



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 09:10 AM EST

PDB ID : 2R6H  
Title : Crystal structure of the domain comprising the NAD binding and the FAD binding regions of the NADH:ubiquinone oxidoreductase, Na translocating, F subunit from Porphyromonas gingivalis  
Authors : Kim, Y.; Mulligan, R.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2007-09-05  
Resolution : 2.95 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

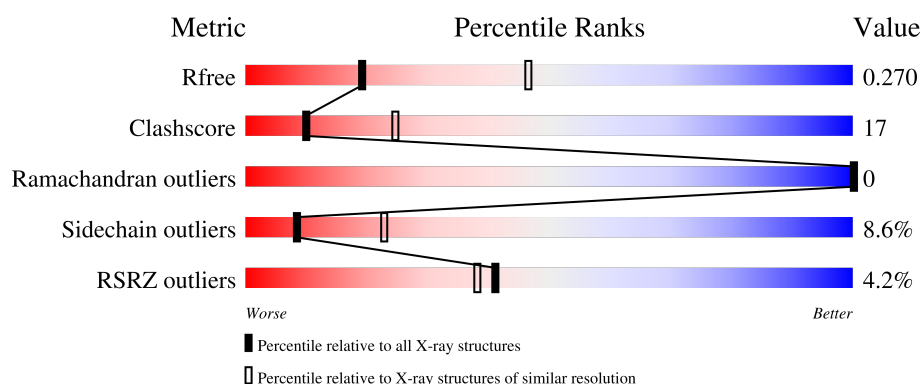
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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	290	<div> <div>3%</div> <div>69%</div> <div>27%</div> <div>• •</div> </div>
1	B	290	<div> <div>6%</div> <div>64%</div> <div>29%</div> <div>6%</div> <div>•</div> </div>
1	C	290	<div> <div>3%</div> <div>66%</div> <div>30%</div> <div>•</div> </div>
1	D	290	<div> <div>4%</div> <div>64%</div> <div>29%</div> <div>• •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9919 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 NADH:ubiquinone oxidoreductase, Na translocating, F subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	4	0
			2349	1505	394	436	3	11			
1	B	286	Total	C	N	O	S	Se	0	1	0
			2331	1499	384	434	3	11			
1	C	289	Total	C	N	O	S	Se	0	6	0
			2397	1538	402	443	3	11			
1	D	284	Total	C	N	O	S	Se	0	2	0
			2321	1489	384	434	3	11			

There are 12 discrepancies between the modelled and reference sequences:

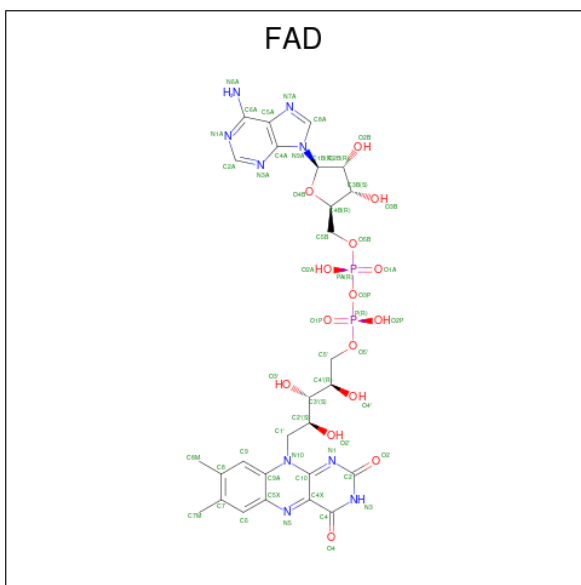
Chain	Residue	Modelled	Actual	Comment	Reference
A	123	SER	-	expression tag	UNP Q7MT22
A	124	ASN	-	expression tag	UNP Q7MT22
A	125	ALA	-	expression tag	UNP Q7MT22
B	123	SER	-	expression tag	UNP Q7MT22
B	124	ASN	-	expression tag	UNP Q7MT22
B	125	ALA	-	expression tag	UNP Q7MT22
C	123	SER	-	expression tag	UNP Q7MT22
C	124	ASN	-	expression tag	UNP Q7MT22
C	125	ALA	-	expression tag	UNP Q7MT22
D	123	SER	-	expression tag	UNP Q7MT22
D	124	ASN	-	expression tag	UNP Q7MT22
D	125	ALA	-	expression tag	UNP Q7MT22

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

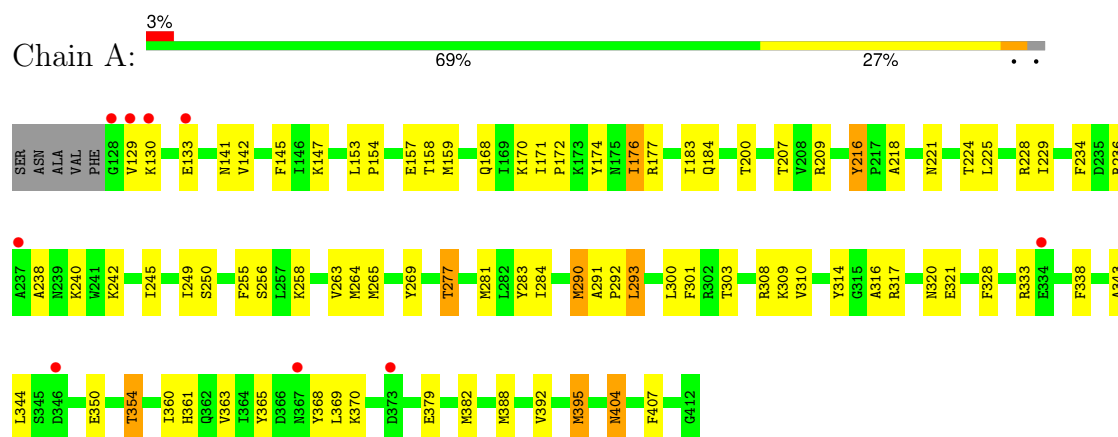
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	58	Total O 58 58	0	0
4	B	51	Total O 51 51	0	0
4	C	80	Total O 80 80	0	0
4	D	65	Total O 65 65	0	0

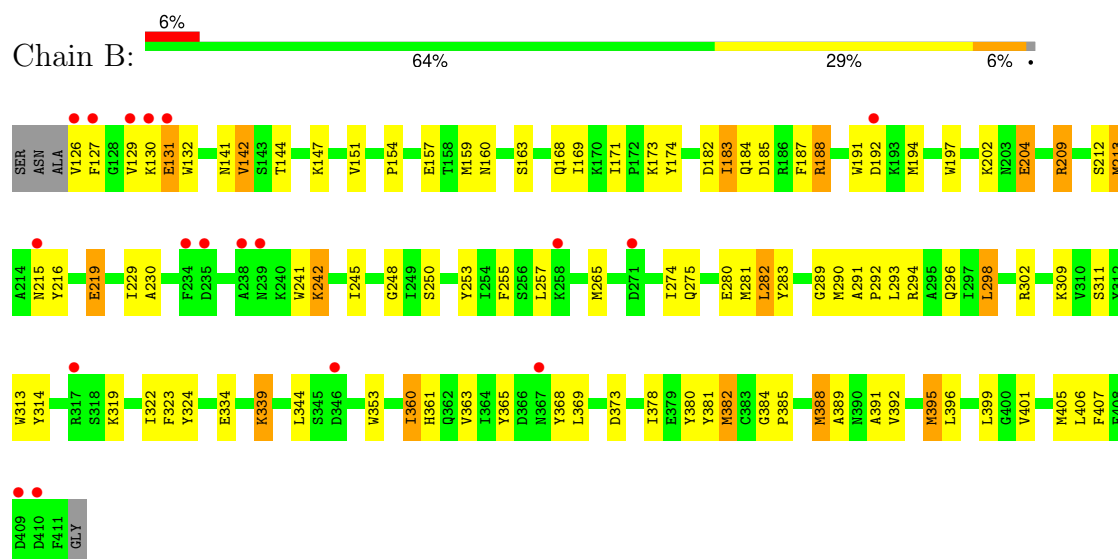
### 3 Residue-property plots

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: NADH:ubiquinone oxidoreductase, Na translocating, F subunit

