Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 04:51 AM EDT

PDB ID	:	2E48
Title	:	Crystal Structure of Human D-Amino Acid Oxidase: Substrate-Free Holoenzyme
Authors	:	Kawazoe, T.; Tsuge, H.; Imagawa, T.; Fukui, K.
Deposited on	:	2006-12-05
Resolution	:	2.90 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

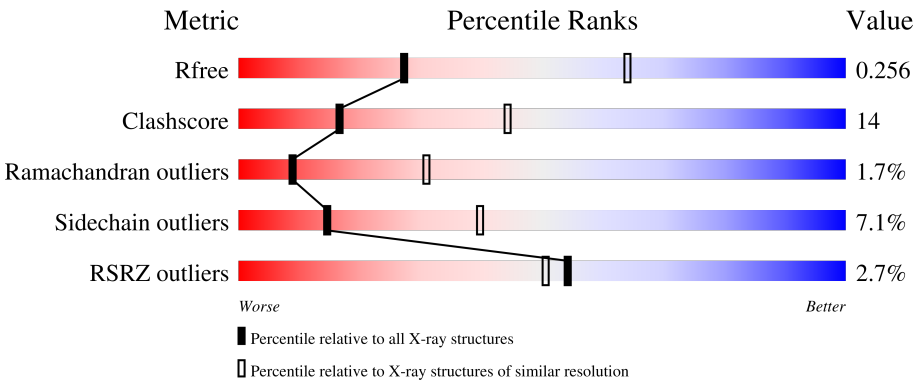
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

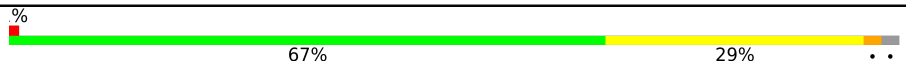
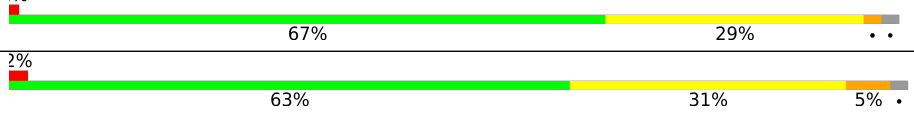
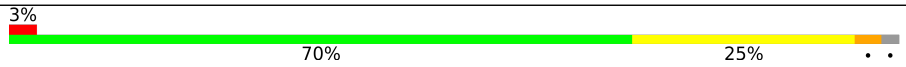
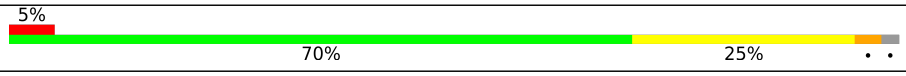
The reported resolution of this entry is 2.90 Å.

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 >=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 <=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 3 unique types of molecules in this entry. The entry contains 11278 atoms, of which 0 are hydrogens and 0 are deuteriums.

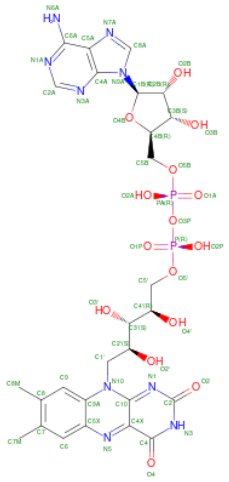
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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	2733	1751	479	494	9	0	0	0
1	B	340	2733	1751	479	494	9	0	0	0
1	C	340	2733	1751	479	494	9	0	0	0
1	D	340	2733	1751	479	494	9	0	0	0

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

FAD



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

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

- Molecule 3 is water.

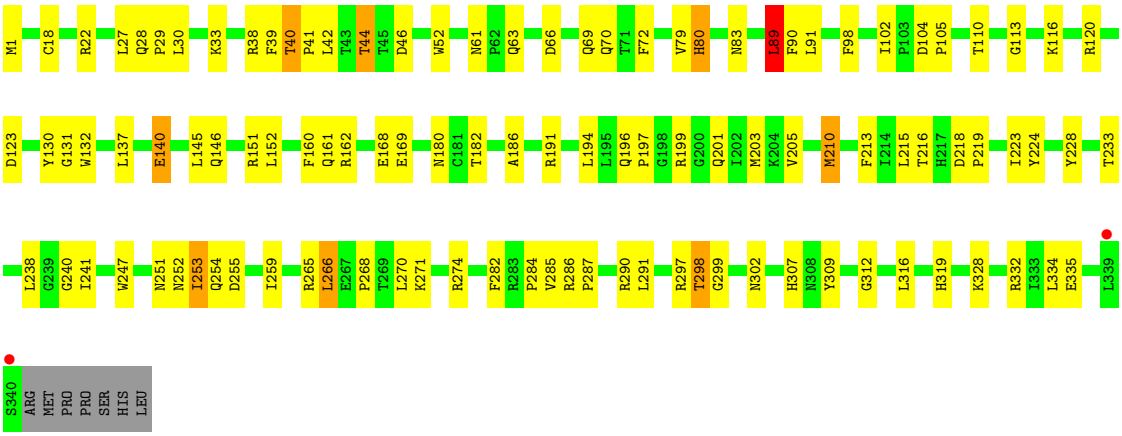
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	39	39	39	0	0
			Total	O		
3	B	33	33	33	0	0
			Total	O		
3	C	27	27	27	0	0
			Total	O		
3	D	35	35	35	0	0

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.

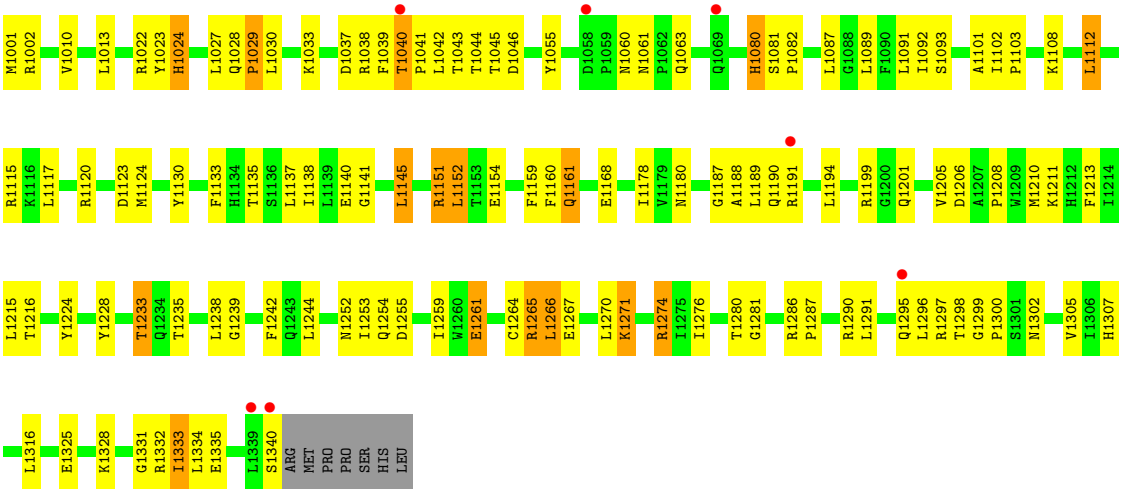
• Molecule 1: D-amino-acid oxidase

Chain A:



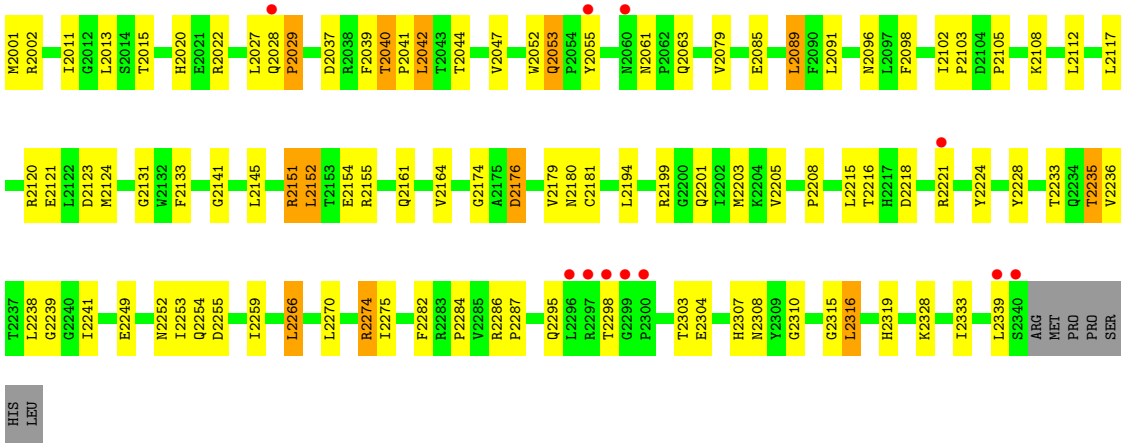
• Molecule 1: D-amino-acid oxidase

Chain B:



