY:HA3	2.53	0.44
1:B:1106:SER:C	1:B:1108:LYS:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1161:GLN:HE21	1:C:2249:GLU:H	1.66	0.44
1:C:2320:TRP:O	1:C:2321:GLY:C	2.60	0.44
1:A:5:VAL:HB	1:A:34:VAL:HG22	2.00	0.44
1:A:223:ILE:HG13	1:A:224:TYR:N	2.33	0.44
1:A:286:ARG:O	1:A:287:PRO:C	2.59	0.44
1:C:2067:TRP:HB2	1:C:2318:ILE:HD11	1.99	0.44
1:B:1017:LEU:HA	1:B:1152:LEU:HD11	1.99	0.43
1:D:3061:ASN:C	1:D:3063:GLN:N	2.74	0.43
1:D:3291:LEU:CD1	1:D:3325:GLU:HG3	2.48	0.43
1:C:2052:TRP:CD1	1:C:2317:THR:HG23	2.53	0.43
1:B:1192:ASP:HA	1:B:1193:PRO:HD3	1.81	0.43
1:D:3264:CYS:HB3	1:D:3271:LYS:HD2	2.00	0.43
1:C:2201:GLN:NE2	1:C:2252:ASN:N	2.65	0.43
1:B:1076:LEU:HB2	1:B:1137:LEU:HD11	2.00	0.43
1:A:161:GLN:HE21	1:A:161:GLN:HB3	1.51	0.43
1:A:189:LEU:HD11	2:A:351:FAD:N6A	2.31	0.43
1:A:197:PRO:HG3	1:A:247:TRP:CZ2	2.53	0.43
1:C:2098:PHE:HD2	1:C:2131:GLY:HA2	1.83	0.43
1:C:2238:LEU:HB3	1:C:2259:ILE:CG2	2.48	0.43
1:D:3040:THR:CG2	1:D:3041:PRO:HD3	2.49	0.43
1:D:3061:ASN:C	1:D:3063:GLN:H	2.26	0.43
1:D:3061:ASN:OD1	1:D:3063:GLN:HB2	2.18	0.43
1:D:3279:ARG:HG3	1:D:3279:ARG:HH11	1.84	0.43
1:D:3203:MET:HE3	1:D:3203:MET:HB2	1.86	0.43
1:C:2020:HIS:CE1	1:C:2155:ARG:HE	2.37	0.43
1:C:2178:ILE:HB	1:C:2305:VAL:HG22	2.00	0.43
1:C:2252:ASN:HD22	1:C:2255:ASP:CG	2.27	0.43
1:D:3136:SER:OG	1:D:3137:LEU:N	2.52	0.43
1:B:1032:ILE:HB	1:B:1157:VAL:HG22	2.01	0.42
1:C:2087:LEU:HD23	1:C:2139:LEU:CD1	2.48	0.42
1:C:2257:ASN:O	1:C:2261:GLU:HB2	2.19	0.42
1:D:3187:GLY:HA2	1:D:3191:ARG:HA	2.01	0.42
1:B:1231:PRO:HB3	1:B:1236:VAL:HG22	2.01	0.42
1:C:2041:PRO:HB2	1:C:2042:LEU:HD23	2.02	0.42
1:C:2048:ALA:HB2	2:C:2351:FAD:O2'	2.20	0.42
1:D:3148:LEU:O	1:D:3149:THR:C	2.63	0.42
1:D:3167:PHE:HB2	1:D:3296:LEU:HD21	2.02	0.42
1:D:3168:GLU:C	1:D:3170:VAL:N	2.77	0.42
1:A:15:THR:HG23	1:A:326:ALA:HB3	2.01	0.42
1:B:1249:GLU:H	1:C:2161:GLN:NE2	2.16	0.42
1:B:1231:PRO:HA	1:B:1236:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2180:ASN:HB3	1:C:2307:HIS:CD2	2.54	0.42
1:C:2329:LEU:C	1:C:2331:GLY:N	2.77	0.42
1:A:242:PHE:HZ	1:A:285:VAL:HG21	1.85	0.42
1:A:27:LEU:HD21	1:A:334:LEU:HD21	2.01	0.42
1:A:144:TYR:CE2	1:A:319:HIS:CE1	3.08	0.42
1:C:2028:GLN:N	1:C:2029:PRO:CD	2.83	0.42
1:A:218:ASP:O	1:A:220:GLU:N	2.53	0.42
1:B:1067:TRP:HB2	1:B:1318:ILE:HD11	2.00	0.42
1:B:1194:LEU:C	1:B:1286:ARG:HG3	2.44	0.42
1:D:3144:TYR:CE2	1:D:3319:HIS:CE1	3.08	0.42
1:D:3161:GLN:HE21	1:D:3161:GLN:HB3	1.68	0.42
1:B:1304:GLU:HG2	4:B:24:HOH:O	2.20	0.42
1:D:3117:LEU:HD12	1:D:3131:GLY:HA3	2.02	0.42
1:A:52:TRP:HE3	1:A:52:TRP:O	2.02	0.42
1:A:136:SER:O	1:A:137:LEU:HD23	2.20	0.42
1:C:2252:ASN:ND2	1:C:2254:GLN:HB3	2.29	0.42
1:D:3291:LEU:HA	1:D:3307:HIS:O	2.20	0.42
1:A:147:TRP:CD1	1:A:151:ARG:HH21	2.38	0.42
1:B:1231:PRO:HA	1:B:1236:VAL:HG13	2.01	0.42
1:D:3336:GLU:C	1:D:3338:LYS:N	2.76	0.42
1:A:199:ARG:HB3	1:A:246:ASN:HB3	2.02	0.41
1:B:1316:LEU:O	1:B:1319:HIS:HD2	2.02	0.41
1:C:2298:THR:CG2	1:C:2299:GLY:N	2.82	0.41
1:D:3032:ILE:O	1:D:3157:VAL:HA	2.18	0.41
1:D:3325:GLU:O	1:D:3328:LYS:HB3	2.19	0.41
1:C:2102:ILE:HD13	4:C:31:HOH:O	2.20	0.41
1:D:3195:LEU:HA	1:D:3286:ARG:HG3	2.01	0.41
1:B:1026:VAL:O	1:B:1027:LEU:HB2	2.19	0.41
1:B:1246:ASN:C	1:B:1248:SER:H	2.29	0.41
1:C:2224:TYR:C	1:C:2226:SER:H	2.28	0.41
1:A:102:ILE:HG23	4:A:356:HOH:O	2.19	0.41
1:A:242:PHE:CZ	1:A:285:VAL:HG21	2.55	0.41
1:C:2289:ILE:N	4:C:2:HOH:O	2.53	0.41
1:B:1252:ASN:HD21	1:B:1254:GLN:HB3	1.85	0.41
1:B:1311:HIS:O	1:B:1312:GLY:C	2.63	0.41
1:C:2184:VAL:HG22	1:C:2247:TRP:CH2	2.56	0.41
1:C:2296:LEU:O	1:C:2302:ASN:HB2	2.20	0.41
1:D:3291:LEU:HD12	1:D:3325:GLU:HG3	2.02	0.41
1:A:118:THR:HB	1:A:119:PRO:HD2	2.01	0.41
1:C:2058:ASP:HA	1:C:2059:PRO:HD3	1.93	0.41
1:C:2117:LEU:HD23	1:C:2133:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3010:VAL:HG21	1:D:3316:LEU:CD1	2.43	0.41
1:D:3156:GLY:O	1:D:3157:VAL:C	2.63	0.41
1:A:35:TYR:HA	1:A:160:PHE:O	2.19	0.41
1:B:1286:ARG:NH1	1:B:1290:ARG:HB2	2.35	0.41
1:B:1320:TRP:O	1:B:1323:ALA:N	2.54	0.41
1:C:2267:GLU:O	1:C:2270:LEU:HB2	2.19	0.41
1:A:47:VAL:HG22	1:A:279:ARG:HB3	2.03	0.41
1:A:316:LEU:HB2	2:A:351:FAD:O2	2.20	0.41
1:B:1169:GLU:HG3	4:B:17:HOH:O	2.21	0.41
1:B:1283:ARG:HD3	1:B:1313:GLY:HA2	2.02	0.41
1:B:1325:GLU:O	1:B:1328:LYS:N	2.54	0.41
1:B:1336:GLU:C	1:B:1338:LYS:N	2.77	0.41
2:B:1351:FAD:H9	2:B:1351:FAD:H1'1	1.51	0.41
1:C:2022:ARG:HD3	4:C:41:HOH:O	2.21	0.41
1:C:2027:LEU:HD22	1:C:2030:LEU:HD12	2.03	0.41
1:C:2180:ASN:HB3	1:C:2307:HIS:HD2	1.86	0.41
1:C:2241:ILE:HD13	1:C:2259:ILE:CD1	2.51	0.41
2:D:3351:FAD:N1	2:D:3351:FAD:C2'	2.84	0.41
1:A:144:TYR:HE2	1:A:319:HIS:CE1	2.38	0.41
1:C:2094:GLY:HA2	1:C:2212:HIS:HB3	2.02	0.41
1:D:3314:TYR:O	1:D:3318:ILE:HG22	2.21	0.41
1:A:192:ASP:OD2	1:A:286:ARG:NH1	2.53	0.40
1:B:1020:HIS:O	1:B:1021:GLU:C	2.64	0.40
1:B:1161:GLN:NE2	1:C:2249:GLU:H	2.18	0.40
1:B:1320:TRP:O	1:B:1322:CYS:N	2.55	0.40
1:A:249:GLU:HB2	1:A:282:PHE:HZ	1.85	0.40
1:A:257:ASN:O	1:A:261:GLU:HB2	2.21	0.40
1:B:1042:LEU:HD23	1:C:2042:LEU:HD22	2.01	0.40
1:B:1152:LEU:HA	1:B:1152:LEU:HD12	1.77	0.40
1:C:2180:ASN:ND2	1:C:2307:HIS:HD2	2.18	0.40
1:A:249:GLU:HB2	1:A:282:PHE:CZ	2.56	0.40
1:B:1018:CYS:SG	1:B:1324:LEU:HA	2.61	0.40
1:B:1290:ARG:HD3	1:B:1309:TYR:OH	2.22	0.40
1:C:2192:ASP:HA	1:C:2193:PRO:HD3	1.98	0.40
1:D:3144:TYR:CE2	1:D:3148:LEU:HD11	2.56	0.40
1:D:3270:LEU:HD12	1:D:3270:LEU:HA	1.96	0.40
1:D:3338:LYS:HB2	1:D:3338:LYS:HE2	1.86	0.40
1:A:17:LEU:HG	1:A:17:LEU:O	2.21	0.40
1:A:268:PRO:C	1:A:270:LEU:N	2.76	0.40
1:A:314:TYR:CD1	1:A:314:TYR:N	2.89	0.40
2:A:351:FAD:H9	2:A:351:FAD:H1'1	1.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1140:GLU:OE2	1:B:1233:THR:HG22	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	338/347 (97%)	284 (84%)	43 (13%)	11 (3%)	3	21
1	B	338/347 (97%)	274 (81%)	51 (15%)	13 (4%)	2	18
1	C	338/347 (97%)	289 (86%)	36 (11%)	13 (4%)	2	18
1	D	338/347 (97%)	278 (82%)	49 (14%)	11 (3%)	3	21
All	All	1352/1388 (97%)	1125 (83%)	179 (13%)	48 (4%)	2	19

