



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 06:14 PM EDT

PDB ID : 6SEM
Title : Crystal Structure of Ancestral Flavin-containing monooxygenase (FMO) 2
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Deposited on : 2019-07-30
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) 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	:	2.37.1
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)	:	2.37.1

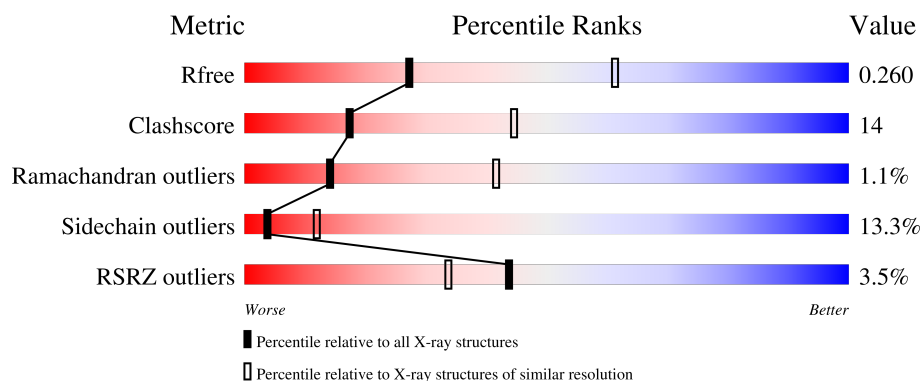
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. 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	535	<div> <div>3%</div> <div>63%</div> <div>29%</div> <div>5%</div> <div>.</div> </div>
1	B	535	<div> <div>5%</div> <div>63%</div> <div>30%</div> <div>5%</div> <div>.</div> </div>
1	C	535	<div> <div>%</div> <div>63%</div> <div>30%</div> <div>.</div> <div>.</div> </div>
1	D	535	<div> <div>4%</div> <div>66%</div> <div>27%</div> <div>.</div> <div>.</div> </div>

2 Entry composition [i](#)

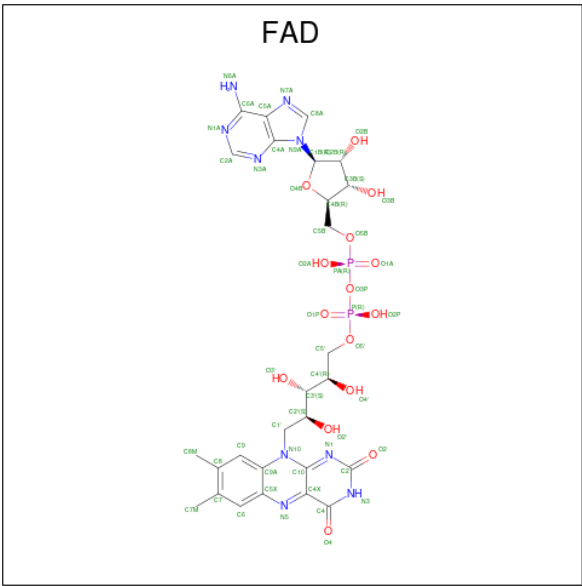
There are 3 unique types of molecules in this entry. The entry contains 16904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ancestral Flavin-containing monooxygenase (FMO) 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	530	Total	C	N	O	S	0	0	0
			4257	2761	706	766	24			
1	A	519	Total	C	N	O	S	0	0	0
			4138	2672	692	750	24			
1	C	520	Total	C	N	O	S	0	0	0
			4128	2662	692	750	24			
1	D	520	Total	C	N	O	S	0	0	0
			4116	2651	691	750	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