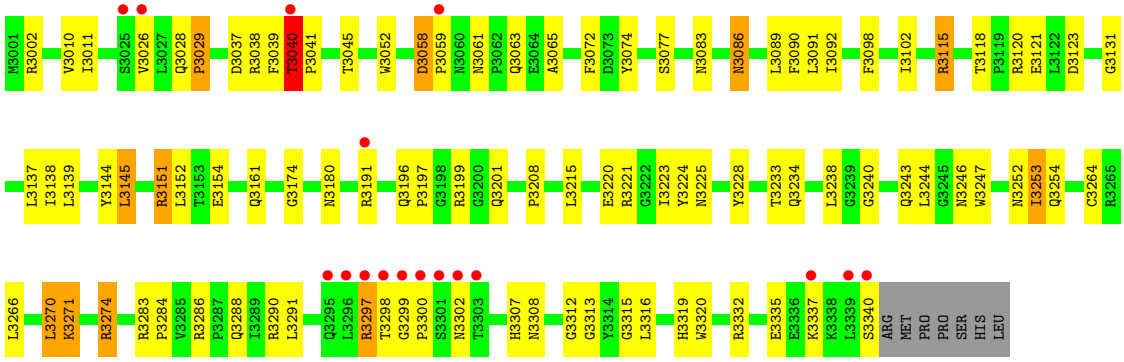
• Molecule 1: D-amino-acid oxidase

Chain C:



- Molecule 1: D-amino-acid oxidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	149.65Å 181.73Å 50.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.94 – 2.89	Depositor EDS
% Data completeness (in resolution range)	96.9 (50.00-2.90) 96.9 (48.94-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.259 0.209 , 0.256	Depositor DCC
R_{free} test set	1578 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11278	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 34.49 % 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 6.7663e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.51	0/2810	0.63	1/3824 (0.0%)
1	B	0.47	0/2810	0.61	0/3824
1	C	0.49	0/2810	0.61	1/3824 (0.0%)
1	D	0.47	0/2810	0.60	0/3824
All	All	0.49	0/11240	0.61	2/15296 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	89	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	2089	LEU	CA-CB-CG	5.24	127.34	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	80	0
1	B	2733	0	2677	86	0
1	C	2733	0	2677	80	0
1	D	2733	0	2677	69	0
2	A	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	4	0
2	C	53	0	31	5	0
2	D	53	0	31	4	0
3	A	39	0	0	4	0
3	B	33	0	0	3	0
3	C	27	0	0	2	0
3	D	35	0	0	6	0
All	All	11278	0	10835	311	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 14.