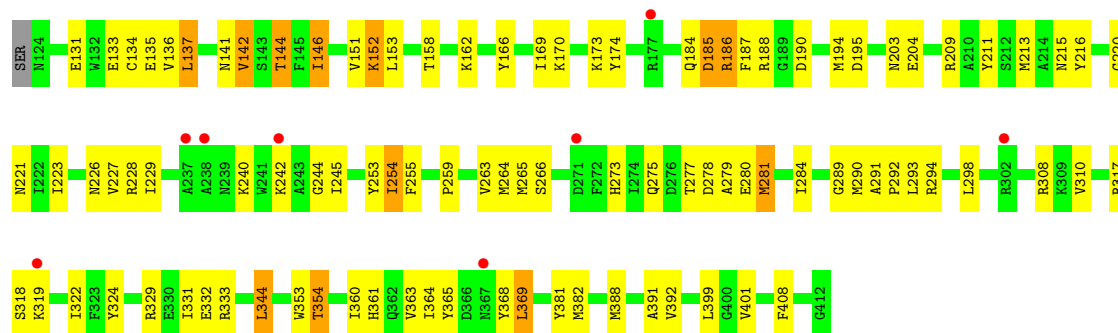


- Molecule 1: NADH:ubiquinone oxidoreductase, Na translocating, F subunit

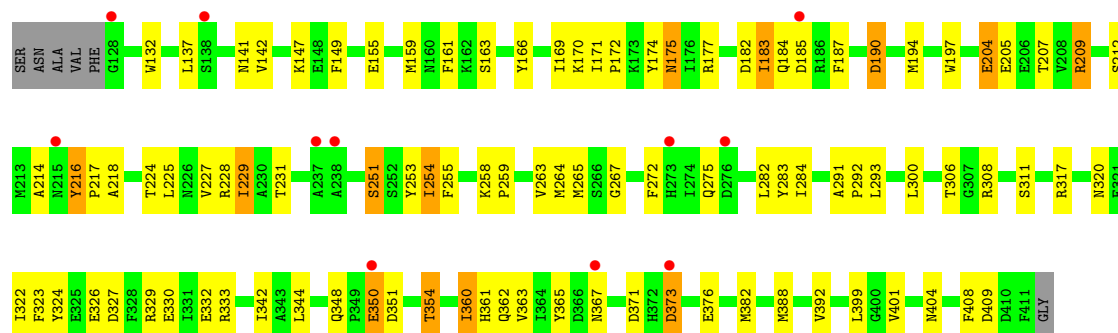


- Molecule 1: NADH:ubiquinone oxidoreductase, Na translocating, F subunit





- Molecule 1: NADH:ubiquinone oxidoreductase, Na translocating, F subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.68Å 175.68Å 244.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.54 – 2.95 47.54 – 2.95	Depositor EDS
% Data completeness (in resolution range)	93.7 (47.54-2.95) 93.7 (47.54-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.06 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.215 , 0.271 0.213 , 0.270	Depositor DCC
$R_{free}$ test set	3826 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.015 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, SO4

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	0.43	0/2405	0.56	0/3232
1	B	0.46	1/2387 (0.0%)	0.50	0/3210
1	C	0.46	0/2453	0.56	0/3294
1	D	0.42	0/2376	0.53	0/3195
All	All	0.44	1/9621 (0.0%)	0.54	0/12931

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368	TYR	CD2-CE2	-5.57	1.30	1.39

There are no bond angle outliers.

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	2349	0	2244	79	0
1	B	2331	0	2229	85	0
1	C	2397	0	2303	91	1
1	D	2321	0	2216	81	1
2	A	15	0	0	0	0
2	B	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	0	1	0
2	D	10	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	0	0
3	C	53	0	31	1	0
3	D	53	0	31	1	0
4	A	58	0	0	3	0
4	B	51	0	0	2	0
4	C	80	0	0	6	0
4	D	65	0	0	5	0
All	All	9919	0	9116	321	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 17.

