Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 11:18 pm GMT

PDB ID	:	2WES
Title	:	Crystal structures of mutant E46Q of tryptophan 5-halogenase (PyrH)
Authors	:	Zhu, X.; Naismith, J.H.
Deposited on	:	2009-04-01
Resolution	:	2.50 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:

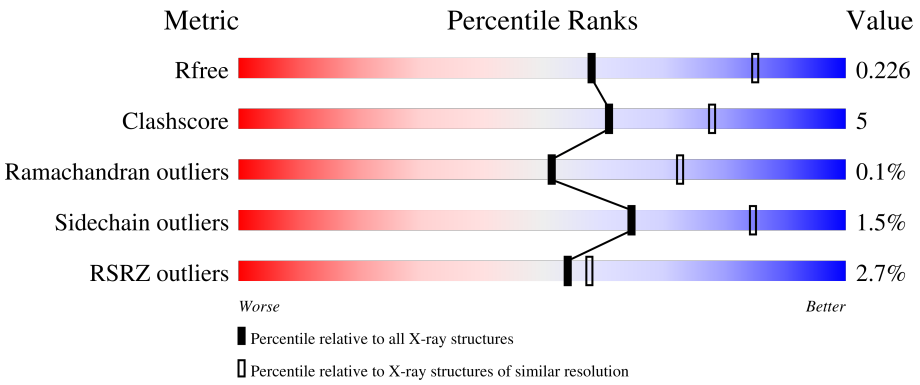
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	511	.% 88% 8% •
1	B	511	2% 89% 8% •
1	C	511	2% 86% 10% •
1	D	511	6% 89% 8% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17104 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 TRYPTOPHAN 5-HALOGENASE.

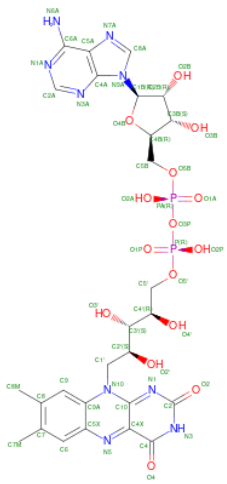
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	496	3987	2535	702	731	19	0	0	0
1	B	496	3987	2535	702	731	19	0	0	0
1	C	496	3987	2535	702	731	19	0	0	0
1	D	496	3987	2535	702	731	19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLN	GLU	engineered mutation	UNP A4D0H5
B	46	GLN	GLU	engineered mutation	UNP A4D0H5
C	46	GLN	GLU	engineered mutation	UNP A4D0H5
D	46	GLN	GLU	engineered mutation	UNP A4D0H5

- 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
2	C	1	52	27	9	14	2	0	0
2	D	1	53	27	9	15	2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	304	304	304	0	0

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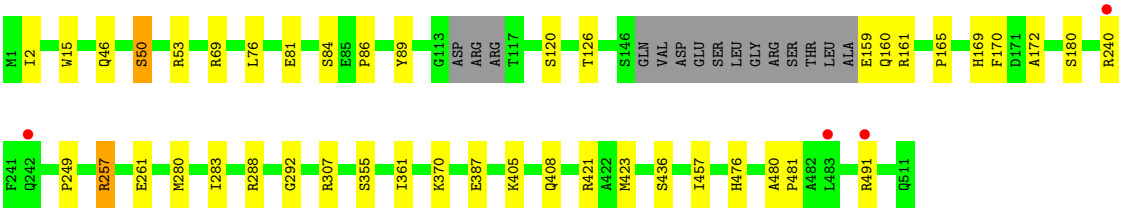
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	239	239	239	0	0
			Total	O		
4	C	203	203	203	0	0
			Total	O		
4	D	195	195	195	0	0

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.

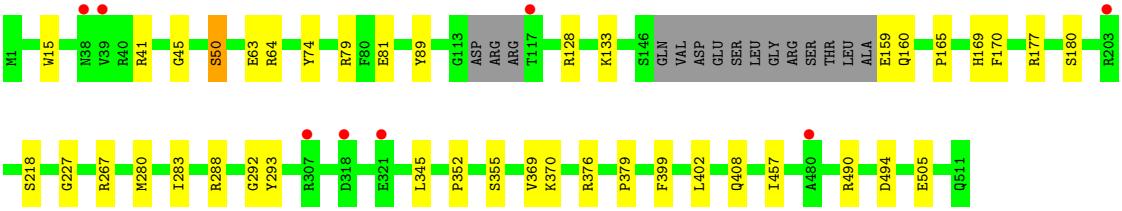
• Molecule 1: TRYPTOPHAN 5-HALOGENASE

Chain A:



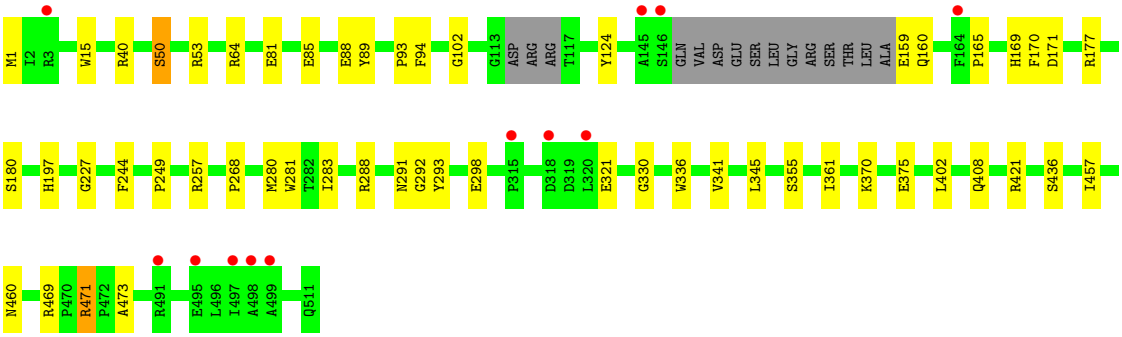
• Molecule 1: TRYPTOPHAN 5-HALOGENASE

Chain B:



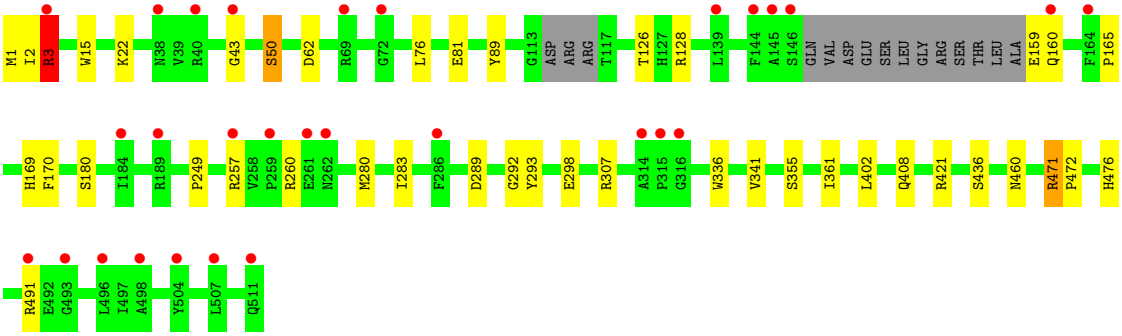
• Molecule 1: TRYPTOPHAN 5-HALOGENASE

Chain C:



• Molecule 1: TRYPTOPHAN 5-HALOGENASE

Chain D:


M1
I2
R3
W15
K22
N38
V39
R40
G43
S50
D62
R69
G72
L76
E81
Y89
G113
ASP
ARG
ARG
T117
T126
H127
R128
L139
F144
A145
S146
GLN
VAL
ASP
GLU
SER
LEU
GLY
ARG
SER
THR
LEU
ALA
E159
Q160
F164
P165
H169
F170
S180
I184
R189
P249
R257
V258
P259
R260
E261
N262
M280
I283
F286
D289
G292
Y293
E298
R307
A314
P315
G316
W336
V341
S355
I361
L402
Q408
R421
S436
N460
R471
P472
H476
R491
E492
G493
L496
I497
A498
Y504
L507
Q511

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	137.57Å 137.57Å 309.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 2.50 46.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.25-2.50) 99.9 (46.40-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.97 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.193 , 0.230 0.191 , 0.226	Depositor DCC
R_{free} test set	5180 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17104	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, CL

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	0.66	0/4094	0.69	0/5550
1	B	0.65	0/4094	0.65	0/5550
1	C	0.64	0/4094	0.64	0/5550
1	D	1.20	2/4094 (0.0%)	0.75	5/5550 (0.1%)
All	All	0.82	2/16376 (0.0%)	0.69	5/22200 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3	ARG	CB-CG	55.12	3.01	1.52
1	D	3	ARG	CA-C	36.14	2.46	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3	ARG	CA-CB-CG	-23.58	61.52	113.40
1	D	3	ARG	CB-CA-C	13.78	137.95	110.40
1	D	3	ARG	CB-CG-CD	-9.65	86.51	111.60
1	D	3	ARG	N-CA-C	-7.51	90.72	111.00
1	D	3	ARG	CA-C-N	-6.05	103.90	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2	ILE	Peptide
1	D	3	ARG	Mainchain,Peptide