All (311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1140:GLU:OE2	1:B:1233:THR:HG22	1.55	1.03
1:B:1028:GLN:HB2	1:B:1029:PRO:HD3	1.40	1.01
1:A:40:THR:HB	1:A:41:PRO:HD3	1.48	0.96
1:D:3040:THR:HB	1:D:3041:PRO:HD3	1.55	0.89
1:A:252:ASN:HD22	1:A:255:ASP:H	1.21	0.85
1:A:140:GLU:OE1	1:A:233:THR:HG22	1.78	0.84
1:D:3091:LEU:HD23	1:D:3137:LEU:HD23	1.59	0.83
1:A:201:GLN:HE22	1:A:252:ASN:H	1.24	0.82
1:A:28:GLN:HB3	1:A:29:PRO:HD3	1.63	0.81
1:C:2001:MET:HE1	1:C:2176:ASP:HB2	1.63	0.80
1:D:3120:ARG:HD3	3:D:37:HOH:O	1.82	0.78
1:D:3059:PRO:HG2	1:D:3065:ALA:HB2	1.64	0.78
1:C:2201:GLN:HE22	1:C:2252:ASN:H	1.33	0.75
1:A:91:LEU:HD23	1:A:137:LEU:HD23	1.69	0.74
1:B:1027:LEU:HD11	1:B:1334:LEU:HD21	1.68	0.74
1:D:3180:ASN:HD22	1:D:3307:HIS:HD2	1.35	0.74
1:A:298:THR:HG22	1:A:302:ASN:HA	1.70	0.73
1:D:3201:GLN:HE22	1:D:3252:ASN:H	1.35	0.73
1:B:1331:GLY:O	1:B:1334:LEU:HB2	1.89	0.73
1:D:3264:CYS:HB3	1:D:3271:LYS:HD3	1.71	0.71
1:C:2001:MET:CE	1:C:2176:ASP:HB2	2.20	0.71
1:B:1252:ASN:HD22	1:B:1255:ASP:H	1.37	0.71
1:A:297:ARG:HA	1:A:302:ASN:CB	2.21	0.71
1:A:120:ARG:HA	1:A:123:ASP:OD2	1.92	0.70
1:D:3252:ASN:HD21	1:D:3254:GLN:HB2	1.58	0.69
1:D:3197:PRO:HG3	1:D:3247:TRP:CE2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:NH2	1:A:169:GLU:OE1	2.27	0.66
1:B:1201:GLN:HE22	1:B:1252:ASN:H	1.42	0.66
1:D:3298:THR:HB	1:D:3302:ASN:HA	1.78	0.65
1:C:2102:ILE:HG13	1:C:2103:PRO:HD2	1.80	0.64
1:C:2028:GLN:HB3	1:C:2029:PRO:HD3	1.80	0.64
1:C:2199:ARG:HH22	1:C:2201:GLN:HE21	1.42	0.64
1:D:3180:ASN:HD22	1:D:3307:HIS:CD2	2.15	0.64
1:C:2199:ARG:HH22	1:C:2201:GLN:NE2	1.95	0.64
1:B:1061:ASN:HD21	1:B:1063:GLN:HE21	1.45	0.64
1:D:3199:ARG:HH22	1:D:3201:GLN:NE2	1.96	0.63
1:B:1091:LEU:HD23	1:B:1137:LEU:HD23	1.80	0.63
1:D:3091:LEU:HD23	1:D:3137:LEU:CD2	2.26	0.63
1:D:3221:ARG:HB3	1:D:3225:ASN:HD22	1.62	0.63
1:A:297:ARG:HA	1:A:302:ASN:HB3	1.80	0.63
1:C:2040:THR:HG23	1:C:2145:LEU:HB3	1.80	0.63
1:C:2039:PHE:O	1:C:2041:PRO:HD2	1.99	0.62
1:B:1091:LEU:HD23	1:B:1137:LEU:CD2	2.29	0.62
1:C:2121:GLU:HA	1:C:2124:MET:HE2	1.80	0.62
1:A:98:PHE:HD2	1:A:131:GLY:HA2	1.64	0.62
1:A:180:ASN:HD22	1:A:307:HIS:CD2	2.18	0.61
1:B:1199:ARG:HH22	1:B:1201:GLN:NE2	1.98	0.61
1:B:1297:ARG:HA	1:B:1302:ASN:HB3	1.83	0.61
1:B:1298:THR:HG22	1:B:1302:ASN:HA	1.81	0.61
1:B:1296:LEU:O	1:B:1302:ASN:HB2	2.01	0.61
1:A:223:ILE:HG13	1:A:224:TYR:CD2	2.36	0.61
1:B:1028:GLN:HB2	1:B:1029:PRO:CD	2.24	0.61
1:B:1252:ASN:HB3	1:B:1255:ASP:HB2	1.84	0.60
1:D:3028:GLN:HB2	1:D:3029:PRO:HD3	1.83	0.60
1:B:1102:ILE:HG13	1:B:1103:PRO:HD2	1.83	0.60
1:A:80:HIS:HB2	3:A:378:HOH:O	2.01	0.60
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.48	0.60
1:C:2120:ARG:O	1:C:2123:ASP:HB2	2.02	0.59
1:A:40:THR:HB	1:A:41:PRO:CD	2.29	0.59
1:A:22:ARG:HH22	1:A:328:LYS:HG3	1.68	0.58
1:A:252:ASN:ND2	1:A:255:ASP:H	1.98	0.58
1:D:3090:PHE:HA	3:D:72:HOH:O	2.02	0.58
1:B:1206:ASP:HB2	1:B:1276:ILE:HD13	1.84	0.58
1:C:2238:LEU:HD11	1:C:2270:LEU:HD21	1.85	0.58
1:C:2252:ASN:ND2	1:C:2255:ASP:H	2.00	0.58
1:A:140:GLU:CD	1:A:233:THR:HG22	2.22	0.58
1:B:1180:ASN:HD22	1:B:1307:HIS:CD2	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1001:MET:HG2	1:B:1002:ARG:N	2.19	0.58
1:A:90:PHE:CE2	1:B:1211:LYS:HE3	2.39	0.57
1:B:1261:GLU:HG3	1:B:1265:ARG:HH12	1.70	0.57
1:D:3028:GLN:OE1	1:D:3028:GLN:HA	2.05	0.57
1:A:161:GLN:HE21	1:C:2249:GLU:H	1.50	0.56
1:A:161:GLN:NE2	1:C:2249:GLU:H	2.03	0.56
1:B:1199:ARG:NH2	1:B:1201:GLN:HE21	2.04	0.56
1:C:2274:ARG:CZ	1:C:2274:ARG:HA	2.36	0.56
1:A:297:ARG:HA	1:A:302:ASN:HB2	1.87	0.56
1:A:42:LEU:HD22	1:C:2042:LEU:HD22	1.88	0.56
1:A:298:THR:H	1:A:302:ASN:HA	1.71	0.56
1:A:199:ARG:HH22	1:A:201:GLN:NE2	2.02	0.56
1:B:1010:VAL:HB	1:B:1045:THR:HG21	1.87	0.56
1:A:116:LYS:HD3	1:A:130:TYR:OH	2.06	0.56
1:D:3238:LEU:HD11	1:D:3270:LEU:HD21	1.88	0.56
1:A:105:PRO:HD3	1:A:132:TRP:CZ2	2.40	0.56
1:A:39:PHE:O	1:A:41:PRO:HD2	2.06	0.55
1:B:1215:LEU:HD23	1:B:1228:TYR:HB2	1.87	0.55
1:C:2151:ARG:O	1:C:2155:ARG:HG3	2.05	0.55
1:D:3221:ARG:O	1:D:3225:ASN:HB3	2.07	0.55
1:D:3233:THR:HG23	1:D:3234:GLN:N	2.21	0.55
1:A:238:LEU:HD11	1:A:270:LEU:HD21	1.89	0.55
1:B:1080:HIS:HB2	3:B:29:HOH:O	2.06	0.55
1:D:3252:ASN:ND2	1:D:3254:GLN:HB2	2.21	0.55
1:C:2201:GLN:NE2	1:C:2252:ASN:H	2.03	0.54
1:C:2180:ASN:HD22	1:C:2307:HIS:CD2	2.25	0.54
1:A:291:LEU:HA	1:A:307:HIS:O	2.08	0.54
1:C:2203:MET:HE3	1:C:2259:ILE:HB	1.90	0.54
1:C:2022:ARG:HH22	1:C:2328:LYS:HA	1.73	0.53
1:B:1120:ARG:HA	1:B:1123:ASP:OD2	2.09	0.53
1:B:1201:GLN:NE2	1:B:1252:ASN:H	2.06	0.53
1:C:2052:TRP:O	1:C:2053:GLN:HB2	2.09	0.53
1:A:252:ASN:HD21	1:A:254:GLN:HB3	1.74	0.53
1:B:1297:ARG:HG2	1:B:1302:ASN:HD22	1.74	0.53
1:C:2002:ARG:HD3	1:C:2174:GLY:O	2.09	0.53
1:C:2098:PHE:HD2	1:C:2131:GLY:HA2	1.72	0.53
1:C:2233:THR:O	1:D:3208:PRO:HB2	2.08	0.53
1:C:2274:ARG:CZ	1:C:2275:ILE:H	2.22	0.53
1:B:1093:SER:HA	1:B:1135:THR:HA	1.91	0.53
1:B:1274:ARG:HA	1:B:1274:ARG:NE	2.23	0.53
1:D:3315:GLY:HA3	2:D:3351:FAD:H4'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1040:THR:HB	1:B:1041:PRO:HD3	1.92	0.52
1:A:182:THR:OG1	1:A:186:ALA:HA	2.10	0.52
1:C:2215:LEU:HD22	1:C:2228:TYR:HB2	1.90	0.52
1:A:241:ILE:HG12	1:A:259:ILE:HD11	1.91	0.52
1:C:2151:ARG:NE	1:C:2154:GLU:OE2	2.42	0.52
1:C:2079:VAL:HG21	1:C:2091:LEU:HG	1.92	0.52
1:B:1242:PHE:CE1	1:B:1244:LEU:HG	2.45	0.52
1:C:2215:LEU:CD2	1:C:2228:TYR:HB2	2.40	0.52
1:A:290:ARG:NH1	1:A:309:TYR:OH	2.43	0.51
1:B:1168:GLU:CD	1:B:1168:GLU:H	2.14	0.51
1:D:3201:GLN:NE2	1:D:3252:ASN:H	2.07	0.51
1:A:27:LEU:HD12	1:A:30:LEU:HD13	1.92	0.51
1:B:1022:ARG:HH22	1:B:1328:LYS:HA	1.75	0.51
1:D:3199:ARG:HH22	1:D:3201:GLN:HE21	1.59	0.51
1:B:1001:MET:HG2	1:B:1002:ARG:H	1.74	0.51
1:C:2218:ASP:CB	1:C:2221:ARG:HH11	2.23	0.51
1:D:3010:VAL:HG21	1:D:3316:LEU:HD13	1.93	0.51
1:B:1255:ASP:O	1:B:1259:ILE:HG12	2.11	0.50
1:A:120:ARG:O	1:A:123:ASP:HB2	2.12	0.50
1:B:1264:CYS:HB3	1:B:1271:LYS:HD3	1.94	0.50
1:A:252:ASN:HD22	1:A:255:ASP:N	2.01	0.50
1:A:91:LEU:HD11	1:B:1124:MET:SD	2.52	0.50
1:D:3221:ARG:HG3	3:D:65:HOH:O	2.12	0.50
1:B:1001:MET:N	1:B:1029:PRO:O	2.44	0.50
1:C:2053:GLN:HE22	1:C:2096:ASN:HD21	1.60	0.50
1:C:2055:TYR:HE1	1:C:2224:TYR:CE2	2.30	0.49
1:B:1101:ALA:HA	1:B:1130:TYR:CD2	2.47	0.49
1:C:2208:PRO:HB2	1:D:3233:THR:O	2.12	0.49
1:D:3010:VAL:HB	1:D:3045:THR:CG2	2.42	0.49
1:D:3038:ARG:O	2:D:3351:FAD:O3B	2.31	0.49
1:A:284:PRO:HD2	1:A:312:GLY:O	2.13	0.49
1:C:2001:MET:HG2	1:C:2027:LEU:HD13	1.94	0.49
1:B:1332:ARG:O	1:B:1333:ILE:C	2.51	0.49
1:D:3074:TYR:O	1:D:3077:SER:OG	2.27	0.49
1:C:2180:ASN:HD22	1:C:2307:HIS:HD2	1.60	0.49
1:D:3283:ARG:HD3	1:D:3313:GLY:HA3	1.94	0.49
1:D:3335:GLU:HA	1:D:3340:SER:HB3	1.94	0.49
1:A:66:ASP:O	1:A:70:GLN:HG3	2.12	0.49
1:C:2039:PHE:O	1:C:2041:PRO:CD	2.59	0.49
1:A:40:THR:O	1:A:46:ASP:OD2	2.30	0.49
1:A:233:THR:O	1:B:1208:PRO:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2216:THR:HG23	1:C:2266:LEU:HD11	1.95	0.49
1:B:1010:VAL:HG21	1:B:1316:LEU:HD13	1.95	0.48
1:D:3118:THR:OG1	1:D:3121:GLU:HG3	2.13	0.48
1:D:3151:ARG:O	1:D:3154:GLU:HG2	2.12	0.48
1:B:1199:ARG:HH22	1:B:1201:GLN:HE21	1.56	0.48
1:C:2316:LEU:O	1:C:2319:HIS:HD2	1.97	0.48
1:D:3286:ARG:CZ	1:D:3290:ARG:HB2	2.42	0.48
1:A:274:ARG:NE	1:A:274:ARG:HA	2.28	0.48
1:B:1037:ASP:HB3	2:B:1351:FAD:O2B	2.13	0.48
1:D:3002:ARG:HD3	1:D:3174:GLY:O	2.13	0.48
1:A:201:GLN:NE2	1:A:252:ASN:H	2.03	0.48
1:D:3284:PRO:HD2	1:D:3312:GLY:O	2.12	0.48