All (321) 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:C:277:THR:HG22	1:C:279:ALA:H	1.07	1.09
1:C:382:MSE:HE1	1:C:392:VAL:HG21	1.31	1.05
1:D:382:MSE:HE2	1:D:388:MSE:HE3	1.40	1.02
1:B:242:LYS:HG2	1:B:245:ILE:HD12	1.43	1.01
1:A:291:ALA:HB3	1:A:292:PRO:HD3	1.37	1.00
1:D:382:MSE:HE1	1:D:392:VAL:HG21	1.47	0.96
1:C:290:MSE:HE2	1:C:324:TYR:HD2	1.31	0.94
1:B:382:MSE:HE1	1:B:392:VAL:HG21	1.50	0.92
1:A:153:LEU:HB2	1:A:221:ASN:HB2	1.52	0.91
1:C:290:MSE:HE2	1:C:324:TYR:CD2	2.08	0.88
1:C:277:THR:HG22	1:C:279:ALA:N	1.89	0.87
1:C:277:THR:HG22	1:C:278:ASP:N	1.91	0.86
1:C:281:MSE:HE2	1:C:381:TYR:CE2	2.13	0.84
1:C:215:ASN:HB3	4:C:432:HOH:O	1.78	0.83
1:C:290:MSE:CE	1:C:324:TYR:HD2	1.92	0.81
1:D:382:MSE:HE1	1:D:392:VAL:CG2	2.12	0.80
1:A:382:MSE:HE2	1:A:388:MSE:HE3	1.62	0.79
1:D:132:TRP:CZ3	1:D:159:MSE:HE3	2.16	0.79
1:D:159:MSE:HG2	1:D:161:PHE:HD2	1.48	0.79
1:A:382:MSE:HE1	1:A:392:VAL:HG21	1.64	0.78
1:B:291:ALA:HB3	1:B:292:PRO:HD3	1.65	0.77
1:C:277:THR:CG2	1:C:279:ALA:H	1.92	0.77
1:C:277:THR:CG2	1:C:278:ASP:N	2.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HG12	1:B:130:LYS:HG2	1.66	0.76
1:C:133:GLU:HG3	1:C:264:MSE:HE1	1.68	0.75
1:C:134:CYS:HB3	1:C:151:VAL:CG1	2.16	0.75
1:C:290:MSE:HE3	1:C:294:ARG:HD2	1.68	0.74
1:C:382:MSE:HE1	1:C:392:VAL:CG2	2.15	0.74
1:A:290:MSE:HE1	1:A:328:PHE:CE2	2.23	0.74
1:B:282:LEU:HD11	1:B:313:TRP:CD1	2.23	0.73
1:D:362:GLN:HG3	4:D:475:HOH:O	1.88	0.73
1:A:354:THR:HG21	1:B:363:VAL:HA	1.68	0.73
1:D:147:LYS:HD2	1:D:255:PHE:CD2	2.24	0.73
1:C:290:MSE:CE	1:C:324:TYR:CD2	2.71	0.71
1:D:329:ARG:HD3	1:D:332:GLU:OE2	1.91	0.71
1:D:132:TRP:HZ3	1:D:159:MSE:HE3	1.54	0.70
1:C:290:MSE:CE	1:C:294:ARG:HD2	2.22	0.70
1:A:141:ASN:HB2	1:A:184:GLN:OE1	1.92	0.69
1:D:382:MSE:CE	1:D:392:VAL:HG21	2.23	0.69
1:B:159:MSE:SE	1:B:213:MSE:HE1	2.43	0.68
1:C:363:VAL:HG22	1:D:354:THR:HG23	1.75	0.68
1:A:207:THR:HG21	1:A:249:ILE:HD11	1.74	0.68
1:C:281:MSE:HE2	1:C:381:TYR:HE2	1.59	0.68
1:B:194:MSE:HE2	1:B:241:TRP:CH2	2.29	0.68
1:B:147:LYS:HD2	1:B:255:PHE:CE2	2.30	0.67
1:D:284:ILE:HG21	1:D:382:MSE:HE3	1.75	0.67
1:D:326:GLU:O	1:D:330:GLU:HG3	1.94	0.67
1:D:291:ALA:HB3	1:D:292:PRO:HD3	1.78	0.66
1:B:274:ILE:HG23	1:B:281:MSE:HE1	1.78	0.66
1:C:280:GLU:OE2	1:C:368:TYR:OH	2.08	0.66
1:C:363:VAL:HA	1:D:354:THR:HG21	1.79	0.65
1:C:277:THR:CG2	1:C:278:ASP:H	2.09	0.65
1:A:290:MSE:HE1	1:A:328:PHE:HE2	1.61	0.65
1:A:236[B]:ARG:NH1	4:A:470:HOH:O	2.29	0.65
1:C:291:ALA:HB3	1:C:292:PRO:HD3	1.79	0.64
1:A:176:ILE:HD12	1:A:256:SER:CB	2.28	0.64
1:B:154:PRO:O	1:B:157:GLU:HB2	1.98	0.63
1:A:281:MSE:HE2	1:A:308:ARG:NE	2.13	0.63
1:B:291:ALA:HB3	1:B:292:PRO:CD	2.28	0.63
1:B:311:SER:HB3	1:B:339:LYS:HD2	1.80	0.63
1:C:319[B]:LYS:HA	1:C:322:ILE:HD12	1.81	0.62
1:B:290:MSE:O	1:B:290:MSE:HG3	1.98	0.62
1:D:216:TYR:CE1	1:D:218:ALA:HB3	2.34	0.62
1:C:354:THR:HG21	1:D:363:VAL:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:PHE:O	1:D:324:TYR:HB2	2.00	0.62
1:C:134:CYS:HB3	1:C:151:VAL:HG13	1.81	0.61
1:A:154:PRO:HB2	1:A:157:GLU:HG3	1.82	0.61
1:D:190:ASP:O	1:D:194:MSE:HG3	2.00	0.61
1:B:188:ARG:HG3	1:B:197:TRP:HZ2	1.65	0.61
1:A:176:ILE:HD12	1:A:256:SER:HB2	1.83	0.60
1:A:168:GLN:HG3	1:A:269:TYR:CE1	2.36	0.60
1:B:174:TYR:CE1	1:B:253:TYR:HB2	2.36	0.60
1:B:204:GLU:HG2	4:B:438:HOH:O	2.00	0.60
1:C:319[A]:LYS:HA	1:C:322:ILE:HD12	1.84	0.60
1:B:323:PHE:O	1:B:324:TYR:HB2	2.01	0.60
1:D:141:ASN:HB2	1:D:184:GLN:OE1	2.02	0.59
1:B:395:MSE:HE3	1:B:399:LEU:HD13	1.84	0.59
1:A:129:VAL:CG1	1:A:130:LYS:N	2.66	0.59
1:C:186:ARG:NH1	2:C:3:SO4:O2	2.36	0.59
1:C:152:LYS:HE2	1:C:153:LEU:O	2.01	0.58
1:A:291:ALA:CB	1:A:292:PRO:HD3	2.20	0.58
1:D:159:MSE:HG2	1:D:161:PHE:CD2	2.36	0.58
1:C:190:ASP:O	1:C:194:MSE:HG3	2.03	0.58
1:A:291:ALA:HB3	1:A:292:PRO:CD	2.24	0.58
1:D:284:ILE:CG2	1:D:382:MSE:HE3	2.33	0.58
1:B:388:MSE:HG3	1:B:389:ALA:N	2.18	0.58
1:B:131:GLU:HG2	1:B:132:TRP:N	2.19	0.57
1:A:170:LYS:HB2	1:A:264:MSE:HB2	1.85	0.57
1:D:149:PHE:HB3	1:D:225:LEU:HB2	1.86	0.57
1:B:131:GLU:CG	1:B:132:TRP:N	2.67	0.57
1:C:344:LEU:HD22	1:C:353:TRP:CE2	2.39	0.57
1:C:185[A]:ASP:OD1	1:C:185[A]:ASP:N	2.35	0.57
1:A:281:MSE:HE1	1:A:300:LEU:HD22	1.87	0.57
1:B:365:TYR:HE1	1:B:399:LEU:HD11	1.70	0.57
1:B:141:ASN:HB2	1:B:184:GLN:OE1	2.05	0.56
1:C:361:HIS:CE1	1:C:391:ALA:HB1	2.41	0.56
1:C:133:GLU:HG3	1:C:264:MSE:CE	2.34	0.56
1:C:290:MSE:HE2	1:C:324:TYR:HB2	1.86	0.56
1:B:163:SER:HB3	1:B:296:GLN:HA	1.88	0.56
1:B:385:PRO:HD2	1:B:388:MSE:HG2	1.87	0.56
1:C:284:ILE:HB	1:C:382:MSE:HE3	1.87	0.56
1:C:365:TYR:HA	1:C:369:LEU:HB2	1.87	0.55
1:C:244:GLY:HA2	4:C:445:HOH:O	2.07	0.55
1:A:238:ALA:HB2	1:C:242[B]:LYS:NZ	2.21	0.55
1:B:130:LYS:HE2	1:B:132:TRP:CZ2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASP:HB2	2:B:11:SO4:O3	2.07	0.55
1:C:344:LEU:HD22	1:C:353:TRP:CD2	2.41	0.55
1:C:382:MSE:HE2	1:C:388:MSE:HE3	1.88	0.55
1:D:224:THR:O	1:D:225:LEU:HD23	2.07	0.55
1:B:380:TYR:CE1	1:B:401:VAL:HG11	2.43	0.54
1:A:157:GLU:O	1:A:221:ASN:HB3	2.08	0.54
1:A:320:ASN:HB2	4:A:415:HOH:O	2.06	0.53
1:B:253:TYR:CZ	1:B:257:LEU:HD21	2.43	0.53
1:C:275:GLN:O	1:C:308:ARG:NH2	2.40	0.53
1:A:207:THR:CG2	1:A:249:ILE:HD11	2.38	0.53
1:A:309:LYS:NZ	1:A:368:TYR:OH	2.41	0.53
1:A:382:MSE:HE2	1:A:388:MSE:CE	2.34	0.53
1:C:281:MSE:HE3	1:C:308:ARG:NH1	2.24	0.53
1:A:129:VAL:HG12	1:A:130:LYS:N	2.24	0.53
1:C:174:TYR:C	1:C:174:TYR:CD2	2.83	0.52
1:D:159:MSE:HE2	1:D:267:GLY:C	2.30	0.52
1:C:289:GLY:O	1:C:292:PRO:HD2	2.08	0.52
1:D:322:ILE:HD11	1:D:342:ILE:CG2	2.40	0.52
1:A:238:ALA:HB1	4:C:485:HOH:O	2.09	0.52
1:B:334:GLU:O	1:B:334:GLU:HG2	2.10	0.52
1:A:171:ILE:HG21	1:A:249:ILE:HD12	1.92	0.52
1:A:284:ILE:HB	1:A:382:MSE:HB2	1.92	0.52
1:B:298:LEU:HD13	1:B:302:ARG:HG3	1.92	0.52
1:D:227:VAL:HG11	1:D:254:ILE:HG13	1.92	0.52
1:A:354:THR:CG2	1:B:363:VAL:HA	2.39	0.52
1:B:173:LYS:HG2	1:B:204:GLU:O	2.10	0.52
1:C:141:ASN:HB2	1:C:184:GLN:OE1	2.10	0.51
1:C:281:MSE:HG3	1:C:310:VAL:HG22	1.92	0.51
1:D:175:ASN:C	1:D:175:ASN:HD22	2.13	0.51
1:C:174:TYR:CE1	1:C:253:TYR:HB2	2.44	0.51
1:A:333:ARG:HD2	1:B:373[B]:ASP:HB2	1.93	0.51
1:B:242:LYS:HG2	1:B:245:ILE:CD1	2.28	0.51
1:D:263:VAL:HG12	4:D:426:HOH:O	2.10	0.51
1:D:291:ALA:HB3	1:D:292:PRO:CD	2.39	0.51
1:C:399:LEU:O	1:C:399:LEU:HD12	2.10	0.51
1:A:277:THR:HG22	4:A:430:HOH:O	2.11	0.51
1:A:240:LYS:HE3	4:C:485:HOH:O	2.09	0.51
1:A:361:HIS:HB2	1:A:395:MSE:HE2	1.92	0.50
1:D:291:ALA:N	1:D:292:PRO:HD2	2.26	0.50
1:A:250:SER:HB3	3:A:1:FAD:O1P	2.12	0.50
1:D:275:GLN:O	1:D:308:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:GLU:CD	1:D:376:GLU:H	2.16	0.50
1:A:216:TYR:CE1	1:A:303:THR:HG23	2.46	0.50
1:A:229:ILE:HG23	1:A:229:ILE:O	2.12	0.50
1:B:142:VAL:HG13	1:B:323:PHE:CG	2.47	0.50
1:C:227:VAL:HG21	1:C:254:ILE:HG21	1.93	0.50
1:A:176:ILE:HD12	1:A:256:SER:HB3	1.94	0.49
1:B:344:LEU:HD12	1:B:353:TRP:CG	2.46	0.49
1:D:183:ILE:HG22	1:D:187:PHE:HB2	1.94	0.49
1:B:313:TRP:HB3	1:B:360:ILE:HD11	1.94	0.49
1:C:364:ILE:HG22	1:C:369:LEU:HG	1.94	0.49
1:D:147:LYS:HD2	1:D:255:PHE:CE2	2.48	0.49
1:B:160:ASN:HA	4:B:418:HOH:O	2.11	0.49
1:B:365:TYR:HA	1:B:369:LEU:HB2	1.94	0.49
1:D:132:TRP:CH2	1:D:159:MSE:HE3	2.48	0.49