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	3987	0	3828	39	1
1	B	3987	0	3828	39	0
1	C	3987	0	3828	42	0
1	D	3987	0	3828	32	1
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	52	0	31	1	0
2	D	53	0	31	1	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	304	0	0	13	0
4	B	239	0	0	17	0
4	C	203	0	0	7	0
4	D	195	0	0	8	0
All	All	17104	0	15436	143	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (143) 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:159:GLU:HG3	1:B:160:GLN:H	1.13	1.06
1:D:159:GLU:HG3	1:D:160:GLN:H	1.21	1.05
1:C:159:GLU:HG3	1:C:160:GLN:H	1.19	1.04
1:B:133:LYS:NZ	4:B:2056:HOH:O	1.90	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLU:HG3	1:A:160:GLN:H	1.22	1.00
1:D:3:ARG:HA	1:D:3:ARG:CG	1.96	0.95
1:A:120:SER:OG	4:A:2080:HOH:O	1.91	0.89
1:A:491:ARG:NH2	4:A:2294:HOH:O	2.06	0.86
1:B:159:GLU:CG	1:B:160:GLN:H	1.89	0.85
1:B:159:GLU:HG3	1:B:160:GLN:N	1.92	0.85
1:D:3:ARG:CA	1:D:3:ARG:C	2.46	0.84
1:C:1:MET:N	1:C:375:GLU:HB2	1.94	0.82
1:B:408:GLN:HG2	4:B:2171:HOH:O	1.81	0.80
1:B:267:ARG:HD3	4:B:2108:HOH:O	1.82	0.80
1:A:159:GLU:CG	1:A:160:GLN:H	1.96	0.79
1:C:159:GLU:CG	1:C:160:GLN:H	1.94	0.79
1:A:161:ARG:NH1	4:A:2095:HOH:O	2.16	0.79
1:D:159:GLU:CG	1:D:160:GLN:H	1.95	0.79
1:D:491:ARG:HG2	4:D:2186:HOH:O	1.83	0.77
1:A:46:GLN:HE21	1:A:172:ALA:HB2	1.49	0.76
1:C:1:MET:H3	1:C:375:GLU:HB2	1.49	0.75
1:A:159:GLU:HG3	1:A:160:GLN:N	2.02	0.74
1:D:159:GLU:HG3	1:D:160:GLN:N	2.00	0.73
1:D:3:ARG:CG	1:D:3:ARG:CA	2.65	0.73
1:C:159:GLU:HG3	1:C:160:GLN:N	1.99	0.73
1:B:159:GLU:HG2	4:B:2063:HOH:O	1.89	0.73
1:C:408:GLN:HG2	4:C:2150:HOH:O	1.90	0.71
1:B:128:ARG:HD2	4:B:2054:HOH:O	1.90	0.71
1:C:257:ARG:CG	1:C:288:ARG:NH1	2.55	0.70
1:A:159:GLU:O	4:A:2092:HOH:O	2.10	0.69
1:A:261:GLU:HB2	4:A:2145:HOH:O	1.92	0.69
1:A:257:ARG:HG2	1:A:288:ARG:HD2	1.74	0.68
1:A:240:ARG:HD2	4:A:2129:HOH:O	1.94	0.68
1:A:50:SER:HB3	1:A:165:PRO:O	1.97	0.65
1:A:288:ARG:HD3	4:A:2158:HOH:O	1.97	0.64
1:B:128:ARG:HD3	4:B:2049:HOH:O	1.98	0.64
1:A:159:GLU:OE1	4:A:2093:HOH:O	2.15	0.63
1:B:41:ARG:NH2	4:B:2010:HOH:O	2.31	0.63
1:A:46:GLN:HE21	1:A:172:ALA:CB	2.12	0.61
1:C:257:ARG:HG3	1:C:288:ARG:NH1	2.15	0.60
1:A:476:HIS:HA	1:D:1:MET:HE3	1.85	0.58
1:A:15:TRP:CE3	1:A:180:SER:HA	2.40	0.57
1:C:53:ARG:HD2	4:C:2019:HOH:O	2.04	0.57
1:D:408:GLN:HG2	4:D:2129:HOH:O	2.05	0.56
1:B:15:TRP:CE3	1:B:180:SER:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ARG:HH11	1:B:288:ARG:HG3	1.70	0.56
1:B:457:ILE:HD11	4:B:2196:HOH:O	2.05	0.56
1:B:45:GLY:HA3	4:B:2115:HOH:O	2.05	0.55
1:B:159:GLU:CG	1:B:160:GLN:N	2.61	0.55
1:B:128:ARG:HG2	4:B:2053:HOH:O	2.06	0.55
1:D:128:ARG:HG2	4:D:2034:HOH:O	2.07	0.55
1:C:321:GLU:HG3	4:C:2101:HOH:O	2.07	0.54
1:C:40:ARG:HG3	4:C:2011:HOH:O	2.08	0.54
1:C:15:TRP:CE3	1:C:180:SER:HA	2.43	0.53
1:B:128:ARG:HG3	4:B:2224:HOH:O	2.09	0.53
1:C:298:GLU:HB2	4:C:2097:HOH:O	2.08	0.53
1:D:15:TRP:CE3	1:D:180:SER:HA	2.43	0.53
1:C:64:ARG:HG3	4:C:2198:HOH:O	2.07	0.53
1:B:490:ARG:CZ	4:B:2225:HOH:O	2.56	0.53
1:A:257:ARG:HD3	4:A:2143:HOH:O	2.10	0.52
1:B:370:LYS:O	1:C:471:ARG:HD3	2.10	0.51
1:A:370:LYS:O	1:D:471:ARG:HD3	2.09	0.51
1:C:257:ARG:CG	1:C:288:ARG:HH11	2.23	0.51
1:B:128:ARG:CD	4:B:2054:HOH:O	2.54	0.51
1:D:307:ARG:HB3	4:D:2078:HOH:O	2.10	0.50
1:A:280:MET:HA	1:A:292:GLY:O	2.11	0.50
1:C:169:HIS:CD2	1:C:283:ILE:HG23	2.47	0.50
1:C:280:MET:HA	1:C:292:GLY:O	2.11	0.50
1:A:361:ILE:HD11	2:A:650:FAD:H5'1	1.95	0.49
1:B:177:ARG:HG3	4:B:2010:HOH:O	2.12	0.49
1:B:159:GLU:HG3	1:B:160:GLN:HG2	1.94	0.49
1:B:280:MET:HA	1:B:292:GLY:O	2.13	0.49
1:B:64:ARG:HD2	4:B:2020:HOH:O	2.12	0.49
1:D:280:MET:HA	1:D:292:GLY:O	2.12	0.49
1:C:1:MET:H2	1:C:375:GLU:HB2	1.73	0.49
1:A:159:GLU:HG3	1:A:160:GLN:HG2	1.95	0.48
1:C:50:SER:HB3	1:C:165:PRO:O	2.13	0.48
1:B:50:SER:HB3	1:B:165:PRO:O	2.13	0.48
1:A:160:GLN:HA	4:A:2092:HOH:O	2.14	0.47
1:A:307:ARG:HD2	1:B:494:ASP:OD2	2.14	0.47
1:D:159:GLU:HG3	1:D:160:GLN:HG2	1.96	0.47
1:A:53:ARG:HD2	4:A:2031:HOH:O	2.14	0.47
1:C:159:GLU:HG3	1:C:160:GLN:HG2	1.95	0.47
1:A:46:GLN:NE2	1:A:172:ALA:HB2	2.25	0.47
1:D:50:SER:HB3	1:D:165:PRO:O	2.14	0.47
4:B:2041:HOH:O	1:C:370:LYS:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:HIS:HB2	4:C:2062:HOH:O	2.14	0.47
1:B:288:ARG:HG3	1:B:288:ARG:NH1	2.30	0.46
1:D:62:ASP:HB3	4:D:2015:HOH:O	2.14	0.46
1:A:457:ILE:HD11	4:A:2256:HOH:O	2.15	0.46
1:C:159:GLU:CG	1:C:160:GLN:N	2.65	0.46
1:A:249:PRO:HG3	1:A:421:ARG:CZ	2.46	0.45
1:D:249:PRO:HG3	1:D:421:ARG:CZ	2.46	0.45
1:C:249:PRO:HG3	1:C:421:ARG:CZ	2.46	0.45
1:C:281:TRP:O	1:C:291:ASN:HA	2.17	0.45
1:D:1:MET:N	4:D:2001:HOH:O	2.46	0.45
1:C:257:ARG:HG2	1:C:288:ARG:HH11	1.81	0.45
1:C:402:LEU:HD11	1:C:460:ASN:OD1	2.17	0.45
1:D:361:ILE:HD11	2:D:650:FAD:H5'1	1.98	0.45
1:C:361:ILE:HD11	2:C:650:FAD:H5'1	1.98	0.44
1:B:399:PHE:O	1:B:402:LEU:HB3	2.16	0.44
1:C:257:ARG:HG3	1:C:288:ARG:HH12	1.82	0.44
1:D:169:HIS:CD2	1:D:283:ILE:HG23	2.53	0.44
1:B:81:GLU:HG3	1:B:89:TYR:HB3	1.98	0.44
1:D:402:LEU:HD11	1:D:460:ASN:OD1	2.18	0.44
1:A:457:ILE:HG21	1:A:457:ILE:HD13	1.68	0.43
1:D:491:ARG:CG	4:D:2186:HOH:O	2.56	0.43
1:A:480:ALA:HB3	1:A:481:PRO:HD3	2.00	0.43
1:A:2:ILE:O	1:D:476:HIS:HE1	2.01	0.43
1:A:159:GLU:CG	1:A:160:GLN:N	2.67	0.43
1:B:227:GLY:HA2	1:B:345:LEU:HB2	2.01	0.43
1:C:93:PRO:HG3	1:C:124:TYR:CD2	2.53	0.43
1:B:376:ARG:HD3	1:C:469:ARG:NH2	2.34	0.43
1:A:169:HIS:CD2	1:A:283:ILE:HG23	2.53	0.42
1:C:457:ILE:HD13	1:C:457:ILE:HG21	1.72	0.42
1:D:43:GLY:O	1:D:257:ARG:NH2	2.51	0.42
1:B:352:PRO:HB3	3:B:700:CL:CL	2.57	0.42
1:B:370:LYS:HE3	1:C:102:GLY:O	2.18	0.42
1:C:85:GLU:HB2	1:C:88:GLU:HB2	2.02	0.42
1:D:81:GLU:HG3	1:D:89:TYR:HB3	2.02	0.42
1:D:22:LYS:HA	1:D:22:LYS:HD3	1.88	0.42
1:D:76:LEU:HB3	1:D:126:THR:HG23	2.02	0.42
1:D:260:ARG:NH1	1:D:289:ASP:OD1	2.53	0.42
1:C:244:PHE:CD2	1:C:330:GLY:HA2	2.55	0.41
1:B:63:GLU:OE2	1:B:74:TYR:OH	2.33	0.41
1:B:79:ARG:NE	1:B:81:GLU:OE1	2.52	0.41
1:D:471:ARG:HA	1:D:472:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LYS:HE3	1:A:423:MET:HG2	2.03	0.41
1:A:69:ARG:HG3	4:A:2045:HOH:O	2.21	0.41
1:A:84:SER:HB2	1:A:408:GLN:HB2	2.03	0.41
1:A:86:PRO:HG2	1:B:505:GLU:CD	2.41	0.41
1:B:369:VAL:O	1:C:473:ALA:HB2	2.21	0.41
1:A:81:GLU:HG3	1:A:89:TYR:HB3	2.02	0.41
1:B:169:HIS:CD2	1:B:283:ILE:HG23	2.56	0.41
1:C:94:PHE:O	1:C:165:PRO:HD2	2.20	0.41
1:D:249:PRO:HD2	4:D:2133:HOH:O	2.20	0.41
1:C:81:GLU:HG3	1:C:89:TYR:HB3	2.02	0.41
1:C:227:GLY:HA2	1:C:345:LEU:HB2	2.02	0.41
1:A:76:LEU:HB3	1:A:126:THR:HG23	2.03	0.40
1:B:218:SER:HB2	4:B:2028:HOH:O	2.22	0.40
1:D:336:TRP:CG	1:D:341:VAL:HG22	2.57	0.40
1:C:171:ASP:OD2	1:C:288:ARG:NH2	2.55	0.40
1:C:336:TRP:CG	1:C:341:VAL:HG22	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:NH2	1:D:298:GLU:O[7_555]	1.74	0.46