1:D:3274:ARG:HA	1:D:3274:ARG:NE	2.28	0.48
1:C:2255:ASP:O	1:C:2259:ILE:HG12	2.13	0.48
1:B:1038:ARG:O	2:B:1351:FAD:O3B	2.32	0.48
1:C:2235:THR:HG23	3:C:31:HOH:O	2.13	0.48
1:C:2241:ILE:HG12	1:C:2259:ILE:HD11	1.95	0.48
1:C:2316:LEU:O	1:C:2319:HIS:CD2	2.66	0.48
1:A:253:ILE:HD13	1:A:253:ILE:O	2.14	0.48
1:D:3223:ILE:HG13	1:D:3224:TYR:CD2	2.49	0.48
1:B:1013:LEU:HD22	1:B:1152:LEU:HD23	1.96	0.47
1:D:3220:GLU:HB2	3:D:65:HOH:O	2.13	0.47
1:C:2102:ILE:HG13	1:C:2103:PRO:CD	2.44	0.47
1:D:3120:ARG:HA	1:D:3123:ASP:OD2	2.13	0.47
1:A:39:PHE:O	1:A:41:PRO:CD	2.62	0.47
1:A:27:LEU:HD11	1:A:334:LEU:HD21	1.96	0.47
1:A:79:VAL:HG21	1:A:91:LEU:HG	1.96	0.47
1:C:2011:ILE:HG21	1:C:2308:ASN:O	2.14	0.47
1:B:1112:LEU:HB2	1:B:1135:THR:HB	1.96	0.47
1:C:2295:GLN:CD	1:C:2295:GLN:H	2.18	0.47
1:D:3196:GLN:HB3	1:D:3244:LEU:HD22	1.97	0.47
1:C:2199:ARG:NH2	1:C:2201:GLN:HE21	2.11	0.47
1:C:2235:THR:OG1	1:C:2236:VAL:N	2.48	0.47
1:D:3040:THR:HB	1:D:3041:PRO:CD	2.35	0.47
1:B:1081:SER:OG	1:B:1082:PRO:HD2	2.14	0.47
2:B:1351:FAD:H6	3:B:5:HOH:O	2.14	0.46
1:C:2218:ASP:HB2	1:C:2221:ARG:HH11	1.78	0.46
1:A:61:ASN:HD21	1:A:63:GLN:HE21	1.63	0.46
1:C:2013:LEU:HD22	1:C:2152:LEU:HD23	1.97	0.46
1:A:215:LEU:HD22	1:A:228:TYR:HB2	1.97	0.46
1:B:1117:LEU:HD23	1:B:1133:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3120:ARG:NH2	3:D:37:HOH:O	2.42	0.46
1:D:3233:THR:CG2	1:D:3234:GLN:N	2.79	0.46
1:A:116:LYS:NZ	3:A:357:HOH:O	2.49	0.46
1:B:1201:GLN:HE22	1:B:1252:ASN:N	2.10	0.46
1:D:3061:ASN:ND2	1:D:3063:GLN:HB2	2.30	0.46
1:A:33:LYS:HG2	1:A:160:PHE:HE1	1.81	0.46
1:B:1039:PHE:HE1	1:B:1159:PHE:HD1	1.62	0.46
1:A:79:VAL:HA	1:A:89:LEU:HD13	1.97	0.46
1:C:2179:VAL:HG12	1:C:2181:CYS:SG	2.56	0.46
1:C:2105:PRO:HD2	1:C:2108:LYS:HB3	1.99	0.45
1:C:2274:ARG:HA	1:C:2274:ARG:NH2	2.30	0.45
1:C:2252:ASN:HD21	1:C:2254:GLN:HB2	1.81	0.45
1:A:298:THR:HG22	1:A:302:ASN:CA	2.43	0.45
1:D:3037:ASP:HB3	2:D:3351:FAD:O2B	2.17	0.45
1:B:1242:PHE:HE1	1:B:1244:LEU:HG	1.80	0.45
1:D:3115:ARG:NH2	1:D:3121:GLU:OE2	2.49	0.45
1:C:2061:ASN:OD1	1:C:2063:GLN:HB2	2.17	0.45
1:B:1187:GLY:C	1:B:1189:LEU:H	2.20	0.45
1:B:1252:ASN:ND2	1:B:1255:ASP:H	2.10	0.45
1:D:3010:VAL:HB	1:D:3045:THR:HG21	1.98	0.45
1:B:1010:VAL:HB	1:B:1045:THR:CG2	2.47	0.45
1:B:1297:ARG:HA	1:B:1302:ASN:CB	2.46	0.45
1:D:3319:HIS:CG	1:D:3320:TRP:N	2.85	0.44
1:B:1190:GLN:HB3	3:B:106:HOH:O	2.17	0.44
1:C:2015:THR:HG21	1:C:2179:VAL:HG11	1.99	0.44
1:B:1178:ILE:HB	1:B:1305:VAL:HG22	2.00	0.44
1:C:2096:ASN:HB2	3:C:122:HOH:O	2.17	0.44
1:B:1224:TYR:HB2	1:B:1242:PHE:HB2	1.99	0.44
1:D:3233:THR:HG23	1:D:3234:GLN:HG2	1.99	0.44
1:B:1194:LEU:HB3	1:B:1287:PRO:CD	2.47	0.44
1:C:2141:GLY:O	1:C:2145:LEU:HB2	2.18	0.44
1:A:332:ARG:HD2	3:A:361:HOH:O	2.17	0.44
1:B:1092:ILE:HG21	1:B:1138:ILE:HG13	1.99	0.44
2:B:1351:FAD:H9	2:B:1351:FAD:H1'1	1.70	0.44
1:C:2047:VAL:HG12	1:C:2047:VAL:O	2.17	0.44
1:D:3332:ARG:O	1:D:3335:GLU:HG2	2.18	0.44
1:B:1033:LYS:HG2	1:B:1160:PHE:HE1	1.83	0.44
1:D:3092:ILE:HG21	1:D:3138:ILE:HG13	2.00	0.44
1:C:2117:LEU:CD2	1:C:2133:PHE:HB2	2.48	0.44
1:B:1199:ARG:NH2	1:B:1201:GLN:NE2	2.63	0.43
1:C:2151:ARG:NH1	1:C:2154:GLU:OE2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3253:ILE:HD13	1:D:3253:ILE:O	2.19	0.43
1:A:104:ASP:OD1	1:A:116:LYS:HE3	2.19	0.43
1:B:1216:THR:HG23	1:B:1266:LEU:HD11	2.00	0.43
2:D:3351:FAD:H9	2:D:3351:FAD:H1'1	1.62	0.43
1:A:69:GLN:OE1	1:A:110:THR:HG23	2.19	0.43
1:A:140:GLU:OE1	1:A:233:THR:CG2	2.60	0.43
1:B:1151:ARG:NH1	1:B:1154:GLU:OE1	2.44	0.43
1:A:197:PRO:HG3	1:A:247:TRP:CE2	2.53	0.43
1:B:1043:THR:O	1:B:1046:ASP:HB2	2.19	0.43
1:B:1141:GLY:O	1:B:1145:LEU:HB2	2.19	0.43
1:C:2022:ARG:NH2	1:C:2328:LYS:HA	2.34	0.43
1:C:2176:ASP:N	1:C:2176:ASP:OD2	2.52	0.43
1:B:1022:ARG:HD3	1:B:1023:TYR:CE2	2.54	0.43
2:A:351:FAD:H9	2:A:351:FAD:H1'1	1.53	0.42
1:D:3011:ILE:HG21	1:D:3308:ASN:O	2.18	0.42
1:A:44:THR:HG21	1:A:282:PHE:O	2.20	0.42
1:A:52:TRP:CE2	1:A:72:PHE:HB2	2.55	0.42
1:D:3145:LEU:HD12	1:D:3145:LEU:HA	1.83	0.42
1:D:3098:PHE:HD2	1:D:3131:GLY:HA2	1.84	0.42
1:D:3274:ARG:HA	1:D:3274:ARG:CZ	2.49	0.42
1:A:203:MET:HE3	1:A:259:ILE:HB	2.01	0.42
1:B:1242:PHE:CD1	1:B:1242:PHE:C	2.93	0.42
1:C:2037:ASP:HB3	2:C:2351:FAD:O2B	2.20	0.42
1:B:1286:ARG:HG2	1:B:1287:PRO:HD2	2.01	0.42
1:C:2164:VAL:H	2:C:2351:FAD:H2A	1.85	0.42
1:D:3139:LEU:HD11	1:D:3144:TYR:CD1	2.55	0.42
1:B:1210:MET:HE1	1:B:1267:GLU:HG2	2.01	0.42
1:A:268:PRO:O	1:A:271:LYS:HB2	2.20	0.42
1:B:1027:LEU:HB2	1:B:1030:LEU:HB2	2.01	0.42
1:C:2053:GLN:NE2	1:C:2096:ASN:HD21	2.17	0.42
1:A:201:GLN:NE2	1:A:251:ASN:HA	2.34	0.42
1:B:1024:HIS:CD2	1:B:1024:HIS:H	2.38	0.42
1:C:2241:ILE:CG1	1:C:2259:ILE:HD11	2.50	0.42
1:A:196:GLN:O	1:A:285:VAL:HB	2.19	0.42
1:A:218:ASP:HA	1:A:219:PRO:HD3	1.89	0.42
1:B:1286:ARG:CZ	1:B:1290:ARG:HB2	2.50	0.42
1:C:2117:LEU:HD21	1:C:2133:PHE:HB2	2.02	0.42
1:C:2284:PRO:HB2	1:C:2310:GLY:HA2	2.01	0.42
1:A:38:ARG:O	2:A:351:FAD:O3B	2.38	0.41
1:A:105:PRO:HA	3:A:366:HOH:O	2.20	0.41
1:A:216:THR:HG23	1:A:266:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2044:THR:HG21	1:C:2282:PHE:O	2.20	0.41
1:A:61:ASN:HD21	1:A:63:GLN:NE2	2.18	0.41
1:B:1239:GLY:HA2	1:B:1259:ILE:HD12	2.01	0.41
1:C:2286:ARG:HG3	1:C:2287:PRO:HD2	2.02	0.41
1:C:2298:THR:HG21	1:C:2303:THR:HG23	2.01	0.41
1:D:3038:ARG:HD2	3:D:8:HOH:O	2.19	0.41
1:D:3215:LEU:HD22	1:D:3228:TYR:HB2	2.02	0.41
1:B:1194:LEU:HB3	1:B:1287:PRO:HD2	2.01	0.41
1:D:3040:THR:CB	1:D:3041:PRO:HD3	2.36	0.41
1:D:3086:ASN:OD1	1:D:3086:ASN:N	2.53	0.41
1:A:213:PHE:CD1	1:A:213:PHE:C	2.94	0.41
1:B:1055:TYR:HE1	1:B:1224:TYR:HH	1.66	0.41
1:C:2164:VAL:H	2:C:2351:FAD:C2A	2.33	0.41
1:A:52:TRP:HE3	1:A:52:TRP:O	2.02	0.41
1:C:2304:GLU:HG3	1:C:2333:ILE:HG23	2.03	0.41
1:D:3052:TRP:CE2	1:D:3072:PHE:HB2	2.55	0.41
1:A:194:LEU:HB3	1:A:287:PRO:HD2	2.02	0.41
1:B:1291:LEU:HD21	1:B:1325:GLU:HB3	2.03	0.41
1:A:210:MET:SD	1:A:270:LEU:HD13	2.60	0.41
1:B:1161:GLN:HE21	1:B:1161:GLN:HB3	1.72	0.41
2:C:2351:FAD:H1'1	2:C:2351:FAD:H9	1.73	0.41
1:B:1013:LEU:HD12	1:B:1145:LEU:HD12	2.02	0.41
1:B:1194:LEU:HD13	1:B:1287:PRO:HG2	2.02	0.41
1:B:1280:THR:HG22	1:B:1281:GLY:N	2.35	0.41
1:B:1335:GLU:HA	1:B:1340:SER:HB2	2.03	0.41
1:C:2274:ARG:NH1	1:C:2275:ILE:H	2.18	0.41
1:A:161:GLN:HG3	1:C:2249:GLU:O	2.20	0.40
1:B:1145:LEU:HD12	1:B:1145:LEU:HA	1.95	0.40
1:D:3061:ASN:HD21	1:D:3063:GLN:HB2	1.85	0.40
1:A:199:ARG:HH22	1:A:201:GLN:HE21	1.68	0.40
1:A:286:ARG:O	1:A:287:PRO:C	2.59	0.40
1:D:3039:PHE:HB3	1:D:3040:THR:H	1.76	0.40
1:D:3291:LEU:HA	1:D:3307:HIS:O	2.21	0.40
1:B:1213:PHE:CD1	1:B:1213:PHE:C	2.95	0.40
1:C:2239:GLY:HA2	1:C:2259:ILE:HD12	2.04	0.40
1:A:316:LEU:O	1:A:319:HIS:HD2	2.04	0.40
1:C:2020:HIS:CE1	1:C:2155:ARG:HB3	2.56	0.40
1:C:2315:GLY:HA3	2:C:2351:FAD:H4'	2.03	0.40
1:D:3243:GLN:NE2	1:D:3246:ASN:HD22	2.20	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%)	309 (91%)	24 (7%)	5 (2%)	10 34
1	B	338/347 (97%)	303 (90%)	27 (8%)	8 (2%)	6 22
1	C	338/347 (97%)	309 (91%)	25 (7%)	4 (1%)	13 40
1	D	338/347 (97%)	301 (89%)	31 (9%)	6 (2%)	8 29
All	All	1352/1388 (97%)	1222 (90%)	107 (8%)	23 (2%)	9 31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	B	1040	THR
1	C	2040	THR
1	D	3040	THR
1	D	3300	PRO
1	A	298	THR
1	B	1029	PRO
1	B	1188	ALA
1	B	1299	GLY
1	C	2339	LEU
1	B	1060	ASN
1	B	1108	LYS
1	B	1300	PRO
1	D	3058	ASP
1	D	3240	GLY
1	D	3297	ARG
1	C	2053	GLN
1	D	3299	GLY
1	A	240	GLY
1	A	299	GLY
1	B	1333	ILE
1	C	2029	PRO
1	A	113	GLY