1:D:272:PHE:CD2	1:D:409:ASP:HB2	2.48	0.49
1:B:382:MSE:HE1	1:B:392:VAL:CG2	2.32	0.48
1:B:289:GLY:O	1:B:292:PRO:HD2	2.14	0.48
1:A:159:MSE:HE1	1:A:265:MSE:HE3	1.94	0.48
1:D:185[B]:ASP:N	1:D:185[B]:ASP:OD1	2.46	0.48
1:A:365:TYR:HA	1:A:369:LEU:HB2	1.95	0.48
1:D:283:TYR:HD2	1:D:293:LEU:HD22	1.78	0.48
1:B:159:MSE:SE	1:B:213:MSE:CE	3.12	0.48
1:B:174:TYR:C	1:B:174:TYR:CD2	2.87	0.48
1:D:284:ILE:HB	1:D:382:MSE:HB2	1.95	0.48
1:B:282:LEU:CD1	1:B:313:TRP:CD1	2.96	0.48
1:A:176:ILE:HG12	1:A:177[B]:ARG:N	2.29	0.47
1:B:283:TYR:CD2	1:B:381:TYR:HB2	2.49	0.47
1:A:176:ILE:HG12	1:A:177[A]:ARG:N	2.29	0.47
1:B:144:THR:HA	1:B:187:PHE:HB3	1.96	0.47
1:C:298:LEU:HD23	1:C:331:ILE:HD11	1.96	0.47
1:A:316:ALA:O	1:A:344:LEU:HA	2.14	0.47
1:A:350:GLU:HB3	1:D:350:GLU:HA	1.95	0.47
1:A:365:TYR:HB2	1:A:395:MSE:SE	2.64	0.47
1:C:170:LYS:HB2	1:C:264:MSE:HB2	1.96	0.47
1:A:159:MSE:CE	1:A:265:MSE:HE3	2.45	0.47
1:B:396:LEU:HD22	1:B:401:VAL:HG21	1.96	0.47
1:A:284:ILE:CG2	1:A:382:MSE:HE3	2.44	0.47
1:C:169:ILE:HD13	1:C:265:MSE:HG3	1.97	0.47
1:C:213:MSE:HG3	1:C:223:ILE:HG23	1.97	0.47
1:D:251:SER:OG	3:D:4:FAD:O2P	2.29	0.47
1:B:130:LYS:HB2	1:B:130:LYS:HE3	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ILE:O	1:B:405:MSE:HG3	2.14	0.47
1:D:147:LYS:HD2	1:D:255:PHE:CG	2.50	0.47
1:D:174:TYR:CE1	1:D:253:TYR:HB2	2.50	0.47
1:A:343:ALA:HB1	1:A:363:VAL:HG21	1.97	0.46
1:D:207:THR:HG21	1:D:209:ARG:NH2	2.30	0.46
1:C:166:TYR:CD1	3:C:413:FAD:HM72	2.50	0.46
1:D:229:ILE:HG23	1:D:231:THR:HG23	1.96	0.46
1:B:384:GLY:HA3	1:B:388:MSE:HE2	1.96	0.46
1:C:329:ARG:HD2	1:D:371:ASP:OD2	2.14	0.46
1:A:379:GLU:HG2	1:A:407:PHE:HE2	1.80	0.46
1:C:322:ILE:HD11	1:C:344:LEU:HD11	1.98	0.46
1:C:290:MSE:HE2	1:C:324:TYR:CB	2.46	0.46
1:A:141:ASN:OD1	1:A:183:ILE:HD13	2.16	0.46
1:B:168:GLN:O	1:B:265:MSE:HG3	2.15	0.46
1:B:365:TYR:CE1	1:B:399:LEU:HD11	2.49	0.46
1:C:333:ARG:HD2	1:D:373:ASP:OD2	2.16	0.46
1:D:322:ILE:CD1	1:D:342:ILE:HG21	2.46	0.46
1:A:291:ALA:CB	1:A:292:PRO:CD	2.91	0.46
1:C:131:GLU:HG3	1:C:266:SER:HB3	1.97	0.46
1:C:277:THR:HG22	1:C:278:ASP:H	1.72	0.46
1:B:361:HIS:HB3	1:B:392:VAL:HG22	1.97	0.45
1:D:182:ASP:HB2	1:D:258:LYS:NZ	2.31	0.45
1:B:280:GLU:HG3	1:B:309:LYS:HB3	1.97	0.45
1:C:382:MSE:HG2	1:C:408:PHE:CD2	2.51	0.45
1:A:129:VAL:CG1	1:A:130:LYS:H	2.29	0.45
1:A:242:LYS:HE3	1:A:245:ILE:HD11	1.98	0.45
1:D:322:ILE:HD11	1:D:342:ILE:HG23	1.98	0.45
1:A:310:VAL:O	1:A:338:PHE:HA	2.15	0.45
1:B:171:ILE:HG12	1:B:250:SER:HA	1.98	0.45
1:D:190:ASP:HB2	4:D:416:HOH:O	2.15	0.45
1:A:290:MSE:HG2	1:A:314:TYR:CE1	2.51	0.45
1:A:283:TYR:HD2	1:A:293:LEU:HG	1.81	0.45
1:A:293:LEU:N	1:A:293:LEU:CD1	2.79	0.45
1:B:365:TYR:OH	1:D:185[B]:ASP:OD2	2.29	0.45
1:C:194:MSE:O	1:C:195:ASP:HB3	2.16	0.45
1:A:145:PHE:O	1:A:228:ARG:HA	2.16	0.45
1:B:399:LEU:HB3	1:B:401:VAL:HG23	1.98	0.45
1:D:171:ILE:HB	1:D:207:THR:HG22	1.98	0.45
1:B:319:LYS:O	1:B:322:ILE:HG12	2.17	0.45
1:C:361:HIS:HB3	1:C:392:VAL:HG22	1.99	0.45
1:C:144:THR:HA	1:C:187:PHE:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ARG:HD2	1:D:371:ASP:CG	2.37	0.44
1:D:137:LEU:O	1:D:259:PRO:HB3	2.18	0.44
1:B:132:TRP:CZ3	1:B:159:MSE:HE2	2.53	0.44
1:B:253:TYR:CE2	1:B:257:LEU:HD21	2.52	0.44
1:D:204:GLU:H	1:D:204:GLU:HG2	1.62	0.44
1:D:348:GLN:O	1:D:351:ASP:HB2	2.17	0.44
1:A:382:MSE:HE1	1:A:392:VAL:CG2	2.42	0.44
1:C:136:VAL:O	1:C:259:PRO:HA	2.18	0.44
1:B:395:MSE:HE2	1:B:396:LEU:HA	2.00	0.44
1:D:214:ALA:HA	1:D:291:ALA:O	2.17	0.44
1:A:234:PHE:HD1	1:A:236[B]:ARG:HD3	1.83	0.44
1:B:294:ARG:HD2	1:B:324:TYR:CD2	2.53	0.44
1:D:320:ASN:HB2	4:D:430:HOH:O	2.17	0.44
1:B:382:MSE:HG2	1:B:406:LEU:HD11	1.98	0.44
1:C:135:GLU:O	1:C:151:VAL:HA	2.17	0.44
1:A:171:ILE:HG12	1:A:250:SER:HA	2.00	0.44
1:C:137:LEU:HD22	1:C:137:LEU:HA	1.86	0.44
1:A:218:ALA:HB2	1:A:303:THR:HG21	2.00	0.43
1:B:202:LYS:HB3	1:B:202:LYS:HE2	1.41	0.43
1:B:242:LYS:NZ	1:B:245:ILE:CD1	2.81	0.43
1:D:322:ILE:CD1	1:D:344:LEU:HD21	2.49	0.43
1:A:224:THR:O	1:A:225:LEU:HD23	2.18	0.43
1:A:301:PHE:CZ	1:A:338:PHE:HB2	2.53	0.43
1:D:171:ILE:HA	1:D:172:PRO:HD2	1.87	0.43
1:D:350:GLU:H	1:D:350:GLU:HG3	1.39	0.43
1:D:324:TYR:O	1:D:327:ASP:HB2	2.18	0.43
1:D:166:TYR:HA	1:D:212:SER:HA	2.01	0.43
1:A:284:ILE:HG21	1:A:382:MSE:HE3	1.99	0.43
1:B:344:LEU:HD12	1:B:353:TRP:CD2	2.54	0.43
1:D:360:ILE:HG22	1:D:361:HIS:N	2.33	0.43
1:A:174:TYR:CD2	1:A:174:TYR:C	2.92	0.43
1:C:162[A]:LYS:HE2	1:C:273:HIS:ND1	2.34	0.43
1:A:147:LYS:HD2	1:A:255:PHE:CD2	2.53	0.43
1:C:318:SER:HA	1:C:344:LEU:HG	2.00	0.43
1:A:281:MSE:HE2	1:A:308:ARG:CZ	2.48	0.42
1:B:369:LEU:HD23	1:B:369:LEU:HA	1.82	0.42
1:D:216:TYR:CD2	1:D:216:TYR:N	2.88	0.42
1:D:170:LYS:HB2	1:D:264:MSE:HB2	2.01	0.42
1:A:404:ASN:C	1:A:404:ASN:HD22	2.22	0.42
1:D:382:MSE:HG2	1:D:408:PHE:HD2	1.83	0.42
1:A:216:TYR:CZ	1:A:218:ALA:HB3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLN:HG3	1:B:407:PHE:CZ	2.54	0.42
1:C:144:THR:HG21	1:C:190:ASP:OD2	2.19	0.42
1:D:300:LEU:O	1:D:306:THR:HG22	2.19	0.42
1:A:293:LEU:N	1:A:293:LEU:HD13	2.34	0.42
1:C:254:ILE:H	1:C:254:ILE:HG12	1.66	0.42
1:B:215:ASN:HD22	1:B:219:GLU:HB2	1.84	0.42
1:B:230:ALA:HB3	1:B:248:GLY:HA3	2.02	0.42
1:C:142:VAL:HG12	1:C:146:ILE:HG13	2.02	0.42
1:C:146:ILE:HD13	1:C:226:ASN:HB3	2.00	0.42
1:C:188:ARG:HD2	4:C:449:HOH:O	2.19	0.42
1:C:228:ARG:HH21	1:C:317:ARG:HH22	1.67	0.42
1:D:322:ILE:HD13	1:D:342:ILE:HD13	2.02	0.42
1:B:183:ILE:HD12	1:B:191:TRP:CE2	2.54	0.42
1:C:229:ILE:HB	1:C:255:PHE:CZ	2.55	0.42
1:D:363:VAL:HG13	1:D:367:ASN:ND2	2.35	0.42
1:A:236[B]:ARG:HD2	1:A:236[B]:ARG:HA	1.53	0.42
1:B:380:TYR:HE1	1:B:401:VAL:HG11	1.83	0.42
1:A:238:ALA:HB2	1:C:242[B]:LYS:HZ3	1.85	0.42
1:B:169:ILE:HG22	1:B:171:ILE:HD12	2.02	0.42
1:D:163:SER:HB3	1:D:217:PRO:HD3	2.01	0.42
1:D:329:ARG:CD	1:D:332:GLU:OE2	2.64	0.42
1:A:238:ALA:HB2	1:C:242[B]:LYS:HZ1	1.85	0.41
1:B:229:ILE:HG23	1:B:229:ILE:O	2.20	0.41
1:B:391:ALA:HA	1:D:197:TRP:CD1	2.55	0.41
1:D:282:LEU:HD23	1:D:282:LEU:C	2.41	0.41
1:A:382:MSE:CE	1:A:388:MSE:HE3	2.43	0.41
1:C:329:ARG:HD3	1:C:332:GLU:OE2	2.20	0.41
1:A:129:VAL:HG13	1:A:130:LYS:H	1.86	0.41
1:C:211:TYR:CE1	1:C:227:VAL:HG13	2.55	0.41
1:B:147:LYS:HD2	1:B:255:PHE:CD2	2.55	0.41
1:C:242[B]:LYS:HB3	1:C:245:ILE:HD12	2.03	0.41
1:D:169:ILE:HG13	1:D:265:MSE:HG3	2.02	0.41
1:B:168:GLN:HA	1:B:209:ARG:O	2.20	0.41
1:B:182:ASP:C	1:B:183:ILE:HG12	2.40	0.41
1:B:290:MSE:HE2	1:B:314:TYR:CD1	2.56	0.41
1:B:242:LYS:HZ1	1:B:245:ILE:HD13	1.86	0.41
1:A:369:LEU:O	1:A:370:LYS:C	2.59	0.41
1:C:152:LYS:HE3	1:C:221:ASN:OD1	2.21	0.41
1:C:173:LYS:HB2	1:C:203:ASN:O	2.21	0.41
1:A:177[A]:ARG:HA	1:A:200:THR:HG22	2.01	0.40
1:B:130:LYS:HE2	1:B:132:TRP:HZ2	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:THR:HG23	1:C:220:GLY:HA3	2.04	0.40
1:C:162[B]:LYS:HB2	1:C:273:HIS:NE2	2.37	0.40
1:C:284:ILE:CB	1:C:382:MSE:HE3	2.51	0.40
1:C:264:MSE:HE1	4:C:446:HOH:O	2.20	0.40
1:C:277:THR:HG23	1:C:278:ASP:H	1.83	0.40
1:B:147:LYS:HD2	1:B:255:PHE:CZ	2.56	0.40
1:D:263:VAL:HA	4:D:426:HOH:O	2.20	0.40
1:B:291:ALA:N	1:B:292:PRO:HD2	2.37	0.40
1:D:329:ARG:O	1:D:333:ARG:HB2	2.21	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:C:185[A]:ASP:OD2	1:D:365:TYR:OH[10_655]	1.90	0.30