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	490/511 (96%)	471 (96%)	19 (4%)	0	100 100
1	B	490/511 (96%)	474 (97%)	16 (3%)	0	100 100
1	C	490/511 (96%)	470 (96%)	19 (4%)	1 (0%)	47 68
1	D	490/511 (96%)	471 (96%)	19 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1960/2044 (96%)	1886 (96%)	73 (4%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	268	PRO

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	411/424 (97%)	405 (98%)	6 (2%)	65 85
1	B	411/424 (97%)	406 (99%)	5 (1%)	71 88
1	C	411/424 (97%)	404 (98%)	7 (2%)	60 82
1	D	411/424 (97%)	405 (98%)	6 (2%)	65 85
All	All	1644/1696 (97%)	1620 (98%)	24 (2%)	65 85

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	A	170	PHE
1	A	257	ARG
1	A	355	SER
1	A	387	GLU
1	A	436	SER
1	B	50	SER
1	B	170	PHE
1	B	293	TYR
1	B	355	SER
1	B	379	PRO
1	C	50	SER
1	C	170	PHE
1	C	177	ARG

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Mol	Chain	Res	Type
1	C	293	TYR
1	C	355	SER
1	C	436	SER
1	C	471	ARG
1	D	50	SER
1	D	170	PHE
1	D	293	TYR
1	D	355	SER
1	D	436	SER
1	D	471	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	C	650	-	50,57,58	1.13	4 (8%)	63,86,89	1.42	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	D	650	-	53,58,58	1.13	4 (7%)	68,89,89	1.34	10 (14%)
2	FAD	A	650	-	53,58,58	1.14	3 (5%)	68,89,89	1.49	10 (14%)
2	FAD	B	650	-	53,58,58	1.18	4 (7%)	68,89,89	1.42	9 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	650	-	-	5/24/48/50	0/6/6/6
2	FAD	D	650	-	-	5/30/50/50	0/6/6/6
2	FAD	A	650	-	-	7/30/50/50	0/6/6/6
2	FAD	B	650	-	-	7/30/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	650	FAD	C4X-N5	4.38	1.39	1.30
2	B	650	FAD	C4X-N5	4.25	1.39	1.30
2	D	650	FAD	C4X-N5	4.12	1.38	1.30
2	B	650	FAD	C2A-N3A	4.02	1.38	1.32
2	C	650	FAD	C4X-N5	3.48	1.37	1.30
2	D	650	FAD	C2A-N3A	3.45	1.37	1.32
2	C	650	FAD	C2A-N3A	3.37	1.37	1.32
2	B	650	FAD	C2A-N1A	3.16	1.39	1.33
2	A	650	FAD	C2A-N3A	3.01	1.36	1.32
2	A	650	FAD	C2A-N1A	2.51	1.38	1.33
2	D	650	FAD	C10-N1	2.42	1.38	1.33
2	D	650	FAD	C2A-N1A	2.37	1.38	1.33
2	C	650	FAD	C10-N1	2.30	1.37	1.33
2	C	650	FAD	C2A-N1A	2.23	1.38	1.33
2	B	650	FAD	C10-N1	2.13	1.37	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	650	FAD	N3A-C2A-N1A	-6.44	118.62	128.68
2	C	650	FAD	N3A-C2A-N1A	-6.31	118.82	128.68
2	B	650	FAD	N3A-C2A-N1A	-6.27	118.87	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	650	FAD	N3A-C2A-N1A	-5.18	120.59	128.68
2	B	650	FAD	C4X-C10-N10	3.32	121.34	116.48
2	C	650	FAD	C4X-C10-N10	3.21	121.17	116.48
2	A	650	FAD	C4X-C10-N10	3.15	121.08	116.48
2	B	650	FAD	C10-C4X-N5	-3.09	118.30	124.86
2	D	650	FAD	C4X-C10-N10	3.08	120.98	116.48
2	A	650	FAD	C10-C4X-N5	-3.07	118.35	124.86
2	C	650	FAD	C4-N3-C2	-3.03	120.05	125.64
2	D	650	FAD	C10-C4X-N5	-2.97	118.55	124.86
2	C	650	FAD	C10-C4X-N5	-2.94	118.61	124.86
2	A	650	FAD	C4-C4X-N5	2.61	121.95	118.23
2	A	650	FAD	C10-N1-C2	2.60	122.09	116.90
2	C	650	FAD	C4X-C4-N3	2.57	119.73	113.19
2	B	650	FAD	O4B-C1B-C2B	-2.47	103.32	106.93
2	C	650	FAD	C4-C4X-N5	2.46	121.73	118.23
2	B	650	FAD	C4-C4X-N5	2.44	121.71	118.23
2	D	650	FAD	C4X-C10-N1	-2.36	119.27	124.73
2	C	650	FAD	C4X-C10-N1	-2.32	119.35	124.73
2	A	650	FAD	C4-N3-C2	-2.32	121.36	125.64
2	D	650	FAD	C4-N3-C2	-2.32	121.36	125.64
2	A	650	FAD	O4'-C4'-C3'	2.30	114.69	109.10
2	B	650	FAD	C1B-N9A-C4A	-2.27	122.65	126.64
2	A	650	FAD	C4X-C10-N1	-2.21	119.60	124.73
2	B	650	FAD	O5'-C5'-C4'	2.20	115.23	109.36
2	D	650	FAD	C10-N1-C2	2.18	121.26	116.90
2	D	650	FAD	C4X-C4-N3	2.17	118.69	113.19
2	B	650	FAD	O4'-C4'-C3'	2.16	114.35	109.10
2	D	650	FAD	C4-C4X-N5	2.13	121.26	118.23
2	C	650	FAD	C10-N1-C2	2.13	121.16	116.90
2	C	650	FAD	O4'-C4'-C3'	2.13	114.27	109.10
2	B	650	FAD	C4A-C5A-N7A	-2.10	107.22	109.40
2	D	650	FAD	C1B-N9A-C4A	-2.07	123.00	126.64
2	A	650	FAD	C4A-C5A-N7A	-2.07	107.24	109.40
2	D	650	FAD	C4-C4X-C10	2.02	120.19	116.79
2	A	650	FAD	C4X-C4-N3	2.01	118.28	113.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	650	FAD	O3'-C3'-C4'-O4'
2	C	650	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	A	650	FAD	C2'-C3'-C4'-C5'
2	B	650	FAD	O3'-C3'-C4'-O4'
2	A	650	FAD	C2'-C3'-C4'-O4'
2	B	650	FAD	C2'-C3'-C4'-O4'
2	D	650	FAD	C2'-C3'-C4'-O4'
2	D	650	FAD	O3'-C3'-C4'-O4'
2	A	650	FAD	O3'-C3'-C4'-C5'
2	B	650	FAD	O3'-C3'-C4'-C5'
2	C	650	FAD	O3'-C3'-C4'-C5'
2	B	650	FAD	C2'-C3'-C4'-C5'
2	D	650	FAD	O3'-C3'-C4'-C5'
2	C	650	FAD	C2'-C3'-C4'-C5'
2	A	650	FAD	O3'-C3'-C4'-O4'
2	B	650	FAD	C5'-O5'-P-O2P
2	D	650	FAD	C2'-C3'-C4'-C5'
2	B	650	FAD	O4B-C4B-C5B-O5B
2	D	650	FAD	O4B-C4B-C5B-O5B
2	A	650	FAD	C5'-O5'-P-O3P
2	B	650	FAD	C5'-O5'-P-O3P
2	A	650	FAD	O4B-C4B-C5B-O5B
2	C	650	FAD	O4B-C4B-C5B-O5B
2	A	650	FAD	C5'-O5'-P-O2P