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	224	TYR
1	B	1040	THR
1	B	1300	PRO
1	C	2040	THR
1	D	3157	VAL
1	A	54	PRO
1	A	105	PRO
1	A	240	GLY
1	A	312	GLY
1	B	1105	PRO
1	C	2113	GLY
1	C	2299	GLY
1	C	2315	GLY

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Mol	Chain	Res	Type
1	D	3027	LEU
1	D	3169	GLU
1	D	3188	ALA
1	A	191	ARG
1	A	219	PRO
1	A	271	LYS
1	A	300	PRO
1	B	1172	ARG
1	B	1191	ARG
1	B	1240	GLY
1	C	2300	PRO
1	C	2338	LYS
1	D	3108	LYS
1	D	3221	ARG
1	B	1224	TYR
1	C	2129	GLY
1	D	3300	PRO
1	B	1027	LEU
1	B	1104	ASP
1	B	1321	GLY
1	C	2029	PRO
1	C	2056	LEU
1	D	3260	TRP
1	D	3339	LEU
1	A	287	PRO
1	B	1029	PRO
1	C	2312	GLY
1	C	2240	GLY
1	C	2284	PRO
1	D	3026	VAL
1	D	3240	GLY
1	C	2223	ILE
1	B	1284	PRO
1	B	1289	ILE

### 5.3.2 Protein sidechains [i](#)

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	292/299 (98%)	260 (89%)	32 (11%)	6	26
1	B	292/299 (98%)	265 (91%)	27 (9%)	8	33
1	C	292/299 (98%)	264 (90%)	28 (10%)	8	32
1	D	292/299 (98%)	264 (90%)	28 (10%)	8	32
All	All	1168/1196 (98%)	1053 (90%)	115 (10%)	7	31