## 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	287/290 (99%)	278 (97%)	9 (3%)	0	100	100
1	B	285/290 (98%)	274 (96%)	11 (4%)	0	100	100
1	C	293/290 (101%)	283 (97%)	10 (3%)	0	100	100
1	D	284/290 (98%)	277 (98%)	7 (2%)	0	100	100
All	All	1149/1160 (99%)	1112 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/236 (105%)	229 (93%)	18 (7%)	11	29
1	B	246/236 (104%)	223 (91%)	23 (9%)	7	20
1	C	252/236 (107%)	231 (92%)	21 (8%)	9	24
1	D	245/236 (104%)	222 (91%)	23 (9%)	7	20
All	All	990/944 (105%)	905 (91%)	85 (9%)	8	23

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	142	VAL
1	A	158	THR
1	A	172	PRO
1	A	176	ILE
1	A	209	ARG
1	A	216	TYR
1	A	258	LYS
1	A	263	VAL
1	A	277	THR
1	A	290	MSE
1	A	293	LEU
1	A	317	ARG
1	A	321	GLU
1	A	354	THR
1	A	360	ILE
1	A	395	MSE
1	A	404	ASN
1	B	126	VAL
1	B	127	PHE
1	B	131	GLU
1	B	142	VAL
1	B	151	VAL
1	B	183	ILE

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Mol	Chain	Res	Type
1	B	188	ARG
1	B	192	ASP
1	B	204	GLU
1	B	209	ARG
1	B	212	SER
1	B	213	MSE
1	B	216	TYR
1	B	219	GLU
1	B	242	LYS
1	B	282	LEU
1	B	293	LEU
1	B	298	LEU
1	B	339	LYS
1	B	360	ILE
1	B	382	MSE
1	B	388	MSE
1	B	395	MSE
1	C	137	LEU
1	C	142	VAL
1	C	144	THR
1	C	146	ILE
1	C	152	LYS
1	C	185[A]	ASP
1	C	185[B]	ASP
1	C	186	ARG
1	C	204	GLU
1	C	209	ARG
1	C	216	TYR
1	C	240	LYS
1	C	254	ILE
1	C	263	VAL
1	C	281	MSE
1	C	293	LEU
1	C	344	LEU
1	C	354	THR
1	C	360	ILE
1	C	369	LEU
1	C	401	VAL
1	D	142	VAL
1	D	155	GLU
1	D	175	ASN
1	D	177	ARG

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Mol	Chain	Res	Type
1	D	183	ILE
1	D	190	ASP
1	D	204	GLU
1	D	205	GLU
1	D	209	ARG
1	D	216	TYR
1	D	228	ARG
1	D	229	ILE
1	D	251	SER
1	D	254	ILE
1	D	311	SER
1	D	317	ARG
1	D	350	GLU
1	D	354	THR
1	D	360	ILE
1	D	373	ASP
1	D	399	LEU
1	D	401	VAL
1	D	404	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	ASN
1	A	404	ASN
1	B	226	ASN
1	D	175	ASN
1	D	348	GLN
1	D	367	ASN
1	D	404	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 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	SO4	A	10	-	4,4,4	0.25	0	6,6,6	0.37	0
2	SO4	D	5	-	4,4,4	0.29	0	6,6,6	0.13	0
2	SO4	B	11	-	4,4,4	0.30	0	6,6,6	0.10	0
2	SO4	C	4	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	A	2	-	4,4,4	0.19	0	6,6,6	0.21	0
3	FAD	B	2	-	54,58,58	1.16	5 (9%)	71,89,89	1.37	8 (11%)
3	FAD	C	413	-	54,58,58	1.27	5 (9%)	71,89,89	1.39	8 (11%)
3	FAD	A	1	-	54,58,58	1.22	5 (9%)	71,89,89	1.45	10 (14%)
2	SO4	A	8	-	4,4,4	0.23	0	6,6,6	0.14	0
3	FAD	D	4	-	54,58,58	1.20	4 (7%)	71,89,89	1.45	10 (14%)
2	SO4	C	7	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SO4	C	9	-	4,4,4	0.21	0	6,6,6	0.30	0
2	SO4	D	6	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	C	3	-	4,4,4	0.23	0	6,6,6	0.44	0
2	SO4	B	1	-	4,4,4	0.28	0	6,6,6	0.22	0

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	FAD	B	2	-	-	4/30/50/50	0/6/6/6
3	FAD	A	1	-	-	2/30/50/50	0/6/6/6
3	FAD	D	4	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	C	413	-	-	1/30/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	FAD	C2A-N3A	4.59	1.39	1.32
3	A	1	FAD	C2A-N3A	4.59	1.39	1.32
3	C	413	FAD	C2A-N3A	4.38	1.38	1.32
3	B	2	FAD	C2A-N3A	4.30	1.38	1.32
3	C	413	FAD	C4X-N5	3.60	1.38	1.30
3	D	4	FAD	C4X-N5	3.45	1.38	1.30
3	A	1	FAD	C4X-N5	3.45	1.38	1.30
3	B	2	FAD	C4X-N5	3.44	1.38	1.30
3	C	413	FAD	PA-O3P	3.26	1.63	1.59
3	A	1	FAD	C2A-N1A	2.92	1.39	1.33
3	C	413	FAD	C2A-N1A	2.89	1.39	1.33
3	D	4	FAD	C2A-N1A	2.84	1.39	1.33
3	B	2	FAD	C2A-N1A	2.81	1.38	1.33
3	A	1	FAD	C10-N1	2.51	1.38	1.33
3	A	1	FAD	PA-O3P	2.42	1.62	1.59
3	B	2	FAD	C10-N1	2.23	1.37	1.33
3	C	413	FAD	C10-N1	2.17	1.37	1.33
3	B	2	FAD	PA-O3P	2.12	1.61	1.59
3	D	4	FAD	C10-N1	2.10	1.37	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	FAD	N3A-C2A-N1A	-6.75	119.51	128.67
3	C	413	FAD	N3A-C2A-N1A	-6.56	119.76	128.67
3	A	1	FAD	N3A-C2A-N1A	-6.54	119.79	128.67
3	B	2	FAD	N3A-C2A-N1A	-6.45	119.91	128.67
3	D	4	FAD	C4X-C10-N10	3.37	121.30	116.48
3	C	413	FAD	C4X-C10-N10	3.33	121.25	116.48
3	A	1	FAD	O4-C4-C4X	-3.20	118.08	126.53
3	B	2	FAD	C4X-C10-N10	3.11	120.94	116.48
3	C	413	FAD	C10-C4X-N5	-2.94	118.81	124.81
3	A	1	FAD	O2A-PA-O3P	2.93	115.19	107.27
3	D	4	FAD	C4-N3-C2	-2.81	120.65	125.64
3	A	1	FAD	C4X-C10-N10	2.78	120.45	116.48
3	C	413	FAD	C4-N3-C2	-2.77	120.72	125.64
3	D	4	FAD	C10-C4X-N5	-2.67	119.36	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	FAD	O4B-C1B-N9A	2.57	112.16	108.75
3	C	413	FAD	O2-C2-N1	-2.57	117.54	121.80
3	B	2	FAD	O4-C4-C4X	-2.56	119.77	126.53
3	A	1	FAD	C4-N3-C2	-2.56	121.09	125.64
3	B	2	FAD	O2A-PA-O3P	2.45	113.89	107.27
3	A	1	FAD	C4'-C3'-C2'	-2.40	109.58	113.57
3	C	413	FAD	C1B-N9A-C4A	-2.38	122.45	126.64
3	B	2	FAD	C4-N3-C2	-2.36	121.46	125.64
3	C	413	FAD	O2A-PA-O3P	2.34	113.61	107.27
3	B	2	FAD	C10-C4X-N5	-2.33	120.04	124.81
3	D	4	FAD	C5X-C9A-N10	2.32	120.07	117.97
3	D	4	FAD	O2-C2-N1	-2.31	117.97	121.80
3	D	4	FAD	O2A-PA-O3P	2.31	113.51	107.27
3	A	1	FAD	O2-C2-N1	-2.21	118.14	121.80
3	A	1	FAD	C4-C4X-C10	2.18	120.68	116.93
3	A	1	FAD	C5X-C9A-N10	2.17	119.93	117.97
3	B	2	FAD	C4X-C4-N3	2.15	118.73	113.25
3	D	4	FAD	O4-C4-C4X	-2.09	121.01	126.53
3	B	2	FAD	C9A-C5X-N5	-2.09	120.24	122.45
3	C	413	FAD	O4-C4-C4X	-2.03	121.18	126.53
3	D	4	FAD	C4-C4X-C10	2.02	120.39	116.93
3	D	4	FAD	C4X-C4-N3	2.01	118.36	113.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