There are no ring outliers.

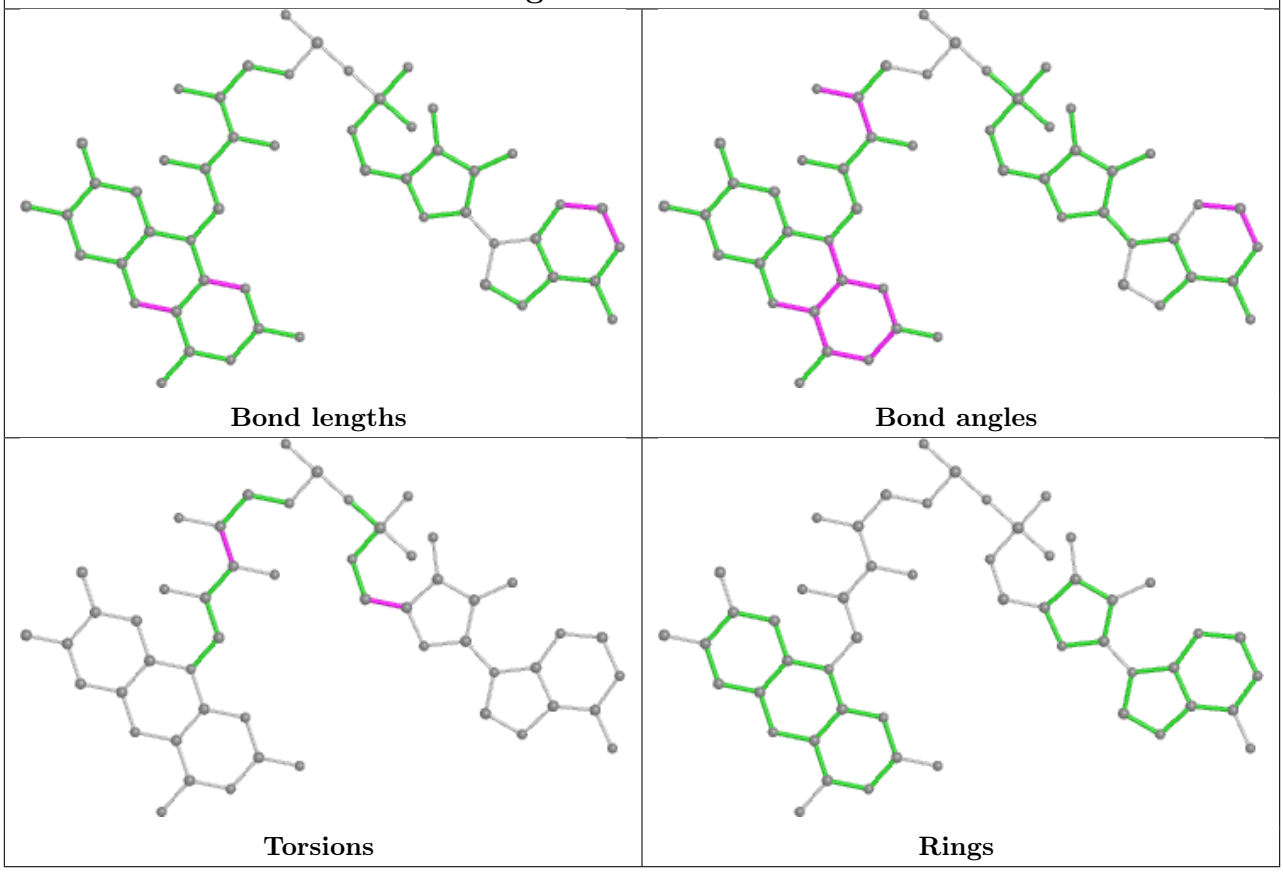
3 monomers are involved in 3 short contacts:

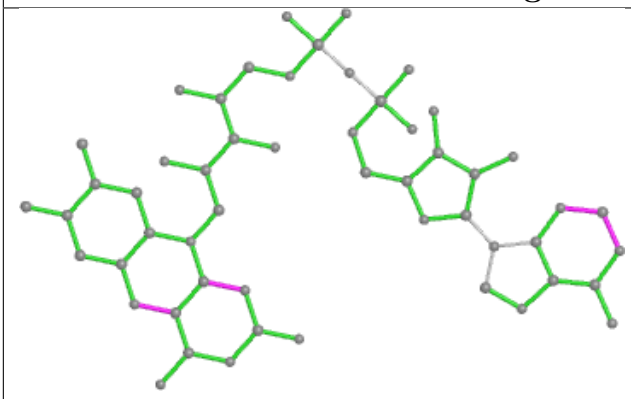
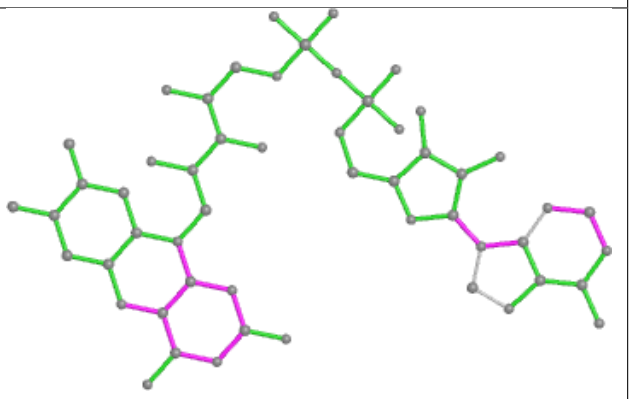
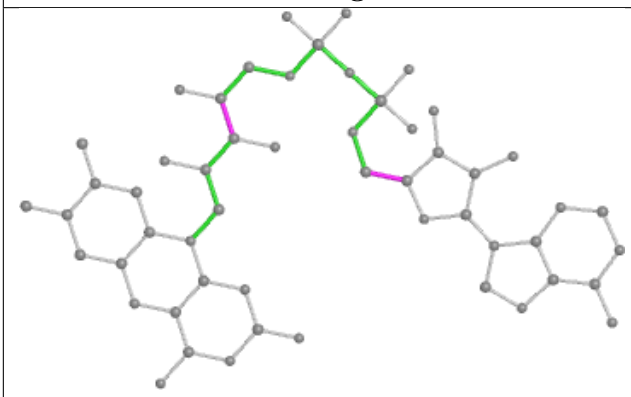
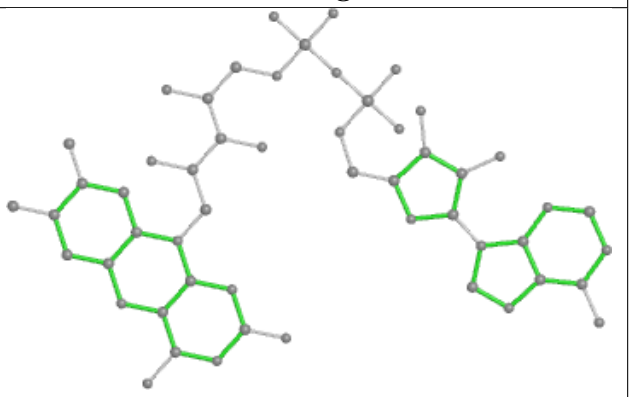
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	650	FAD	1	0
2	D	650	FAD	1	0
2	A	650	FAD	1	0

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

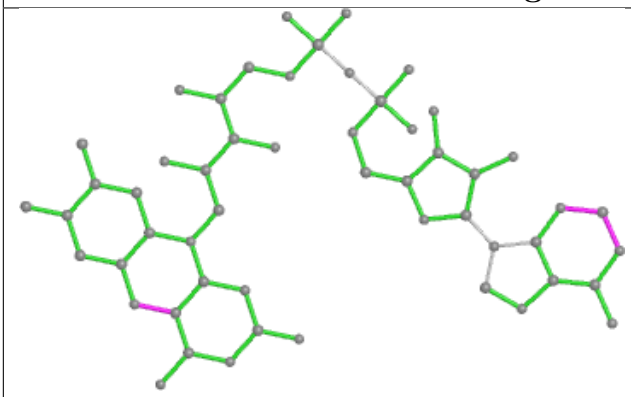
equivalents in the CSD to analyse the geometry.