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%)	272 (93%)	20 (7%)	16	42
1	B	292/299 (98%)	266 (91%)	26 (9%)	9	29
1	C	292/299 (98%)	277 (95%)	15 (5%)	24	56
1	D	292/299 (98%)	270 (92%)	22 (8%)	13	37
All	All	1168/1196 (98%)	1085 (93%)	83 (7%)	14	40

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	CYS
1	A	44	THR
1	A	80	HIS
1	A	83	ASN
1	A	89	LEU
1	A	102	ILE
1	A	140	GLU
1	A	145	LEU
1	A	146	GLN
1	A	151	ARG
1	A	152	LEU
1	A	168	GLU
1	A	191	ARG
1	A	205	VAL
1	A	210	MET
1	A	253	ILE
1	A	265	ARG
1	A	266	LEU
1	A	335	GLU
1	B	1024	HIS
1	B	1042	LEU
1	B	1044	THR
1	B	1080	HIS

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Mol	Chain	Res	Type
1	B	1087	LEU
1	B	1089	LEU
1	B	1112	LEU
1	B	1115	ARG
1	B	1145	LEU
1	B	1151	ARG
1	B	1152	LEU
1	B	1161	GLN
1	B	1191	ARG
1	B	1205	VAL
1	B	1233	THR
1	B	1235	THR
1	B	1238	LEU
1	B	1253	ILE
1	B	1254	GLN
1	B	1261	GLU
1	B	1265	ARG
1	B	1266	LEU
1	B	1270	LEU
1	B	1271	LYS
1	B	1274	ARG
1	B	1295	GLN
1	C	2042	LEU
1	C	2085	GLU
1	C	2089	LEU
1	C	2112	LEU
1	C	2151	ARG
1	C	2152	LEU
1	C	2161	GLN
1	C	2176	ASP
1	C	2194	LEU
1	C	2205	VAL
1	C	2235	THR
1	C	2253	ILE
1	C	2266	LEU
1	C	2274	ARG
1	C	2316	LEU
1	D	3026	VAL
1	D	3029	PRO
1	D	3040	THR
1	D	3058	ASP
1	D	3083	ASN

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Mol	Chain	Res	Type
1	D	3086	ASN
1	D	3089	LEU
1	D	3102	ILE
1	D	3115	ARG
1	D	3145	LEU
1	D	3151	ARG
1	D	3152	LEU
1	D	3161	GLN
1	D	3191	ARG
1	D	3253	ILE
1	D	3266	LEU
1	D	3270	LEU
1	D	3271	LYS
1	D	3274	ARG
1	D	3288	GLN
1	D	3297	ARG
1	D	3337	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	63	GLN
1	A	161	GLN
1	A	201	GLN
1	A	243	GLN
1	A	252	ASN
1	A	272	ASN
1	A	307	HIS
1	A	319	HIS
1	B	1024	HIS
1	B	1063	GLN
1	B	1083	ASN
1	B	1161	GLN
1	B	1201	GLN
1	B	1243	GLN
1	B	1252	ASN
1	B	1295	GLN
1	B	1302	ASN
1	B	1307	HIS
1	B	1319	HIS
1	C	2053	GLN

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Mol	Chain	Res	Type
1	C	2069	GLN
1	C	2146	GLN
1	C	2161	GLN
1	C	2201	GLN
1	C	2252	ASN
1	C	2307	HIS
1	C	2319	HIS
1	D	3069	GLN
1	D	3099	HIS
1	D	3161	GLN
1	D	3201	GLN
1	D	3243	GLN
1	D	3252	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	351	-	53,58,58	0.95	2 (3%)	68,89,89	1.81	17 (25%)
2	FAD	B	1351	-	53,58,58	0.94	3 (5%)	68,89,89	1.72	10 (14%)
2	FAD	C	2351	-	53,58,58	0.92	3 (5%)	68,89,89	1.69	10 (14%)
2	FAD	D	3351	-	53,58,58	0.93	3 (5%)	68,89,89	1.74	14 (20%)

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	351	-	-	9/30/50/50	0/6/6/6
2	FAD	B	1351	-	-	9/30/50/50	0/6/6/6
2	FAD	C	2351	-	-	7/30/50/50	0/6/6/6
2	FAD	D	3351	-	-	9/30/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2351	FAD	C9A-N10	-3.38	1.35	1.41
2	A	351	FAD	C9A-N10	-3.24	1.35	1.41
2	A	351	FAD	C4X-N5	2.95	1.36	1.30
2	B	1351	FAD	C4X-N5	2.77	1.36	1.30
2	D	3351	FAD	C4X-N5	2.54	1.35	1.30
2	D	3351	FAD	C9A-N10	-2.36	1.37	1.41
2	B	1351	FAD	C9A-N10	-2.25	1.37	1.41
2	B	1351	FAD	C4-N3	-2.11	1.34	1.38
2	D	3351	FAD	C5X-N5	-2.08	1.35	1.39
2	C	2351	FAD	C4X-N5	2.05	1.34	1.30
2	C	2351	FAD	C5X-N5	-2.02	1.35	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2351	FAD	P-O3P-PA	-7.93	105.63	132.83
2	B	1351	FAD	P-O3P-PA	-7.55	106.90	132.83
2	A	351	FAD	P-O3P-PA	-7.22	108.06	132.83
2	D	3351	FAD	P-O3P-PA	-6.88	109.21	132.83
2	A	351	FAD	N3A-C2A-N1A	-5.21	120.53	128.68
2	D	3351	FAD	N3A-C2A-N1A	-5.02	120.84	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1351	FAD	N3A-C2A-N1A	-4.67	121.38	128.68
2	C	2351	FAD	N3A-C2A-N1A	-4.57	121.54	128.68
2	B	1351	FAD	C5X-C9A-N10	3.68	121.75	117.95
2	A	351	FAD	C5X-C9A-N10	3.64	121.72	117.95
2	D	3351	FAD	C4X-C10-N1	-3.58	116.43	124.73
2	D	3351	FAD	C5X-C9A-N10	3.52	121.59	117.95
2	C	2351	FAD	C5X-C9A-N10	3.12	121.18	117.95
2	A	351	FAD	C4X-C10-N1	-3.10	117.55	124.73
2	B	1351	FAD	C4X-C10-N1	-3.09	117.56	124.73
2	D	3351	FAD	C10-N1-C2	3.08	123.06	116.90
2	A	351	FAD	C1B-N9A-C4A	-3.06	121.26	126.64
2	A	351	FAD	C4-C4X-N5	2.99	122.48	118.23
2	A	351	FAD	C10-N1-C2	2.89	122.67	116.90
2	C	2351	FAD	C4X-C10-N1	-2.87	118.08	124.73
2	C	2351	FAD	C4-C4X-N5	2.80	122.21	118.23
2	D	3351	FAD	C4-C4X-N5	2.75	122.15	118.23
2	B	1351	FAD	C4-C4X-N5	2.51	121.81	118.23
2	A	351	FAD	C4A-C5A-N7A	-2.51	106.78	109.40
2	A	351	FAD	C10-C4X-N5	-2.50	119.56	124.86
2	C	2351	FAD	O4-C4-C4X	-2.48	120.01	126.60
2	D	3351	FAD	C4-N3-C2	-2.45	121.11	125.64
2	D	3351	FAD	C10-C4X-N5	-2.41	119.75	124.86
2	C	2351	FAD	C10-N1-C2	2.40	121.69	116.90
2	B	1351	FAD	C10-N1-C2	2.38	121.67	116.90
2	C	2351	FAD	C10-C4X-N5	-2.37	119.82	124.86
2	A	351	FAD	C4X-C10-N10	2.33	119.88	116.48
2	B	1351	FAD	O5'-C5'-C4'	2.32	115.55	109.36
2	A	351	FAD	C4-N3-C2	-2.31	121.37	125.64
2	C	2351	FAD	C4A-C5A-N7A	-2.31	106.99	109.40
2	D	3351	FAD	N10-C10-N1	2.29	124.92	118.35
2	B	1351	FAD	C4A-C5A-N7A	-2.26	107.04	109.40
2	A	351	FAD	P-O5'-C5'	-2.25	108.47	121.68
2	D	3351	FAD	C4A-C5A-N7A	-2.23	107.07	109.40
2	C	2351	FAD	C4-N3-C2	-2.23	121.52	125.64
2	D	3351	FAD	O4-C4-C4X	-2.18	120.82	126.60
2	B	1351	FAD	C10-C4X-N5	-2.17	120.25	124.86
2	A	351	FAD	C1'-N10-C9A	-2.16	116.91	120.51
2	D	3351	FAD	C4X-C4-N3	2.12	118.56	113.19
2	D	3351	FAD	O2P-P-O1P	2.11	122.65	112.24
2	A	351	FAD	O2P-P-O1P	2.09	122.58	112.24
2	D	3351	FAD	C1B-N9A-C4A	-2.09	122.97	126.64
2	A	351	FAD	C4'-C3'-C2'	-2.04	109.12	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1351	FAD	O4B-C1B-C2B	-2.02	103.97	106.93
2	A	351	FAD	O2-C2-N1	-2.01	118.50	121.83
2	A	351	FAD	O4-C4-C4X	-2.00	121.29	126.60