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	ILE
1	A	17	LEU
1	A	26	VAL
1	A	30	LEU
1	A	31	ASP
1	A	40	THR
1	A	42	LEU
1	A	45	THR
1	A	58	ASP
1	A	89	LEU
1	A	91	LEU
1	A	92	ILE
1	A	102	ILE
1	A	151	ARG
1	A	152	LEU
1	A	161	GLN
1	A	179	VAL
1	A	190	GLN
1	A	215	LEU
1	A	219	PRO
1	A	221	ARG
1	A	238	LEU
1	A	241	ILE
1	A	250	LEU
1	A	254	GLN
1	A	270	LEU
1	A	288	GLN
1	A	298	THR
1	A	334	LEU
1	A	335	GLU
1	A	338	LYS
1	B	1027	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1031	ASP
1	B	1044	THR
1	B	1060	ASN
1	B	1068	SER
1	B	1069	GLN
1	B	1085	GLU
1	B	1087	LEU
1	B	1092	ILE
1	B	1099	HIS
1	B	1102	ILE
1	B	1107	TRP
1	B	1115	ARG
1	B	1146	GLN
1	B	1151	ARG
1	B	1152	LEU
1	B	1196	GLN
1	B	1205	VAL
1	B	1210	MET
1	B	1215	LEU
1	B	1238	LEU
1	B	1241	ILE
1	B	1258	THR
1	B	1261	GLU
1	B	1266	LEU
1	B	1288	GLN
1	B	1332	ARG
1	C	2003	VAL
1	C	2019	ILE
1	C	2028	GLN
1	C	2032	ILE
1	C	2058	ASP
1	C	2080	HIS
1	C	2087	LEU
1	C	2089	LEU
1	C	2106	SER
1	C	2108	LYS
1	C	2112	LEU
1	C	2151	ARG
1	C	2152	LEU
1	C	2161	GLN
1	C	2169	GLU
1	C	2184	VAL

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Mol	Chain	Res	Type
1	C	2210	MET
1	C	2226	SER
1	C	2237	THR
1	C	2238	LEU
1	C	2241	ILE
1	C	2244	LEU
1	C	2250	LEU
1	C	2258	THR
1	C	2266	LEU
1	C	2274	ARG
1	C	2292	GLU
1	C	2295	GLN
1	D	3027	LEU
1	D	3028	GLN
1	D	3042	LEU
1	D	3056	LEU
1	D	3060	ASN
1	D	3068	SER
1	D	3083	ASN
1	D	3102	ILE
1	D	3112	LEU
1	D	3115	ARG
1	D	3117	LEU
1	D	3120	ARG
1	D	3143	ASN
1	D	3145	LEU
1	D	3151	ARG
1	D	3176	ASP
1	D	3179	VAL
1	D	3210	MET
1	D	3221	ARG
1	D	3233	THR
1	D	3266	LEU
1	D	3270	LEU
1	D	3274	ARG
1	D	3291	LEU
1	D	3297	ARG
1	D	3334	LEU
1	D	3335	GLU
1	D	3337	LYS

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

Mol	Chain	Res	Type
1	A	69	GLN
1	A	83	ASN
1	A	86	ASN
1	A	134	HIS
1	A	161	GLN
1	A	201	GLN
1	A	225	ASN
1	A	234	GLN
1	A	243	GLN
1	A	254	GLN
1	A	288	GLN
1	A	302	ASN
1	A	307	HIS
1	A	319	HIS
1	B	1053	GLN
1	B	1063	GLN
1	B	1069	GLN
1	B	1134	HIS
1	B	1161	GLN
1	B	1190	GLN
1	B	1201	GLN
1	B	1212	HIS
1	B	1243	GLN
1	B	1252	ASN
1	B	1288	GLN
1	B	1302	ASN
1	B	1307	HIS
1	B	1308	ASN
1	B	1311	HIS
1	B	1319	HIS
1	C	2053	GLN
1	C	2070	GLN
1	C	2096	ASN
1	C	2134	HIS
1	C	2161	GLN
1	C	2180	ASN
1	C	2201	GLN
1	C	2234	GLN
1	C	2243	GLN
1	C	2252	ASN
1	C	2307	HIS
1	C	2319	HIS
1	D	3096	ASN

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Mol	Chain	Res	Type
1	D	3161	GLN
1	D	3201	GLN
1	D	3243	GLN
1	D	3288	GLN
1	D	3307	HIS
1	D	3319	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 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$
3	MH6	D	3352	-	5,6,6	7.31	3 (60%)	2,7,7	4.54	1 (50%)
2	FAD	B	1351	-	58,58,58	3.29	7 (12%)	85,89,89	2.14	24 (28%)
2	FAD	C	2351	-	58,58,58	1.99	9 (15%)	85,89,89	2.05	25 (29%)
3	MH6	A	352	-	5,6,6	1.49	0	2,7,7	2.11	1 (50%)
3	MH6	B	1352	-	5,6,6	1.30	0	2,7,7	0.96	0
2	FAD	A	351	-	58,58,58	2.54	9 (15%)	85,89,89	2.10	26 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MH6	C	2352	-	5,6,6	1.97	2 (40%)	2,7,7	2.72	1 (50%)
2	FAD	D	3351	-	58,58,58	4.30	11 (18%)	85,89,89	2.28	22 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MH6	D	3352	-	-	3/3/6/6	-
2	FAD	B	1351	-	-	7/34/50/50	0/6/6/6
2	FAD	C	2351	-	-	3/34/50/50	0/6/6/6
3	MH6	A	352	-	-	1/3/6/6	-
3	MH6	B	1352	-	-	1/3/6/6	-
2	FAD	A	351	-	-	4/34/50/50	0/6/6/6
3	MH6	C	2352	-	-	1/3/6/6	-
2	FAD	D	3351	-	-	4/34/50/50	0/6/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3351	FAD	C5'-C4'	30.36	1.93	1.51
2	B	1351	FAD	C5'-C4'	20.57	1.79	1.51
2	A	351	FAD	C5'-C4'	12.98	1.69	1.51
3	D	3352	MH6	CB-CA	10.93	1.65	1.50
2	B	1351	FAD	O4'-C4'	10.64	1.65	1.43
3	D	3352	MH6	OG-CB	9.47	1.72	1.41
2	A	351	FAD	O4'-C4'	8.61	1.61	1.43
2	C	2351	FAD	C5'-C4'	8.53	1.63	1.51
3	D	3352	MH6	CA-N	7.36	1.44	1.27
2	A	351	FAD	P-O3P	6.73	1.66	1.59
2	C	2351	FAD	O4'-C4'	6.17	1.56	1.43
2	D	3351	FAD	P-O3P	6.07	1.66	1.59
2	C	2351	FAD	P-O3P	5.98	1.66	1.59
2	D	3351	FAD	O4'-C4'	5.65	1.55	1.43
2	B	1351	FAD	P-O3P	4.82	1.64	1.59
2	A	351	FAD	PA-O3P	3.96	1.63	1.59
2	A	351	FAD	C9A-N10	-3.64	1.34	1.41
2	B	1351	FAD	C9A-N10	-3.55	1.35	1.41
2	B	1351	FAD	PA-O3P	3.47	1.63	1.59
2	C	2351	FAD	C9A-N10	-3.26	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2351	FAD	P-O1P	3.19	1.61	1.50
3	C	2352	MH6	OG-CB	3.08	1.51	1.41
2	C	2351	FAD	O5'-C5'	3.05	1.56	1.44
2	D	3351	FAD	PA-O3P	2.75	1.62	1.59
2	D	3351	FAD	C9A-N10	-2.64	1.36	1.41
2	D	3351	FAD	P-O1P	2.60	1.59	1.50
2	A	351	FAD	P-O1P	2.59	1.59	1.50
2	C	2351	FAD	C4-N3	-2.45	1.34	1.38
3	C	2352	MH6	CB-CA	2.39	1.53	1.50
2	C	2351	FAD	C8A-N7A	2.36	1.36	1.31
2	D	3351	FAD	C5X-N5	-2.35	1.35	1.39
2	D	3351	FAD	O5'-C5'	2.31	1.53	1.44
2	D	3351	FAD	C5A-N7A	-2.26	1.35	1.39
2	A	351	FAD	C8A-N7A	2.24	1.36	1.31
2	D	3351	FAD	C8A-N9A	-2.24	1.33	1.37
2	A	351	FAD	C4X-N5	2.23	1.35	1.30
2	D	3351	FAD	C4X-N5	2.17	1.35	1.30
2	B	1351	FAD	C5X-N5	-2.11	1.35	1.39
2	B	1351	FAD	C8A-N7A	2.09	1.35	1.31
2	A	351	FAD	C4A-N9A	-2.09	1.33	1.37
2	C	2351	FAD	C4A-N9A	-2.02	1.33	1.37