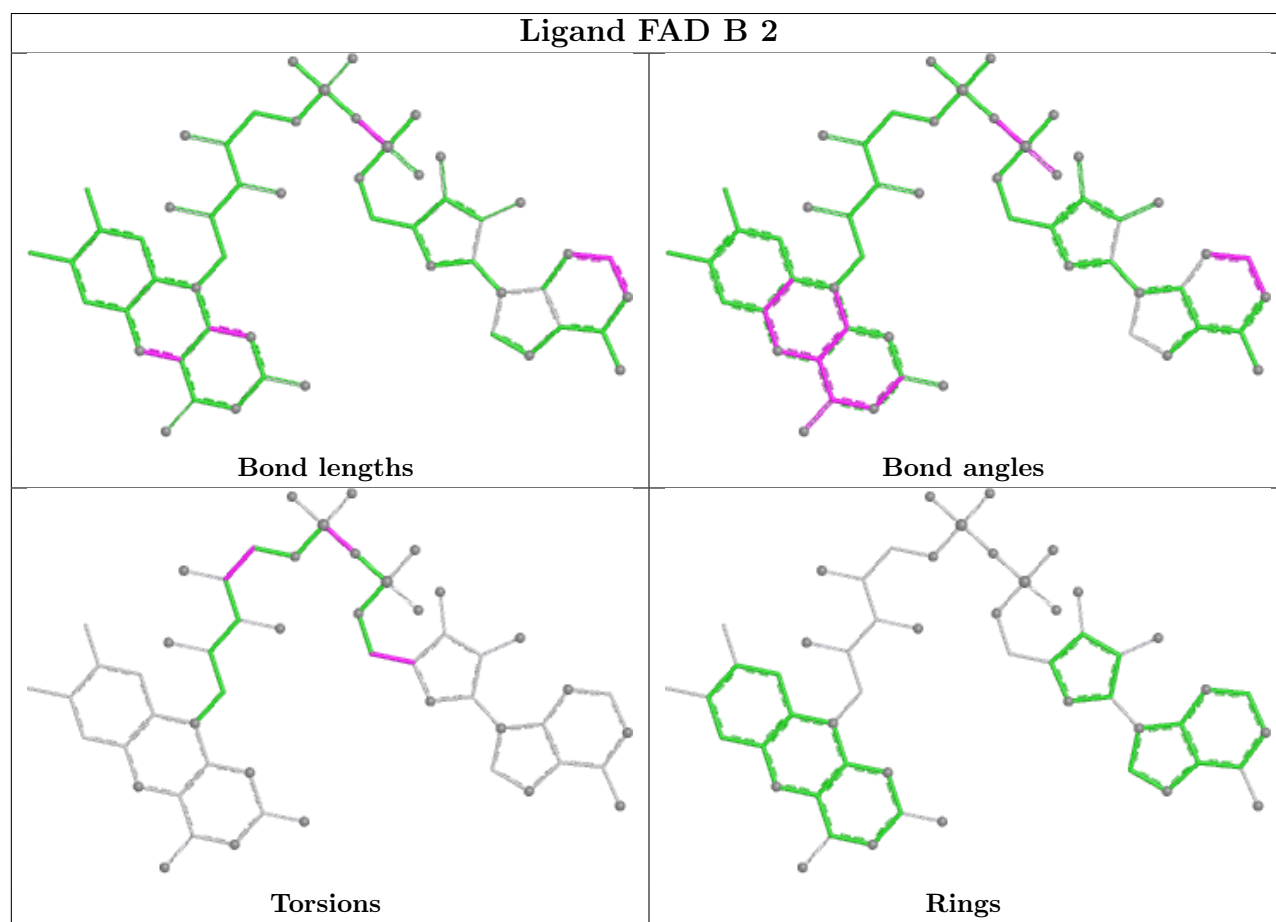
Mol	Chain	Res	Type	Atoms
3	D	4	FAD	C5B-O5B-PA-O1A
3	D	4	FAD	C5B-O5B-PA-O3P
3	B	2	FAD	O4B-C4B-C5B-O5B
3	B	2	FAD	C3B-C4B-C5B-O5B
3	B	2	FAD	C3'-C4'-C5'-O5'
3	A	1	FAD	O2'-C2'-C3'-C4'
3	A	1	FAD	C1'-C2'-C3'-C4'
3	C	413	FAD	PA-O3P-P-O2P
3	B	2	FAD	PA-O3P-P-O2P
3	D	4	FAD	PA-O3P-P-O2P

There are no ring outliers.

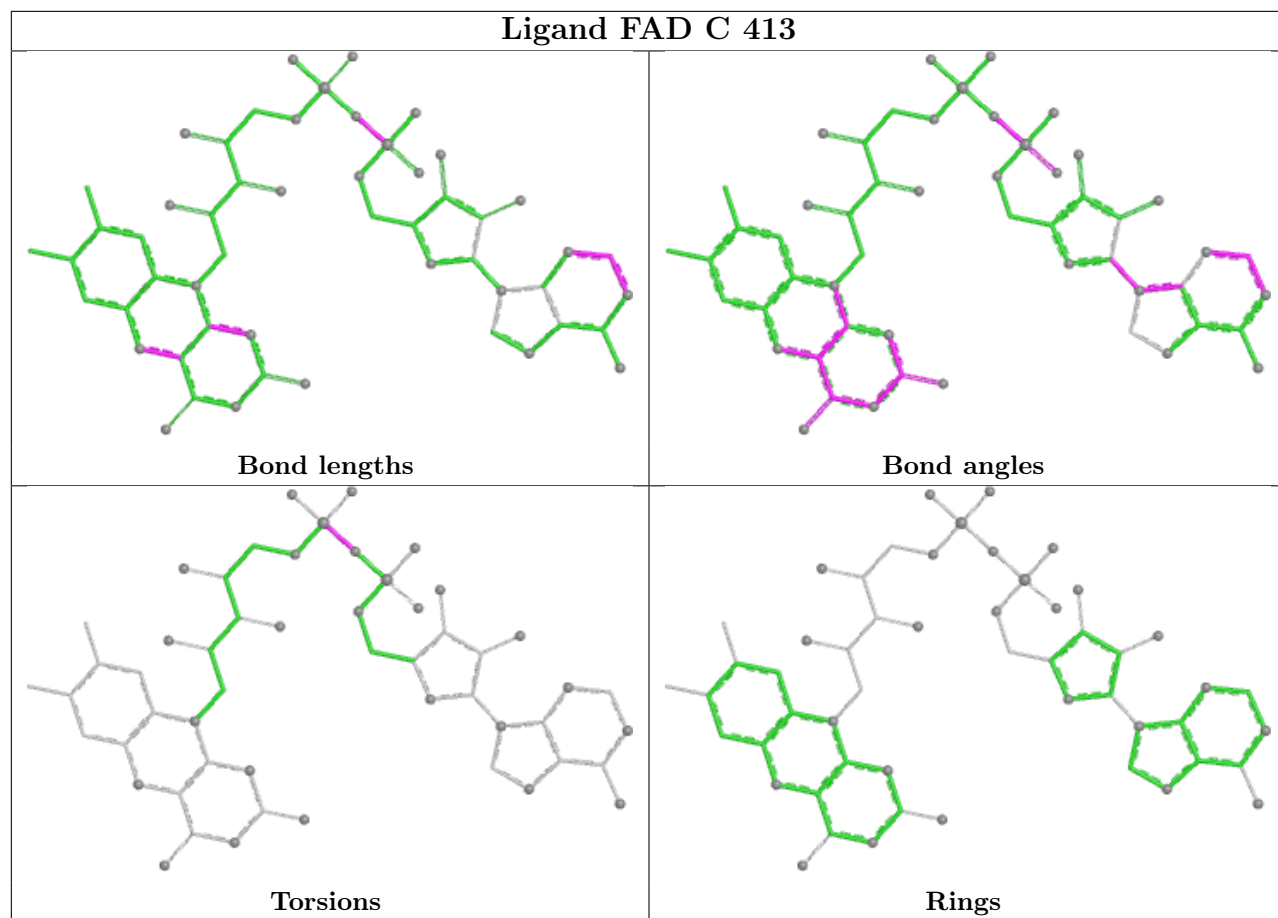
5 monomers are involved in 5 short contacts:

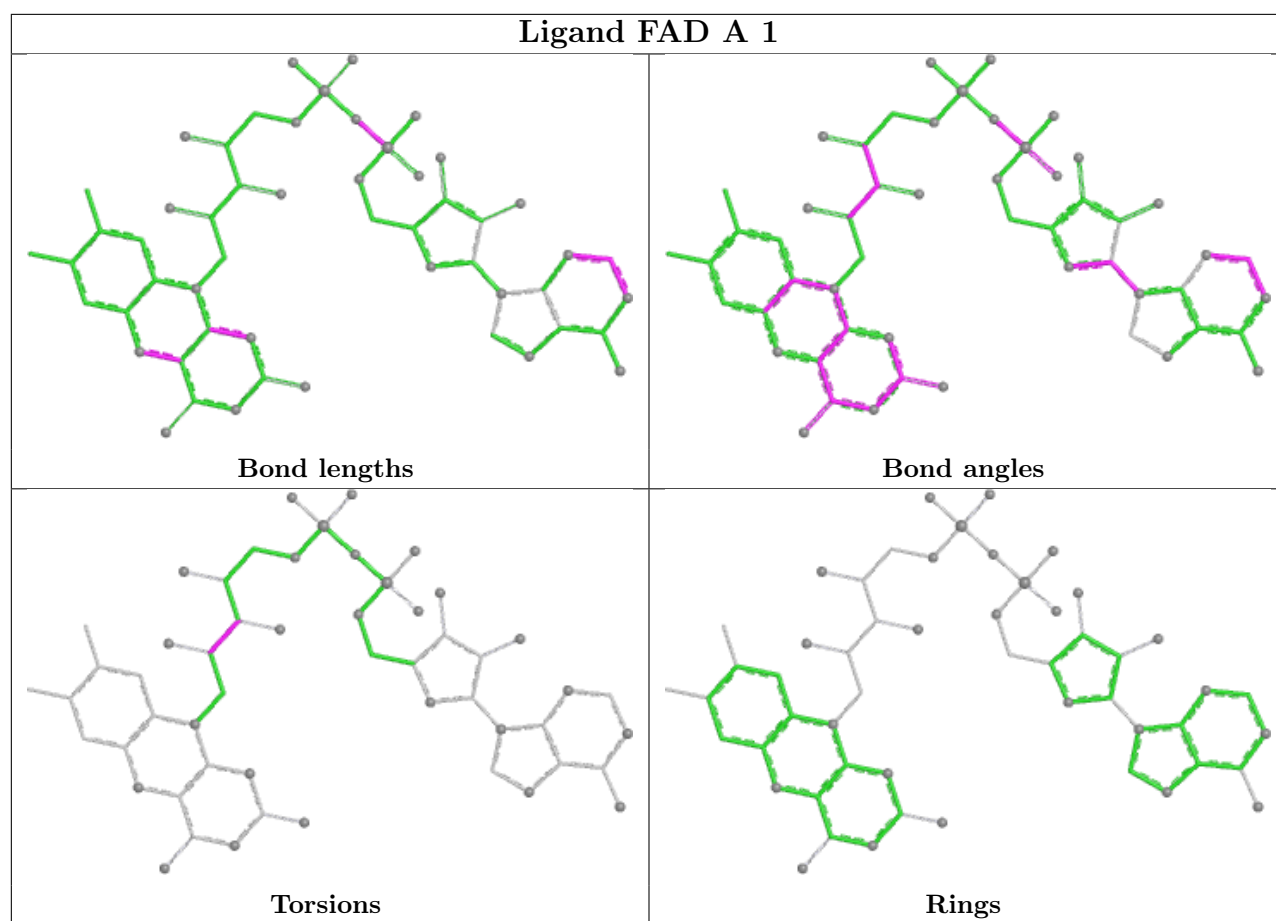
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	11	SO4	1	0
3	C	413	FAD	1	0
3	A	1	FAD	1	0
3	D	4	FAD	1	0
2	C	3	SO4	1	0

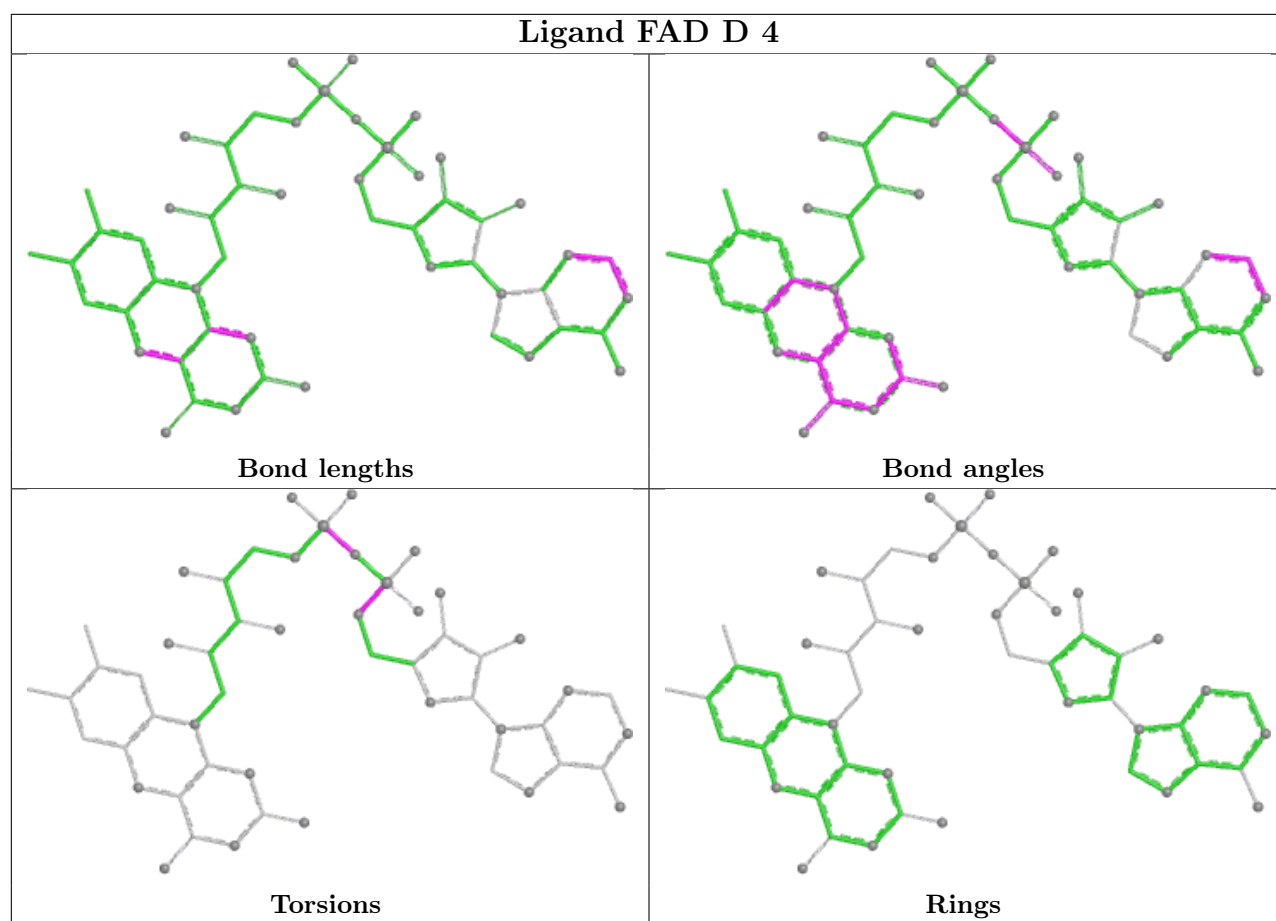
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



## Ligand FAD C 413







## 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	274/290 (94%)	-0.02	9 (3%)	49	47	21, 41, 77, 129	4 (1%)
1	B	275/290 (94%)	0.30	18 (6%)	26	24	22, 49, 87, 110	1 (0%)
1	C	278/290 (95%)	-0.05	8 (2%)	54	50	18, 37, 65, 99	6 (2%)
1	D	273/290 (94%)	0.05	11 (4%)	43	40	20, 45, 77, 105	2 (0%)
All	All	1100/1160 (94%)	0.07	46 (4%)	41	38	18, 43, 79, 129	13 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	VAL	5.5
1	A	130	LYS	5.4
1	B	367	ASN	5.0
1	B	215	ASN	4.1
1	A	129	VAL	4.0
1	A	367	ASN	4.0
1	D	367	ASN	3.8
1	B	127	PHE	3.6
1	D	238	ALA	3.6
1	A	133	GLU	3.4
1	D	373	ASP	3.2
1	D	215[A]	ASN	3.2
1	C	367	ASN	3.2
1	B	346	ASP	3.2
1	B	131	GLU	3.1
1	C	302[A]	ARG	3.1
1	D	138	SER	3.0
1	B	129	VAL	2.9
1	A	334	GLU	2.9
1	D	237	ALA	2.8
1	A	128	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	237	ALA	2.7
1	A	346	ASP	2.7
1	C	242[A]	LYS	2.6
1	C	238	ALA	2.6
1	B	234	PHE	2.5
1	B	130	LYS	2.5
1	D	128	GLY	2.4
1	B	238	ALA	2.3
1	B	258	LYS	2.3
1	D	350	GLU	2.2
1	B	235	ASP	2.2
1	B	317	ARG	2.2
1	B	192	ASP	2.2
1	D	185[A]	ASP	2.2
1	C	319[A]	LYS	2.2
1	B	271	ASP	2.2
1	B	410	ASP	2.2
1	D	276	ASP	2.2
1	C	237	ALA	2.1
1	A	373[A]	ASP	2.1
1	C	271	ASP	2.1
1	B	239	ASN	2.0
1	B	409	ASP	2.0
1	C	177[A]	ARG	2.0
1	D	273	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