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	351	FAD	C5B-O5B-PA-O1A
2	A	351	FAD	C5B-O5B-PA-O3P
2	A	351	FAD	C3B-C4B-C5B-O5B
2	A	351	FAD	O4'-C4'-C5'-O5'
2	A	351	FAD	C5'-O5'-P-O1P
2	B	1351	FAD	C5B-O5B-PA-O1A
2	B	1351	FAD	C5B-O5B-PA-O3P
2	B	1351	FAD	O4B-C4B-C5B-O5B
2	B	1351	FAD	C3B-C4B-C5B-O5B
2	B	1351	FAD	O4'-C4'-C5'-O5'
2	B	1351	FAD	C5'-O5'-P-O1P
2	B	1351	FAD	C5'-O5'-P-O3P
2	C	2351	FAD	C5B-O5B-PA-O3P
2	C	2351	FAD	O4B-C4B-C5B-O5B
2	C	2351	FAD	C3B-C4B-C5B-O5B
2	C	2351	FAD	C5'-O5'-P-O1P
2	C	2351	FAD	C5'-O5'-P-O3P
2	D	3351	FAD	C5B-O5B-PA-O3P
2	D	3351	FAD	C3B-C4B-C5B-O5B
2	D	3351	FAD	O4'-C4'-C5'-O5'
2	D	3351	FAD	C5'-O5'-P-O1P
2	A	351	FAD	O4B-C4B-C5B-O5B
2	D	3351	FAD	O4B-C4B-C5B-O5B
2	D	3351	FAD	C3'-C4'-C5'-O5'
2	A	351	FAD	C2'-C1'-N10-C10
2	D	3351	FAD	C2'-C1'-N10-C10
2	C	2351	FAD	C5B-O5B-PA-O1A
2	D	3351	FAD	C5B-O5B-PA-O1A
2	C	2351	FAD	O4'-C4'-C5'-O5'
2	A	351	FAD	C5'-O5'-P-O3P
2	D	3351	FAD	C5'-O5'-P-O3P
2	B	1351	FAD	C4'-C5'-O5'-P
2	A	351	FAD	C3'-C4'-C5'-O5'
2	B	1351	FAD	C3'-C4'-C5'-O5'

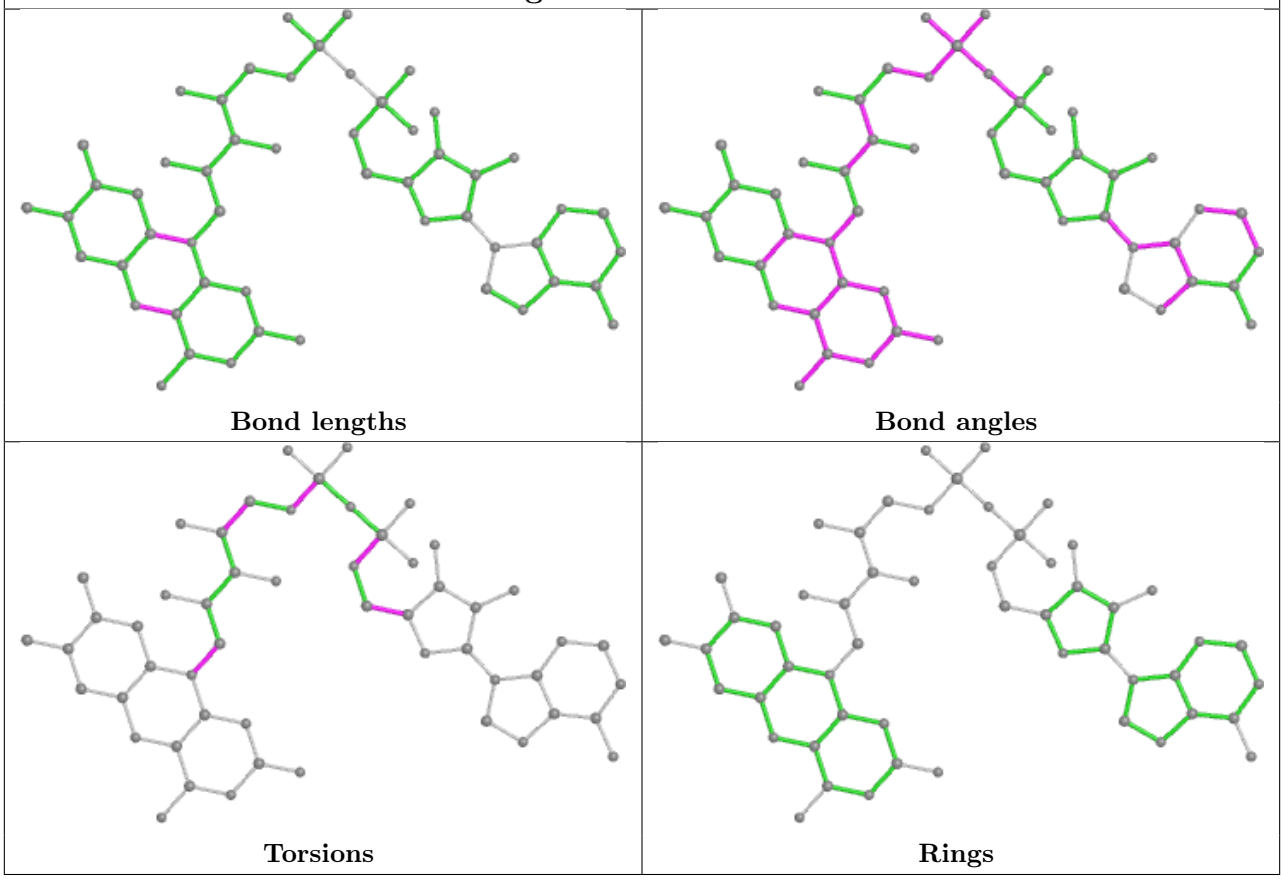
There are no ring outliers.

4 monomers are involved in 15 short contacts:

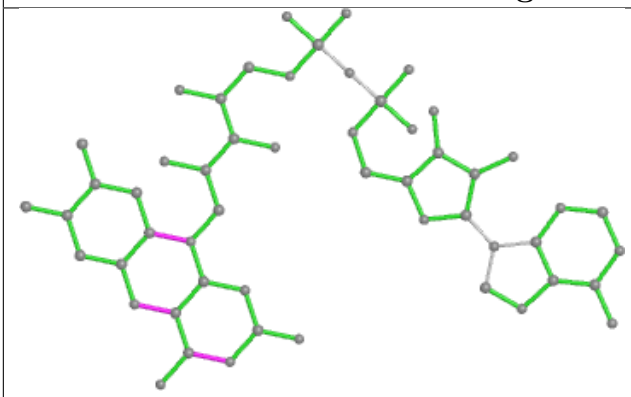
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	351	FAD	2	0
2	B	1351	FAD	4	0
2	C	2351	FAD	5	0
2	D	3351	FAD	4	0

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 then 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.