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3351	FAD	C5'-C4'-C3'	-6.70	99.59	112.22
2	B	1351	FAD	O4'-C4'-C5'	-6.53	95.60	109.99
2	D	3351	FAD	P-O5'-C5'	-6.51	84.03	121.35
3	D	3352	MH6	OG-CB-CA	-6.34	98.66	111.77
2	D	3351	FAD	O4'-C4'-C5'	-6.30	96.09	109.99
2	D	3351	FAD	C5A-C4A-N3A	-5.96	118.50	126.72
2	C	2351	FAD	P-O5'-C5'	-5.45	90.12	121.35
2	A	351	FAD	N3A-C2A-N1A	-5.42	120.37	128.58
2	C	2351	FAD	N3A-C2A-N1A	-5.31	120.54	128.58
2	D	3351	FAD	O5'-C5'-C4'	-5.27	95.29	109.36
2	C	2351	FAD	C5'-C4'-C3'	-5.26	102.30	112.22
2	B	1351	FAD	P-O5'-C5'	-5.22	91.45	121.35
2	B	1351	FAD	N3A-C2A-N1A	-5.17	120.76	128.58
2	A	351	FAD	C5'-C4'-C3'	-5.05	102.68	112.22
2	A	351	FAD	C5A-C4A-N3A	-4.90	119.97	126.72
2	B	1351	FAD	C5A-C4A-N3A	-4.83	120.06	126.72
2	A	351	FAD	P-O5'-C5'	-4.81	93.79	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3351	FAD	N3A-C2A-N1A	-4.62	121.58	128.58
2	A	351	FAD	C4-C4X-N5	4.59	124.55	118.21
2	B	1351	FAD	C5X-C9A-N10	4.54	122.08	117.97
2	C	2351	FAD	N9A-C8A-N7A	-4.29	107.86	113.94
2	B	1351	FAD	C5'-C4'-C3'	-4.28	104.15	112.22
2	B	1351	FAD	N9A-C8A-N7A	-4.23	107.94	113.94
2	C	2351	FAD	C5A-C4A-N3A	-4.20	120.94	126.72
2	D	3351	FAD	N3A-C4A-N9A	4.20	134.31	127.17
2	D	3351	FAD	O4B-C1B-N9A	4.10	115.97	108.09
2	A	351	FAD	N9A-C8A-N7A	-4.06	108.17	113.94
2	C	2351	FAD	C4'-C3'-C2'	-3.96	106.98	113.57
2	B	1351	FAD	C4A-N9A-C8A	3.82	109.75	105.74
2	A	351	FAD	C2A-N3A-C4A	3.72	120.91	111.83
2	D	3351	FAD	C2A-N3A-C4A	3.71	120.88	111.83
2	D	3351	FAD	C5X-C9A-N10	3.70	121.31	117.97
2	A	351	FAD	O4'-C4'-C5'	-3.69	101.86	109.99
3	C	2352	MH6	OG-CB-CA	-3.68	104.17	111.77
2	B	1351	FAD	O4B-C1B-N9A	3.67	115.13	108.09
2	C	2351	FAD	O4'-C4'-C5'	-3.62	102.00	109.99
2	C	2351	FAD	C4A-N9A-C8A	3.61	109.53	105.74
2	A	351	FAD	C10-C4X-N5	-3.61	117.43	124.81
2	A	351	FAD	C4'-C3'-C2'	-3.60	107.58	113.57
2	B	1351	FAD	C2A-N3A-C4A	3.57	120.55	111.83
2	C	2351	FAD	C2A-N3A-C4A	3.49	120.34	111.83
2	A	351	FAD	C5X-C9A-N10	3.48	121.11	117.97
2	D	3351	FAD	O4'-C4'-C3'	-3.48	101.11	109.25
2	D	3351	FAD	N9A-C8A-N7A	-3.44	109.06	113.94
2	B	1351	FAD	N3A-C4A-N9A	3.42	132.98	127.17
2	A	351	FAD	O4B-C1B-N9A	3.41	114.64	108.09
2	B	1351	FAD	C4'-C3'-C2'	-3.41	107.90	113.57
2	A	351	FAD	C4A-N9A-C8A	3.29	109.19	105.74
2	D	3351	FAD	C4-C4X-N5	3.26	122.72	118.21
2	B	1351	FAD	O5'-C5'-C4'	-3.23	100.74	109.36
2	A	351	FAD	C4A-C5A-N7A	-3.17	106.95	110.58
2	C	2351	FAD	C4X-C10-N1	-3.17	116.81	124.59
2	C	2351	FAD	C4A-C5A-N7A	-3.16	106.97	110.58
2	C	2351	FAD	O4'-C4'-C3'	-3.15	101.87	109.25
2	A	351	FAD	O4'-C4'-C3'	-3.14	101.89	109.25
2	C	2351	FAD	O5'-C5'-C4'	-3.11	101.06	109.36
2	C	2351	FAD	C5X-C9A-N10	3.09	120.76	117.97
2	B	1351	FAD	C2B-C1B-N9A	-3.06	105.70	113.30
2	A	351	FAD	N3A-C4A-N9A	3.01	132.29	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2351	FAD	O4B-C1B-N9A	3.00	113.86	108.09
2	C	2351	FAD	C5B-C4B-C3B	-3.00	104.41	115.21
2	D	3351	FAD	C4X-C10-N1	-2.96	117.32	124.59
2	A	351	FAD	C4X-C10-N1	-2.96	117.33	124.59
2	C	2351	FAD	C5A-N7A-C8A	2.89	107.99	103.45
2	A	351	FAD	C5A-N7A-C8A	2.86	107.95	103.45
2	C	2351	FAD	C1'-N10-C9A	-2.81	115.18	120.63
2	B	1351	FAD	C5A-N7A-C8A	2.79	107.84	103.45
2	D	3351	FAD	C4A-C5A-N7A	-2.77	107.42	110.58
2	D	3351	FAD	C4A-N9A-C8A	2.76	108.63	105.74
2	D	3351	FAD	C5A-N7A-C8A	2.71	107.70	103.45
2	B	1351	FAD	O2-C2-N1	-2.69	117.32	121.80
2	B	1351	FAD	C4A-C5A-N7A	-2.69	107.51	110.58
2	C	2351	FAD	C4A-N9A-C1B	-2.67	120.39	126.63
2	A	351	FAD	C1'-N10-C9A	-2.66	115.47	120.63
2	A	351	FAD	C10-N1-C2	2.65	122.58	116.85
2	D	3351	FAD	C10-C4X-N5	-2.63	119.44	124.81
2	B	1351	FAD	C4X-C10-N1	-2.62	118.17	124.59
2	D	3351	FAD	C10-N1-C2	2.56	122.38	116.85
2	D	3351	FAD	C1'-N10-C9A	-2.53	115.71	120.63
2	C	2351	FAD	N3A-C4A-N9A	2.50	131.41	127.17
2	C	2351	FAD	PA-O5B-C5B	-2.45	107.30	121.35
2	C	2351	FAD	C10-C4X-N5	-2.43	119.84	124.81
2	B	1351	FAD	C9-C9A-N10	-2.42	118.59	121.85
2	A	351	FAD	O2-C2-N1	-2.41	117.80	121.80
2	A	351	FAD	C5B-C4B-C3B	-2.40	106.59	115.21
2	D	3351	FAD	C5B-C4B-C3B	-2.37	106.67	115.21
2	B	1351	FAD	O3P-P-O1P	-2.36	103.60	110.70
3	A	352	MH6	OG-CB-CA	-2.34	106.93	111.77
2	C	2351	FAD	C10-N1-C2	2.34	121.91	116.85
2	C	2351	FAD	C4-C4X-N5	2.30	121.39	118.21
2	A	351	FAD	O5'-C5'-C4'	-2.28	103.27	109.36
2	B	1351	FAD	C10-C4X-N5	-2.28	120.15	124.81
2	B	1351	FAD	C5B-C4B-C3B	-2.28	107.00	115.21
2	D	3351	FAD	C4'-C3'-C2'	-2.27	109.79	113.57
2	B	1351	FAD	C4-C4X-N5	2.25	121.31	118.21
2	C	2351	FAD	C2B-C3B-C4B	2.16	106.78	102.61
2	A	351	FAD	C4X-C10-N10	2.14	119.55	116.48
2	A	351	FAD	PA-O5B-C5B	-2.06	109.53	121.35
2	B	1351	FAD	C4X-C10-N10	2.05	119.42	116.48
2	A	351	FAD	C4-N3-C2	-2.05	122.00	125.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	351	FAD	C2'-C1'-N10-C10
2	B	1351	FAD	C2'-C1'-N10-C10
2	C	2351	FAD	C2'-C1'-N10-C10
2	D	3351	FAD	C2'-C1'-N10-C10
3	A	352	MH6	C-CA-CB-OG
3	B	1352	MH6	C-CA-CB-OG
3	D	3352	MH6	O-C-CA-CB
3	D	3352	MH6	OXT-C-CA-CB
3	D	3352	MH6	C-CA-CB-OG
2	B	1351	FAD	C3B-C4B-C5B-O5B
2	C	2351	FAD	C3'-C4'-C5'-O5'
2	A	351	FAD	C3B-C4B-C5B-O5B
2	D	3351	FAD	O3'-C3'-C4'-O4'
2	D	3351	FAD	C2'-C3'-C4'-O4'
2	A	351	FAD	C5'-O5'-P-O1P
2	B	1351	FAD	C5B-O5B-PA-O1A
2	B	1351	FAD	C5'-O5'-P-O1P
2	C	2351	FAD	C5'-O5'-P-O1P
2	D	3351	FAD	C5'-O5'-P-O1P
2	B	1351	FAD	O4B-C4B-C5B-O5B
2	B	1351	FAD	C2'-C3'-C4'-O4'
3	C	2352	MH6	C-CA-CB-OG
2	A	351	FAD	O4B-C4B-C5B-O5B
2	B	1351	FAD	O3'-C3'-C4'-O4'