Ligand FAD C 650

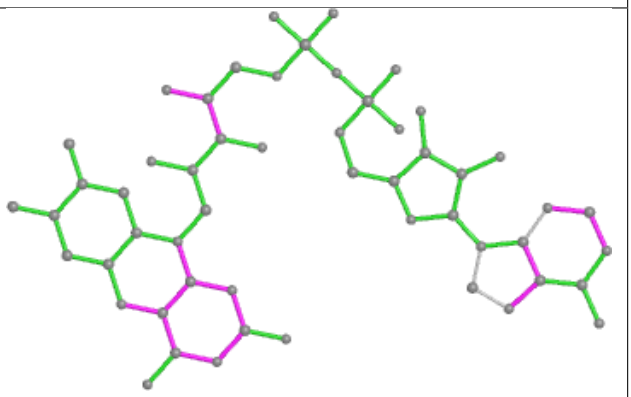


Ligand FAD D 650	
 Bond lengths	 Bond angles
 Torsions	 Rings

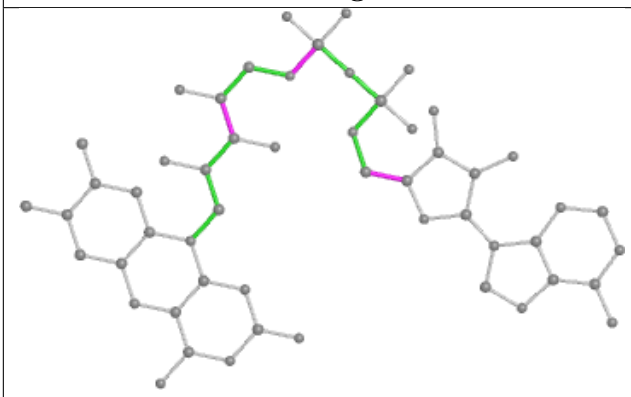
Ligand FAD A 650



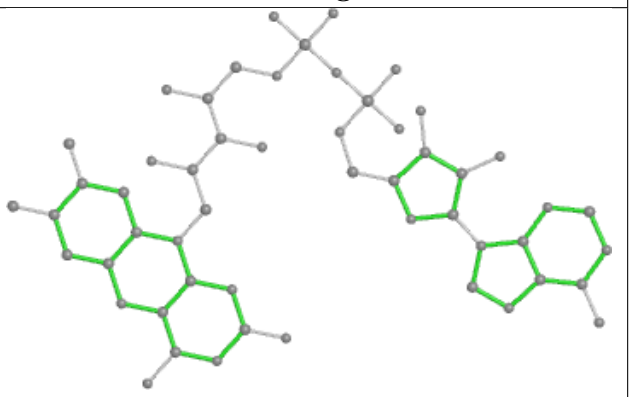
Bond lengths



Bond angles

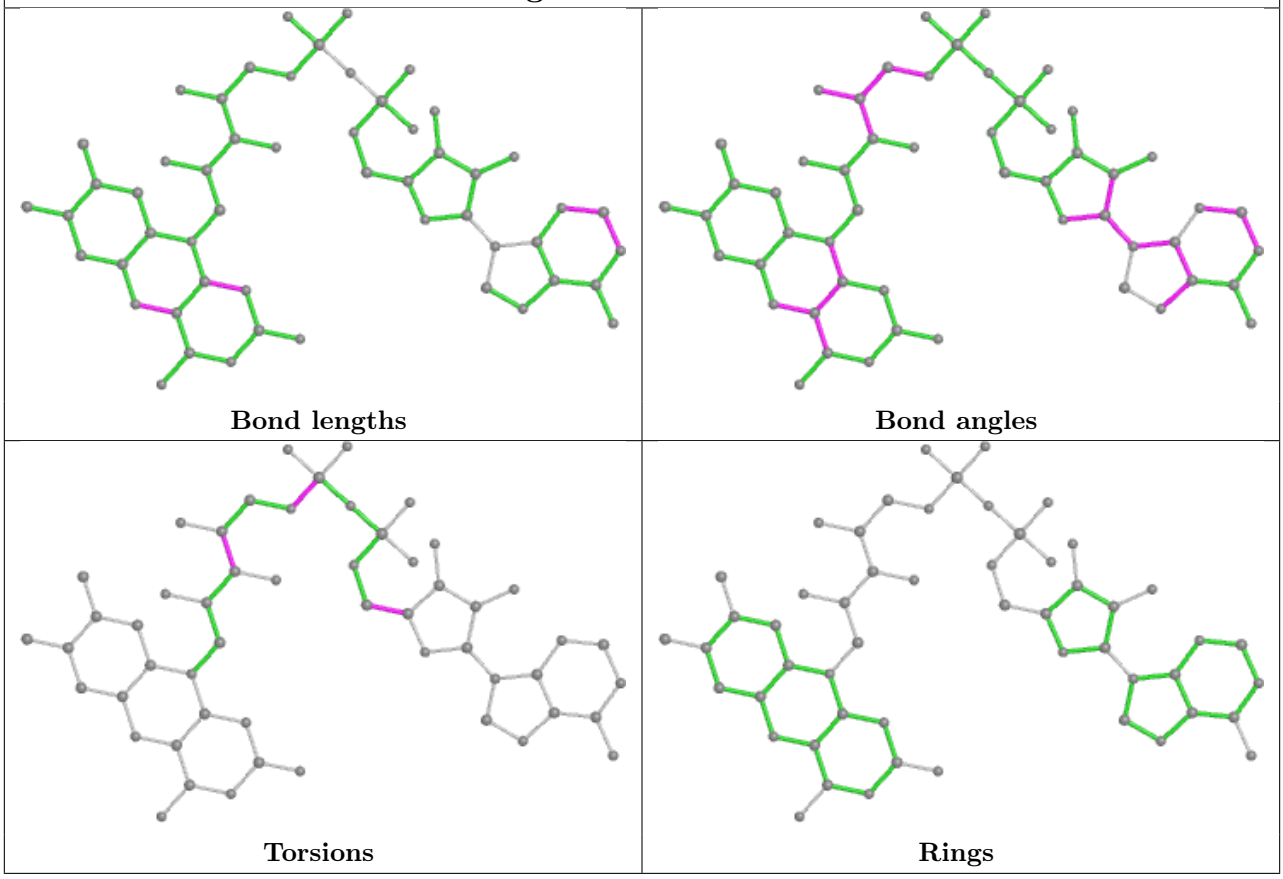


Torsions



Rings

Ligand FAD B 650



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	496/511 (97%)	-0.05	4 (0%)	86	87	22, 36, 58, 76	0
1	B	496/511 (97%)	-0.05	8 (1%)	72	74	22, 36, 58, 76	0
1	C	496/511 (97%)	-0.03	12 (2%)	59	62	22, 36, 59, 76	0
1	D	496/511 (97%)	0.16	29 (5%)	23	24	22, 36, 59, 76	0
All	All	1984/2044 (97%)	0.01	53 (2%)	54	58	22, 36, 58, 76	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	164	PHE	5.9
1	D	144	PHE	4.7
1	C	498	ALA	4.5
1	D	43	GLY	3.9
1	D	316	GLY	3.6
1	D	491	ARG	3.5
1	D	139	LEU	3.4
1	A	483	LEU	3.3
1	D	3	ARG	3.2
1	D	261	GLU	3.2
1	D	498	ALA	3.2
1	C	497	ILE	3.2
1	D	504	TYR	3.1
1	C	164	PHE	3.0
1	D	507	LEU	2.8
1	B	318	ASP	2.7
1	D	160	GLN	2.7
1	D	40	ARG	2.7
1	C	491	ARG	2.7
1	D	69	ARG	2.6
1	D	38	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	3	ARG	2.6
1	D	314	ALA	2.5
1	D	493	GLY	2.5
1	D	145	ALA	2.5
1	A	242	GLN	2.5
1	D	257	ARG	2.4
1	B	117	THR	2.4
1	B	307	ARG	2.4
1	C	145	ALA	2.4
1	C	146	SER	2.4
1	D	146	SER	2.4
1	B	38	ASN	2.4
1	D	286	PHE	2.4
1	C	499	ALA	2.4
1	B	39	VAL	2.3
1	D	72	GLY	2.3
1	C	318	ASP	2.3
1	C	495	GLU	2.3
1	A	240	ARG	2.2
1	D	496	LEU	2.2
1	B	480	ALA	2.2
1	C	315	PRO	2.2
1	D	262	ASN	2.2
1	B	321	GLU	2.2
1	C	320	LEU	2.1
1	D	184	ILE	2.1
1	D	259	PRO	2.1
1	D	511	GLN	2.1
1	D	315	PRO	2.1
1	A	491	ARG	2.1
1	B	203	ARG	2.0
1	D	189	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