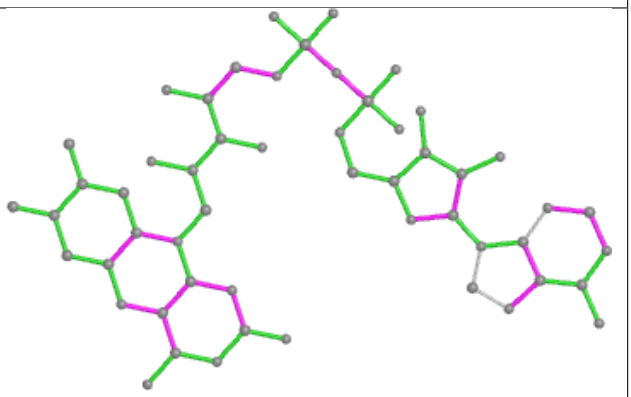
Ligand FAD A 351



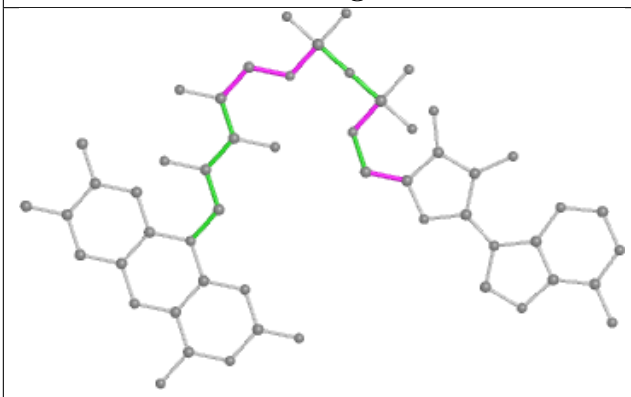
Ligand FAD B 1351



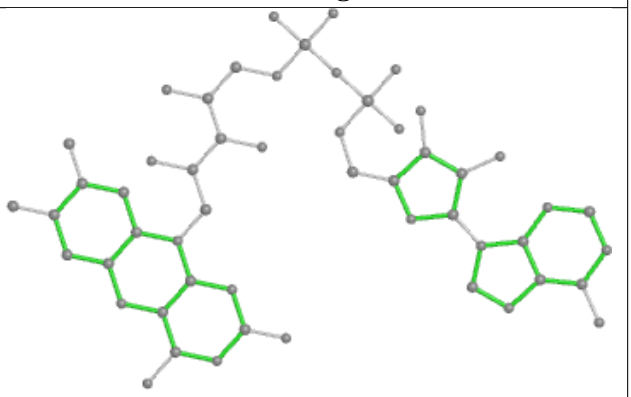
Bond lengths



Bond angles

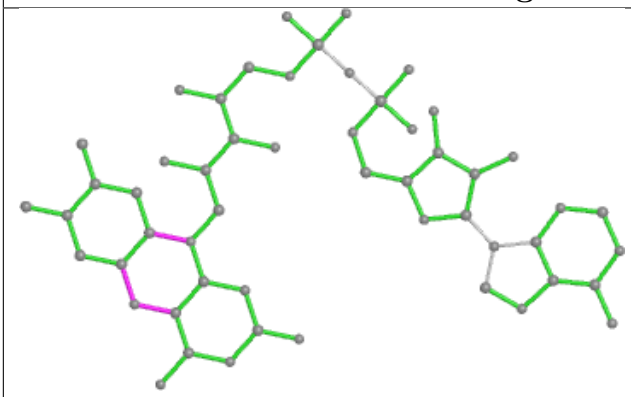


Torsions

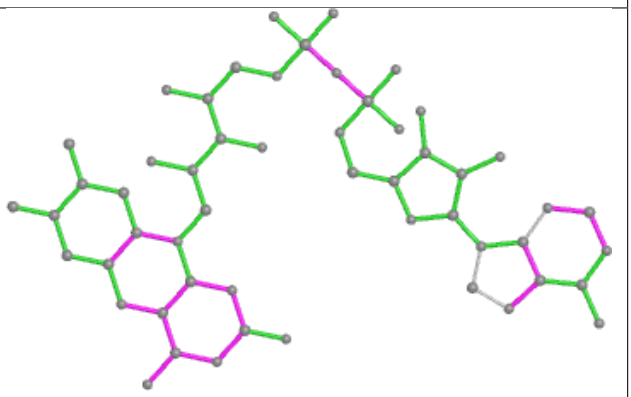


Rings

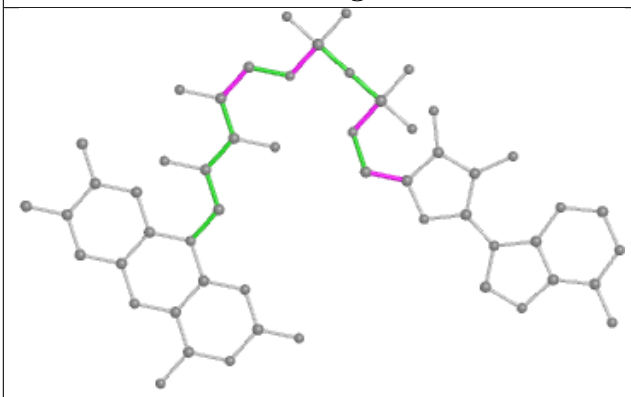
Ligand FAD C 2351



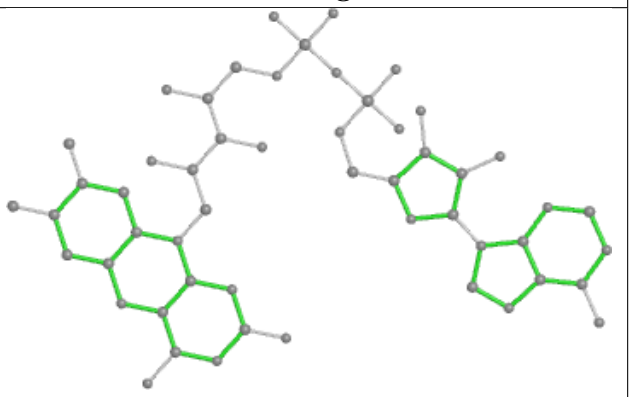
Bond lengths



Bond angles

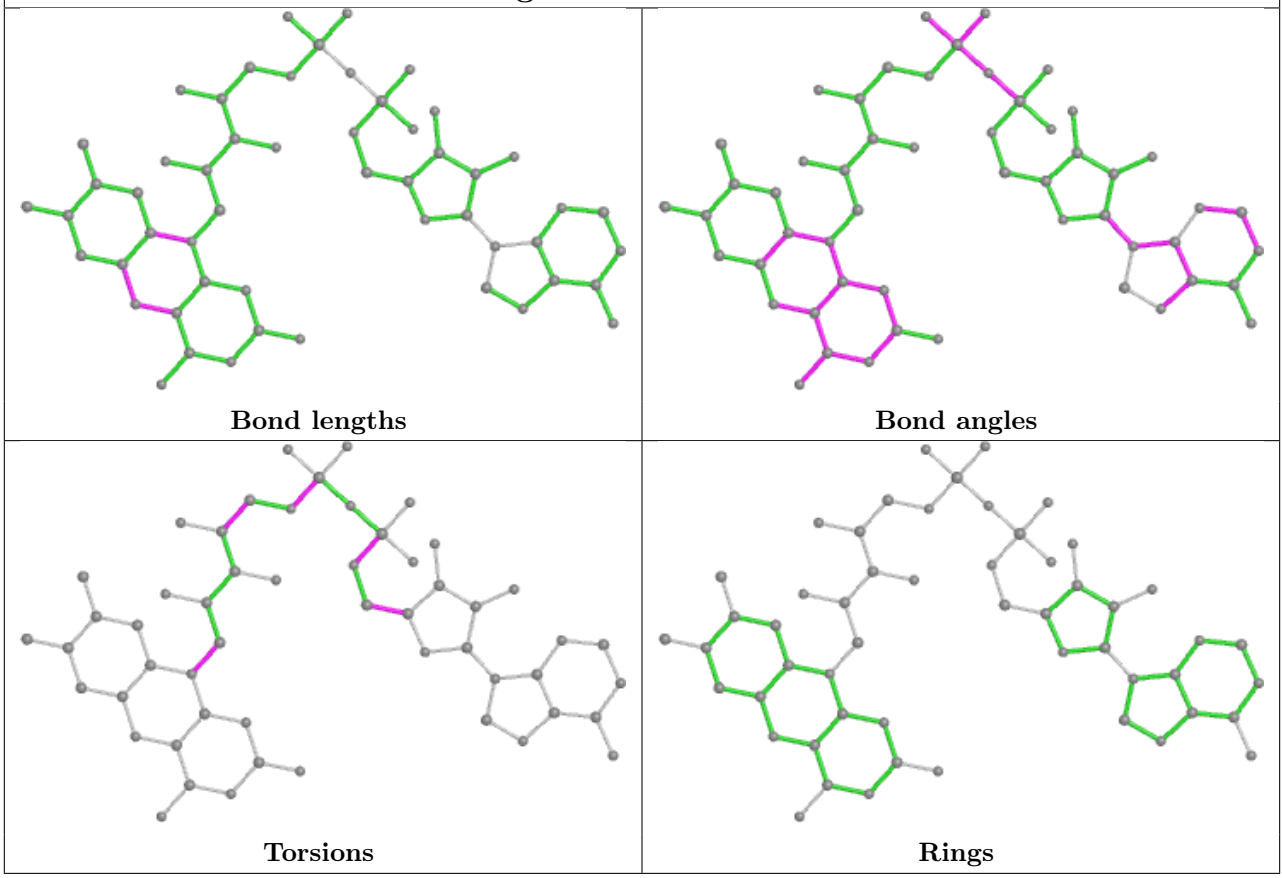


Torsions



Rings

Ligand FAD D 3351



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	340/347 (97%)	-0.22	2 (0%)	89	89	13, 27, 50, 68	0
1	B	340/347 (97%)	-0.15	7 (2%)	63	61	16, 31, 56, 68	0
1	C	340/347 (97%)	0.02	11 (3%)	47	43	18, 32, 58, 75	0
1	D	340/347 (97%)	0.09	17 (5%)	28	25	20, 35, 63, 81	0
All	All	1360/1388 (97%)	-0.07	37 (2%)	54	50	13, 31, 58, 81	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2298	THR	5.9
1	D	3300	PRO	5.5
1	D	3301	SER	5.4
1	A	340	SER	4.9
1	D	3302	ASN	4.8
1	D	3295	GLN	4.3
1	D	3298	THR	4.2
1	D	3296	LEU	4.1
1	C	2340	SER	4.0
1	D	3339	LEU	3.9
1	D	3297	ARG	3.9
1	B	1340	SER	3.8
1	C	2339	LEU	3.7
1	C	2299	GLY	3.5
1	C	2300	PRO	3.5
1	D	3026	VAL	3.5
1	C	2297	ARG	3.4
1	D	3340	SER	3.3
1	C	2296	LEU	3.1
1	B	1040	THR	3.0
1	D	3337	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	3040	THR	2.7
1	B	1069	GLN	2.6
1	D	3191	ARG	2.6
1	D	3303	THR	2.6
1	D	3059	PRO	2.5
1	B	1058	ASP	2.5
1	C	2055	TYR	2.4
1	B	1295	GLN	2.4
1	C	2060	ASN	2.3
1	A	339	LEU	2.3
1	D	3299	GLY	2.2
1	D	3025	SER	2.2