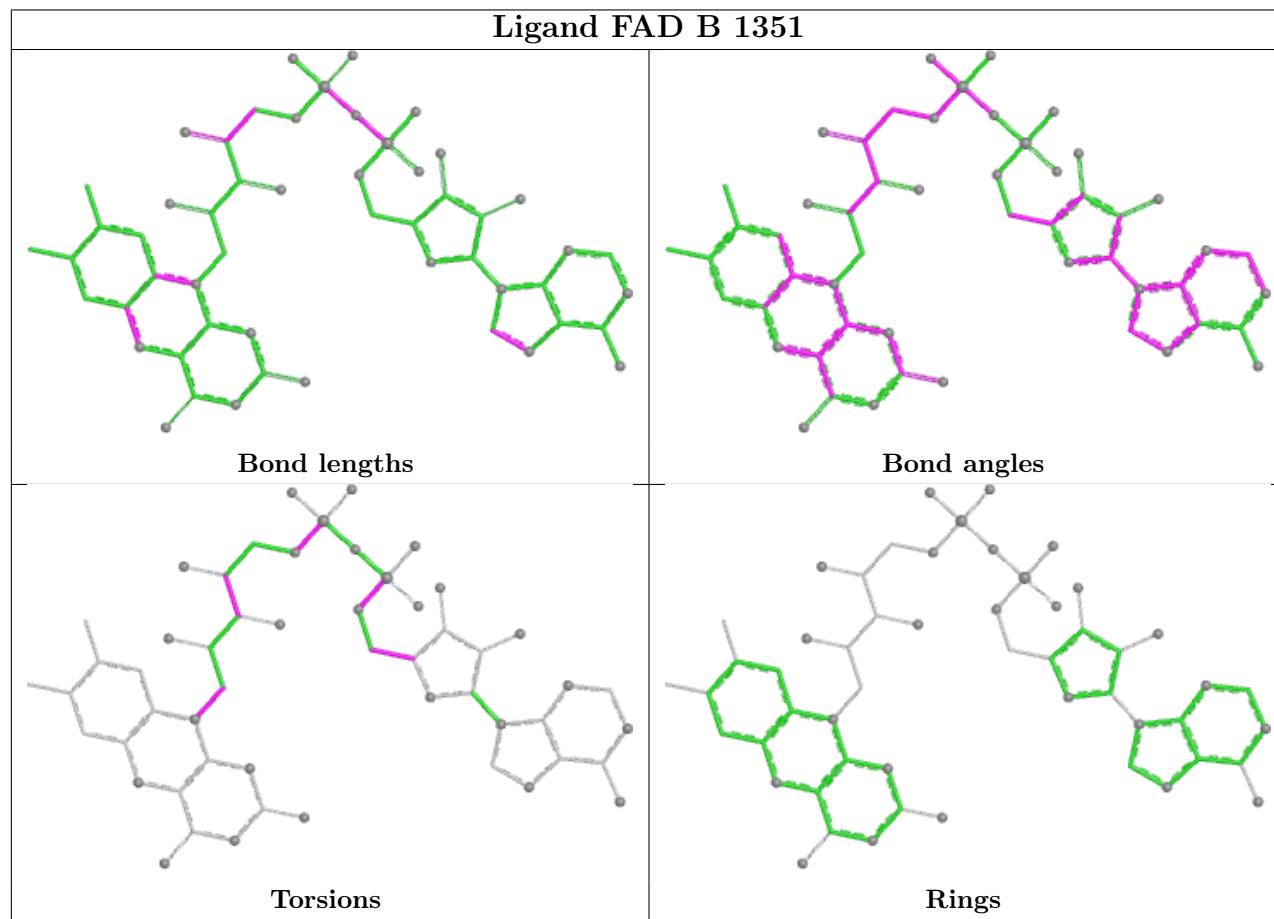
There are no ring outliers.