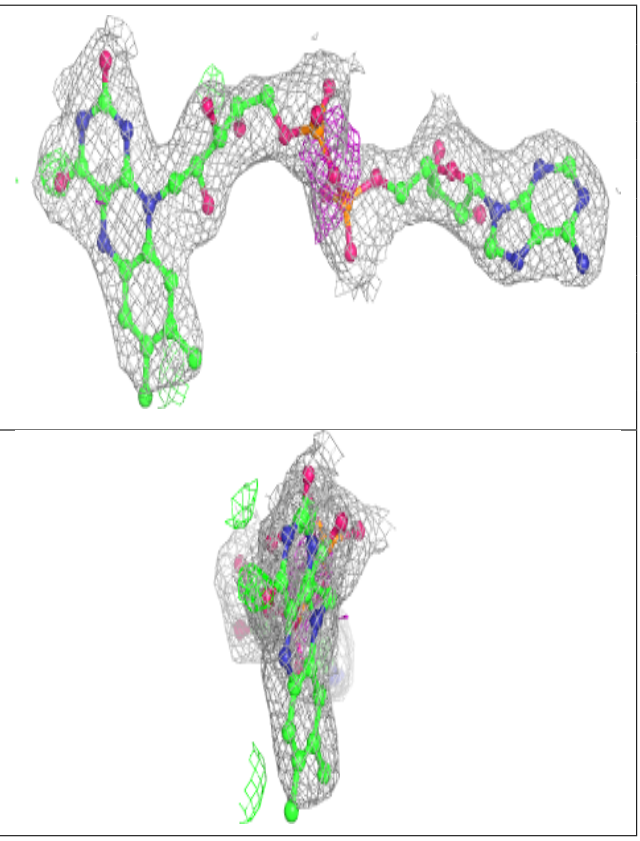
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	650	53/53	0.94	0.14	22,33,38,43	0
3	CL	C	700	1/1	0.95	0.10	44,44,44,44	0
3	CL	B	700	1/1	0.96	0.13	44,44,44,44	0
2	FAD	B	650	53/53	0.96	0.12	22,32,38,43	0
2	FAD	C	650	52/53	0.97	0.15	22,33,38,43	0
2	FAD	A	650	53/53	0.97	0.16	22,32,38,43	0
3	CL	D	700	1/1	0.98	0.06	45,45,45,45	0
3	CL	A	700	1/1	0.99	0.19	43,43,43,43	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.

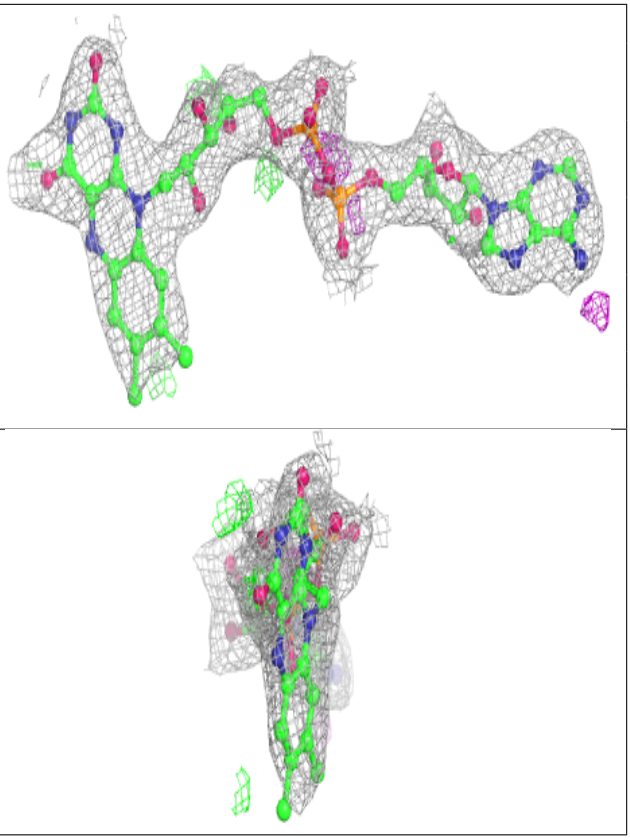
Electron density around FAD D 650:

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



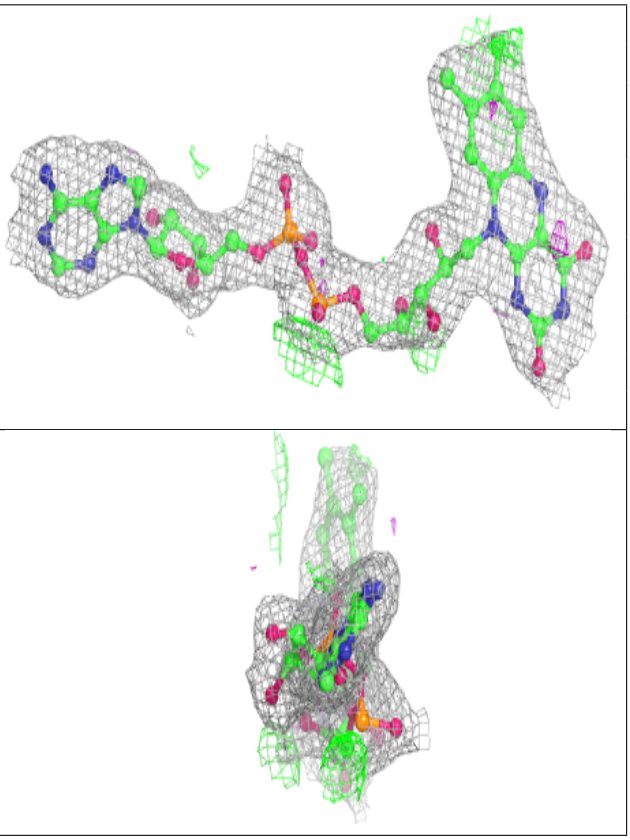
Electron density around FAD B 650:

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



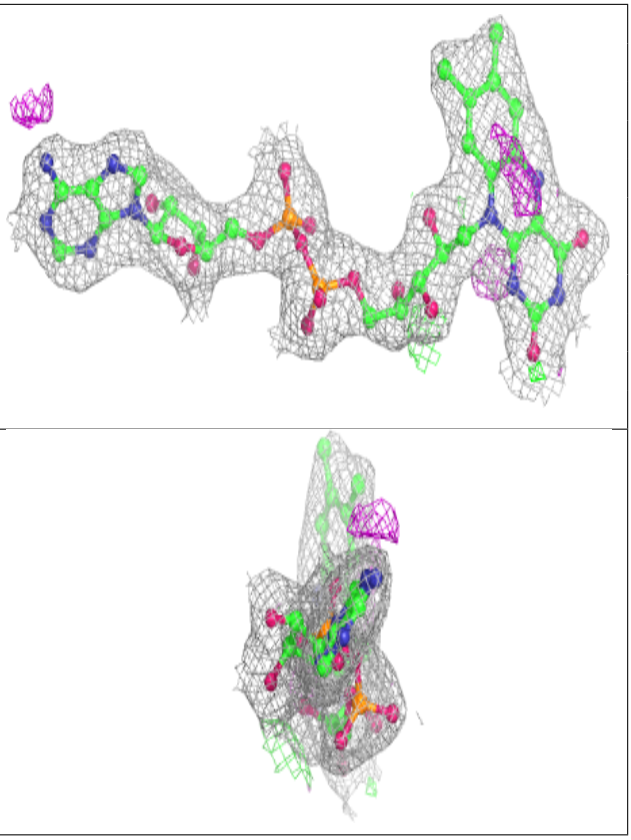
Electron density around FAD C 650:

$2mF_o$-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 650:

$2mF_o$-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.