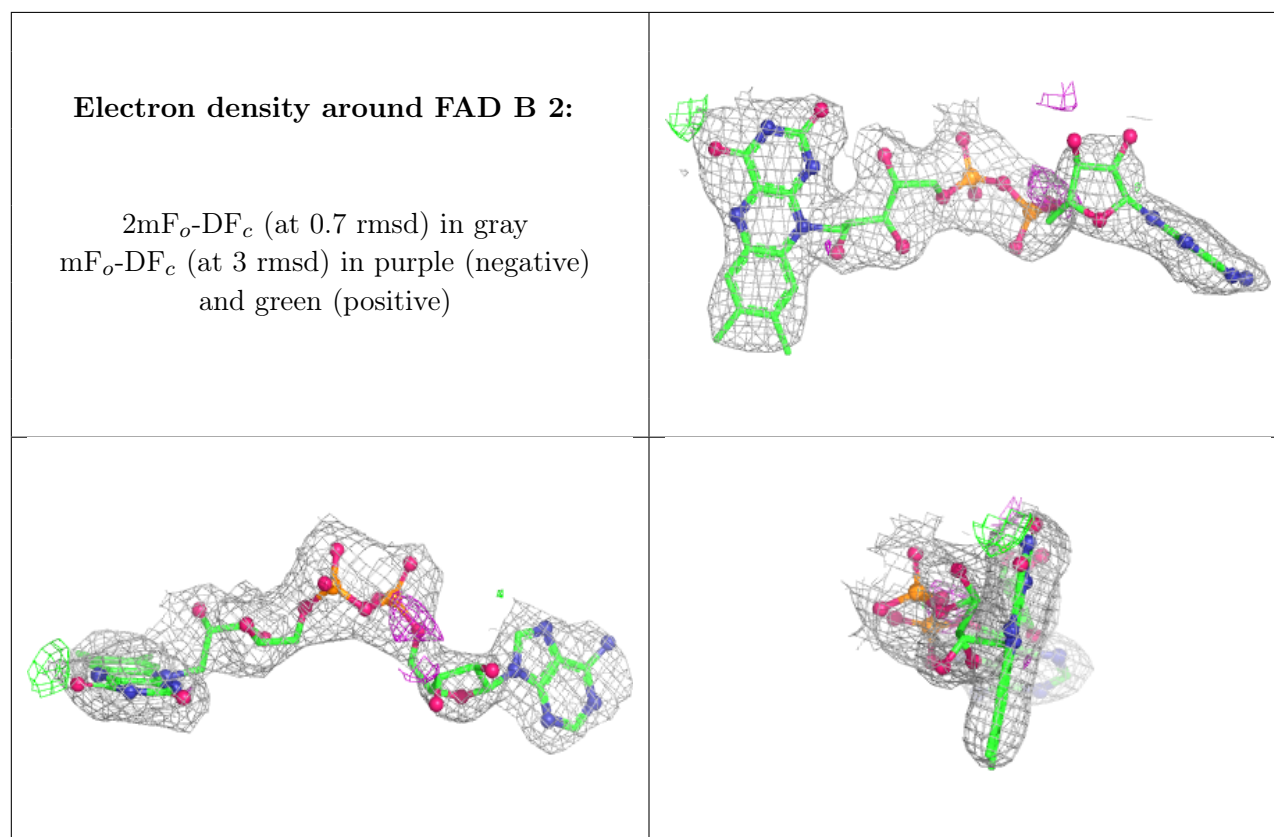
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	SO4	D	6	5/5	0.68	0.20	118,119,120,120	0
2	SO4	C	4	5/5	0.69	0.18	136,136,137,137	0
2	SO4	C	7	5/5	0.75	0.18	117,118,118,118	0
2	SO4	A	8	5/5	0.75	0.16	128,128,128,129	0
2	SO4	A	10	5/5	0.78	0.26	130,130,130,130	0
2	SO4	C	9	5/5	0.81	0.14	102,102,102,102	0
2	SO4	D	5	5/5	0.81	0.14	84,84,85,85	0
2	SO4	B	11	5/5	0.81	0.14	138,138,138,138	0
2	SO4	B	1	5/5	0.84	0.15	80,81,81,83	0
2	SO4	C	3	5/5	0.88	0.12	87,89,89,90	0
2	SO4	A	2	5/5	0.91	0.10	75,76,77,78	0
3	FAD	B	2	53/53	0.93	0.11	48,54,75,75	0
3	FAD	A	1	53/53	0.94	0.10	30,48,85,85	0
3	FAD	C	413	53/53	0.94	0.09	25,37,51,54	0
3	FAD	D	4	53/53	0.94	0.09	33,43,73,74	0

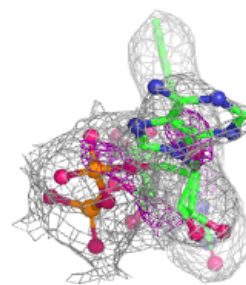
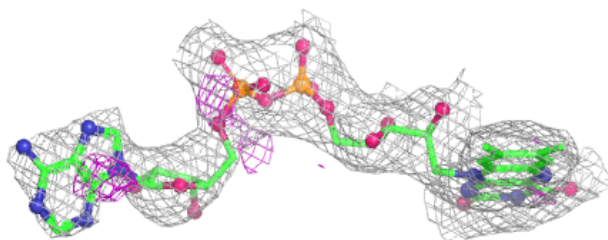
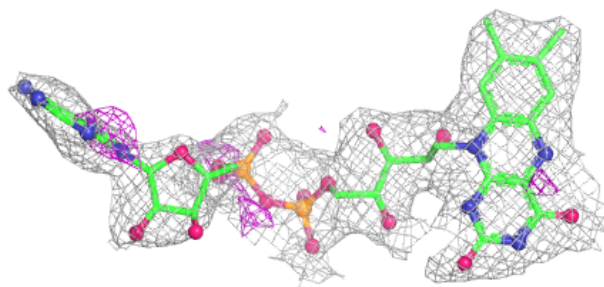
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



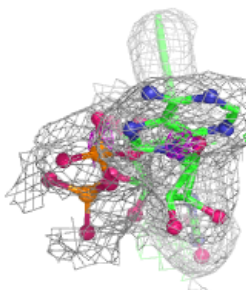
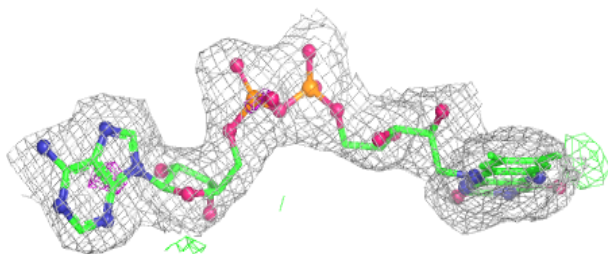
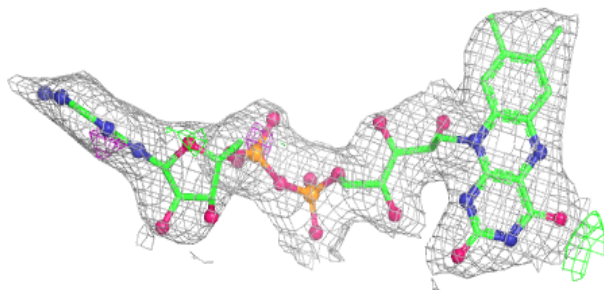


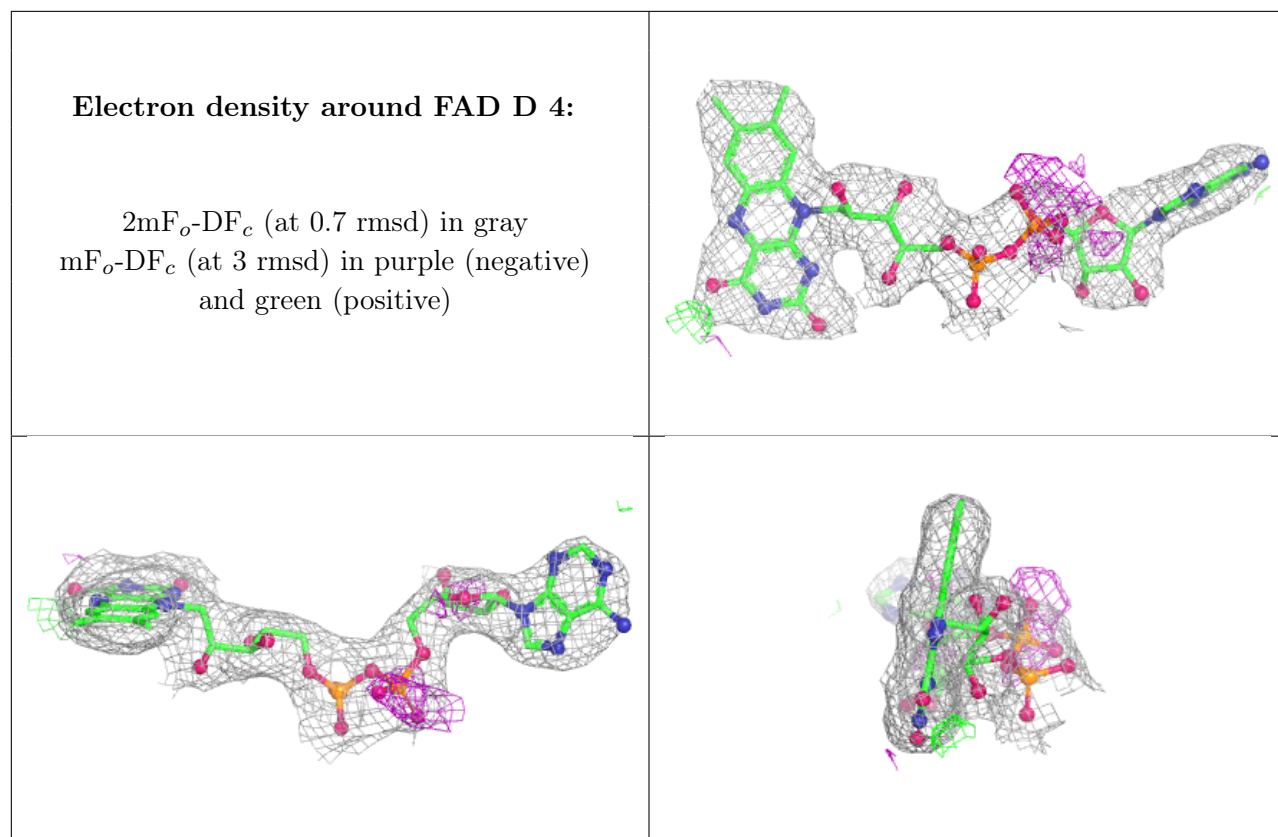
**Electron density around FAD A 1:**

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

**Electron density around FAD C 413:**

$2mF_o-DF_c$  (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.