1	B	1339	LEU	2.2
1	B	1191	ARG	2.2
1	C	2221	ARG	2.1
1	C	2028	GLN	2.1

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 monosaccharides 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, 95th 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.

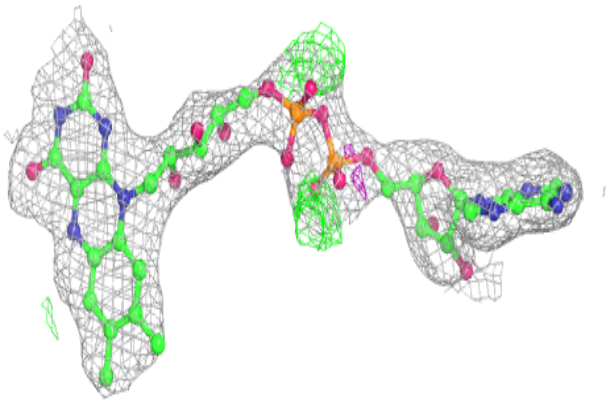
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	D	3351	53/53	0.93	0.20	22,35,40,43	0
2	FAD	C	2351	53/53	0.94	0.18	16,24,33,35	0
2	FAD	A	351	53/53	0.94	0.18	11,24,30,33	0
2	FAD	B	1351	53/53	0.95	0.17	19,25,29,31	0

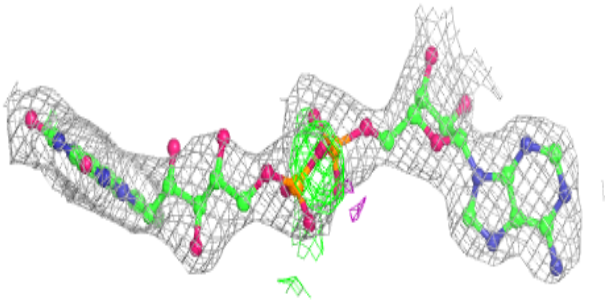
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

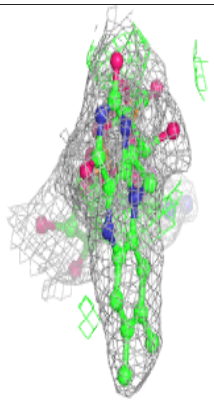
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD 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)

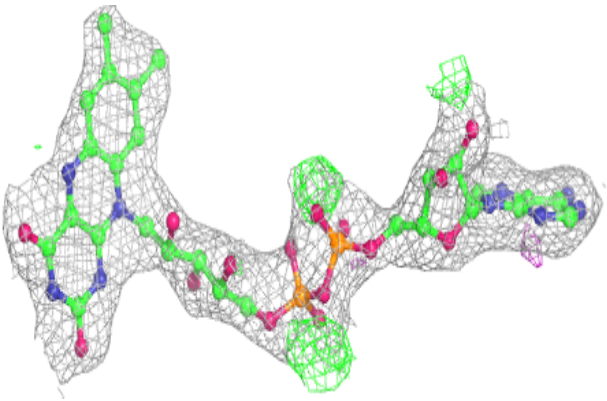


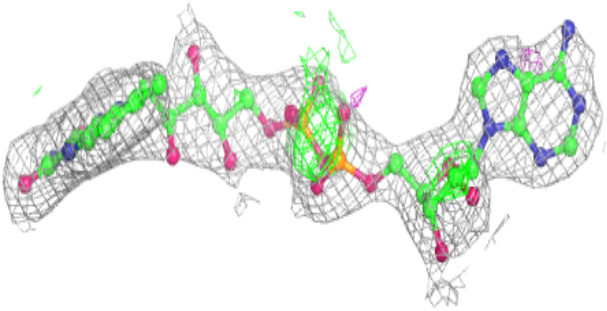


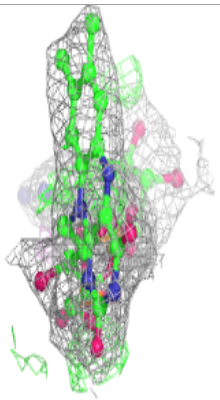


Electron density around FAD C 2351:

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

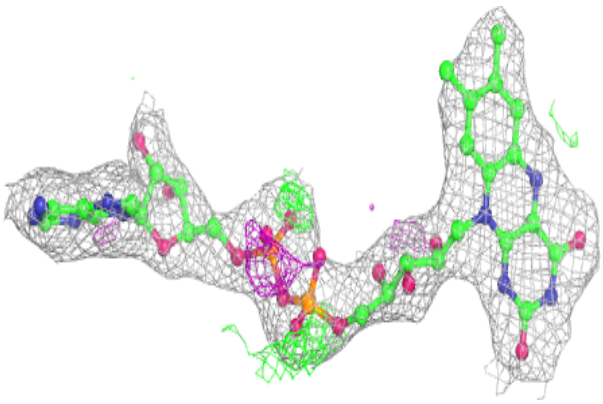


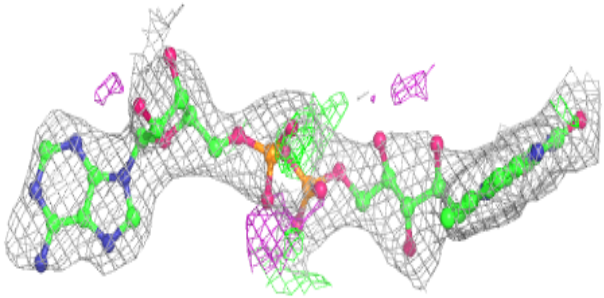


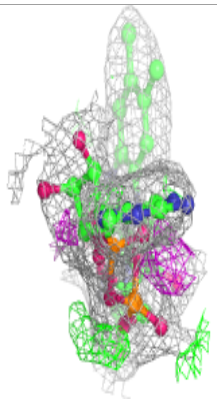


Electron density around FAD A 351:

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

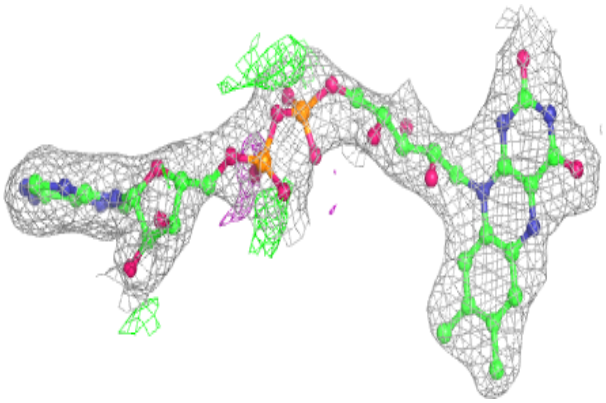


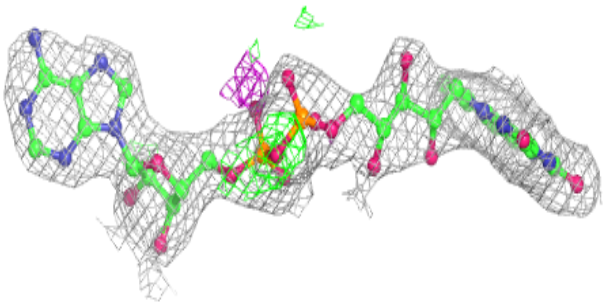


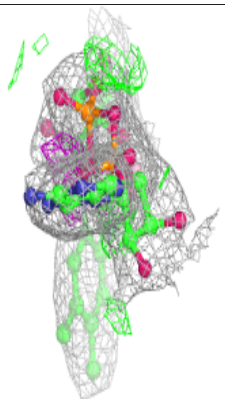


Electron density around FAD B 1351:

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







6.5 Other polymers (i)

There are no such residues in this entry.