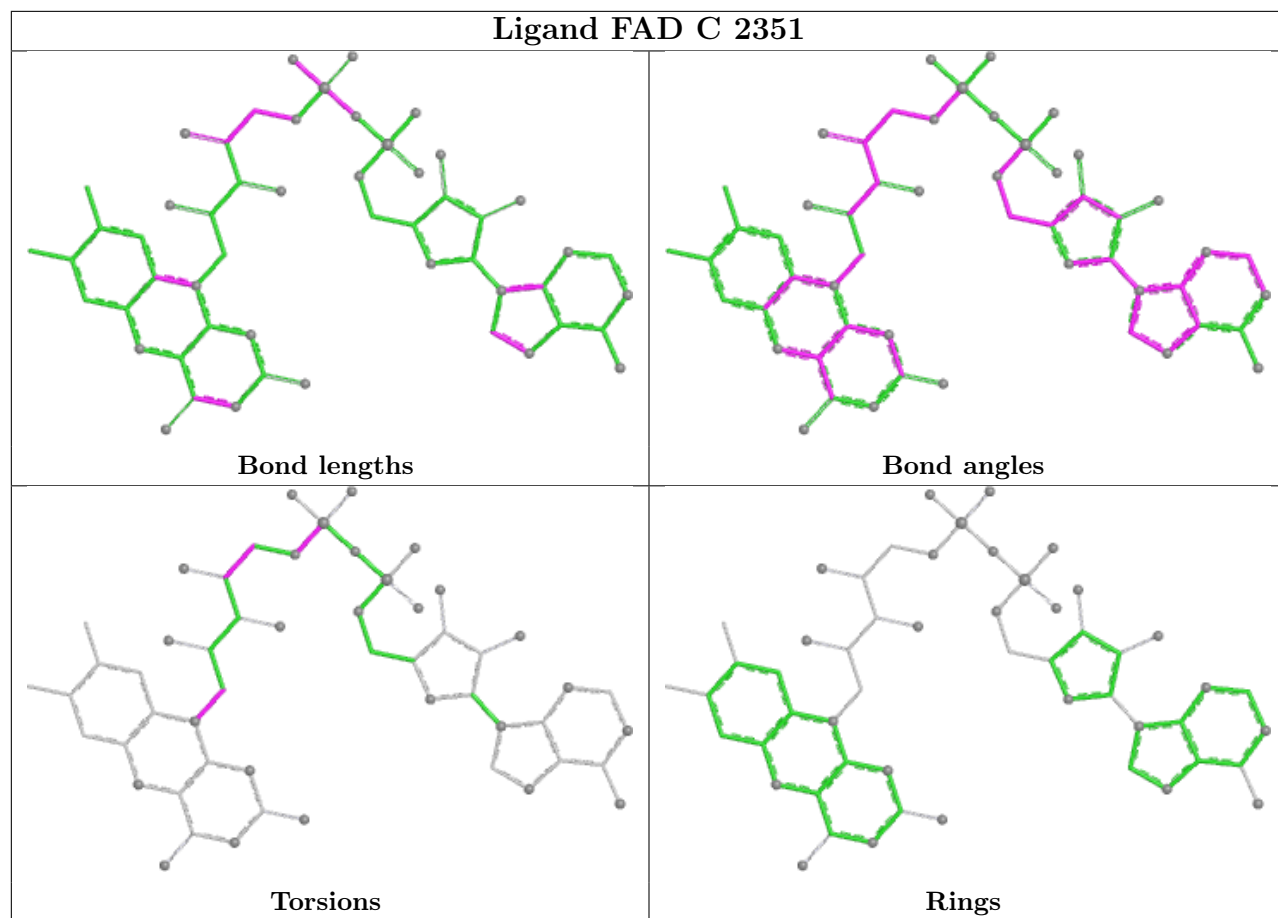
5 monomers are involved in 37 short contacts:

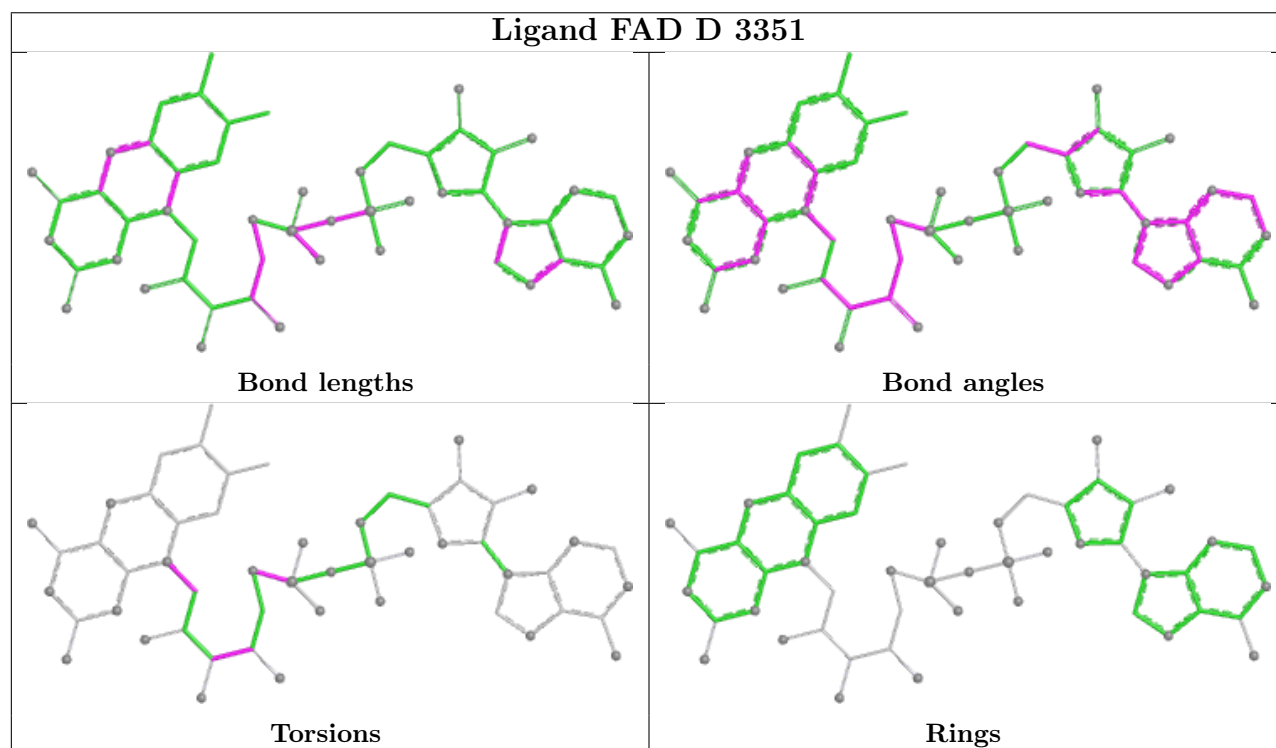
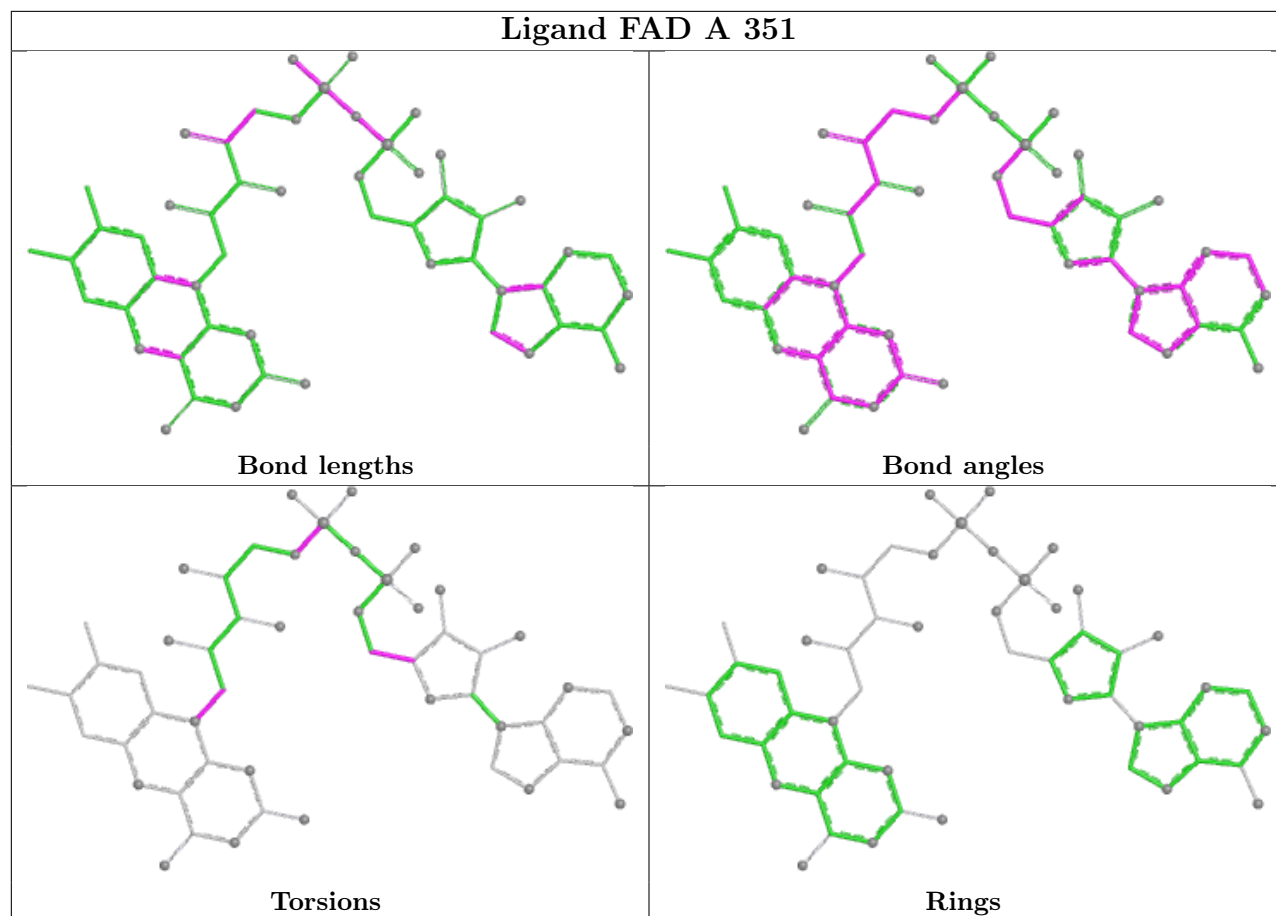
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3352	MH6	2	0
2	B	1351	FAD	11	0
2	C	2351	FAD	5	0
2	A	351	FAD	8	0
2	D	3351	FAD	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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	340/347 (97%)	0.12	6 (1%) 67 48	21, 43, 69, 80	0
1	B	340/347 (97%)	0.07	7 (2%) 63 43	21, 38, 60, 66	0
1	C	340/347 (97%)	-0.00	2 (0%) 85 73	19, 35, 57, 76	0
1	D	340/347 (97%)	0.16	5 (1%) 72 52	19, 39, 61, 72	0
All	All	1360/1388 (97%)	0.09	20 (1%) 72 52	19, 38, 62, 80	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3183	GLY	5.8
1	C	2183	GLY	4.1
1	B	1183	GLY	3.8
1	A	29	PRO	3.4
1	D	3191	ARG	3.3
1	C	2311	HIS	3.2
1	A	339	LEU	2.7
1	B	1182	THR	2.7
1	B	1299	GLY	2.6
1	B	1240	GLY	2.6
1	A	311	HIS	2.6
1	D	3068	SER	2.6
1	D	3044	THR	2.6
1	B	1300	PRO	2.5
1	A	40	THR	2.5
1	B	1339	LEU	2.2
1	D	3298	THR	2.2
1	A	321	GLY	2.2
1	A	310	GLY	2.0
1	B	1301	SER	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

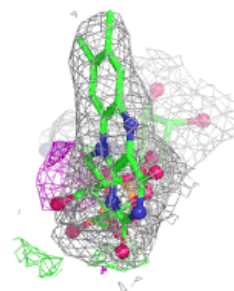
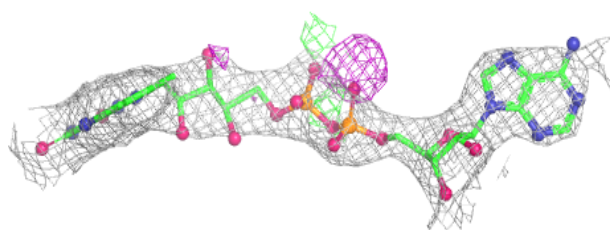
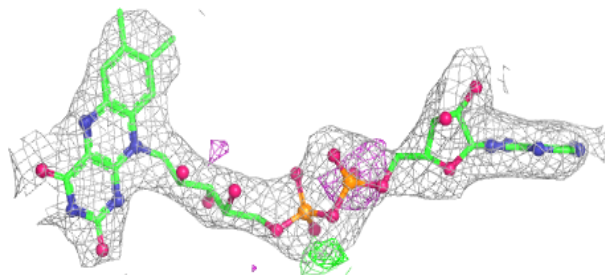
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MH6	A	352	7/7	0.87	0.15	81,81,82,82	0
3	MH6	D	3352	7/7	0.88	0.17	81,81,81,81	0
2	FAD	A	351	53/53	0.89	0.12	30,40,46,47	0
2	FAD	D	3351	53/53	0.89	0.11	21,31,36,38	0
2	FAD	B	1351	53/53	0.90	0.12	22,33,46,49	0
3	MH6	B	1352	7/7	0.91	0.10	54,54,55,55	0
2	FAD	C	2351	53/53	0.91	0.12	19,31,38,41	0
3	MH6	C	2352	7/7	0.95	0.11	67,67,67,67	0

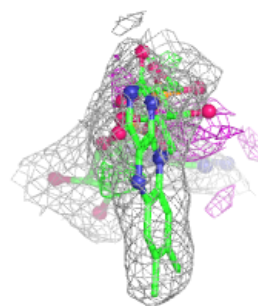
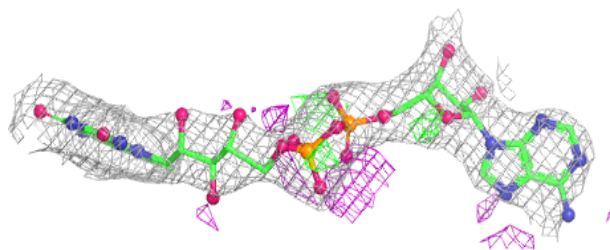
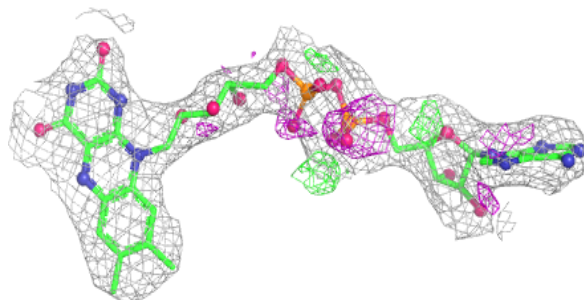
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around FAD A 351:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

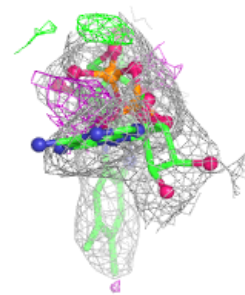
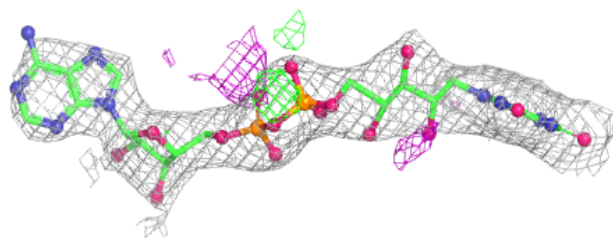
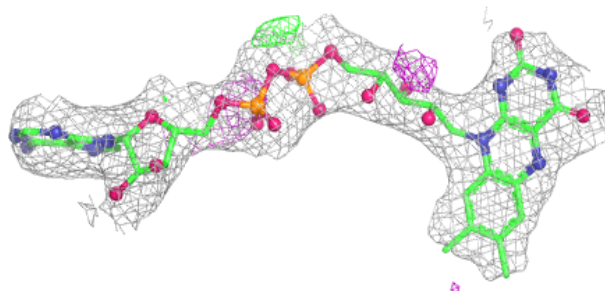
**Electron density around FAD D 3351:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

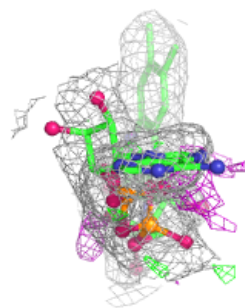
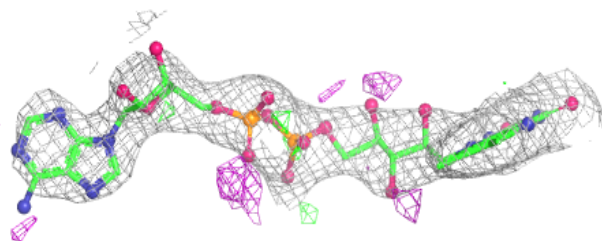
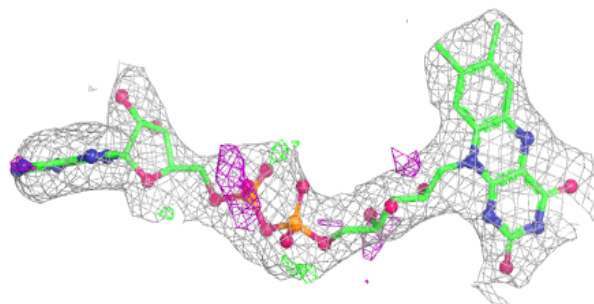


**Electron density around FAD B 1351:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FAD C 2351:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.