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

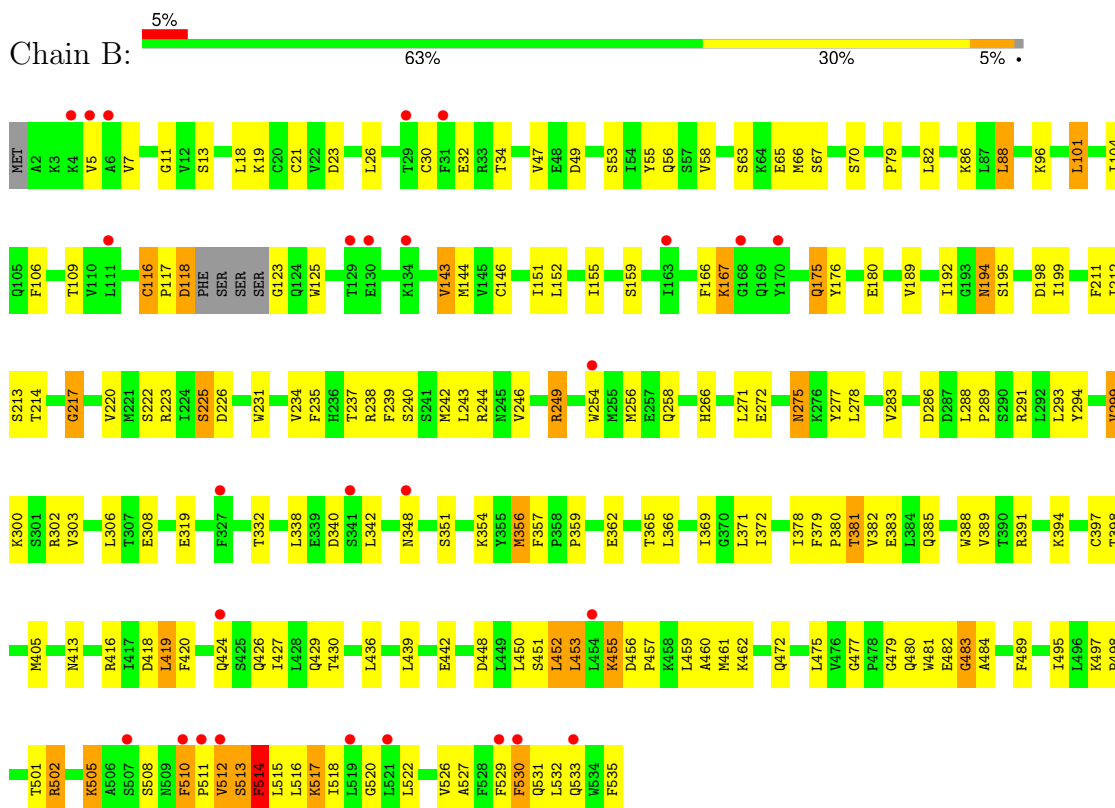
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	16	Total	O	0	0
			16	16		
3	A	10	Total	O	0	0
			10	10		
3	C	15	Total	O	0	0
			15	15		
3	D	12	Total	O	0	0
			12	12		

3 Residue-property plots

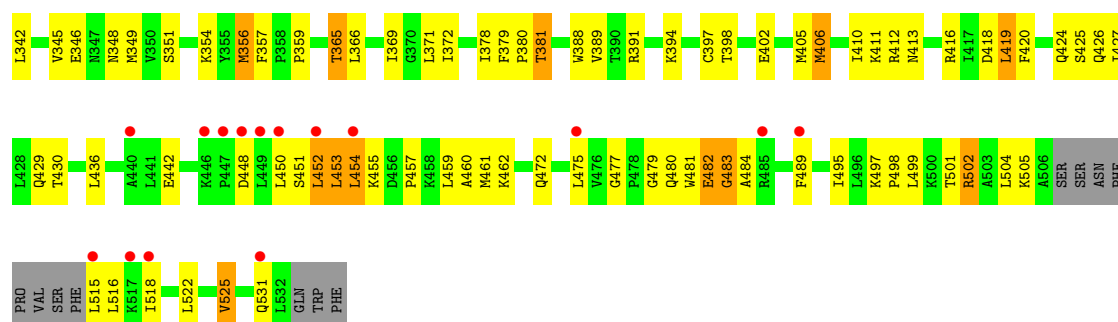
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ancestral Flavin-containing monooxygenase (FMO) 2

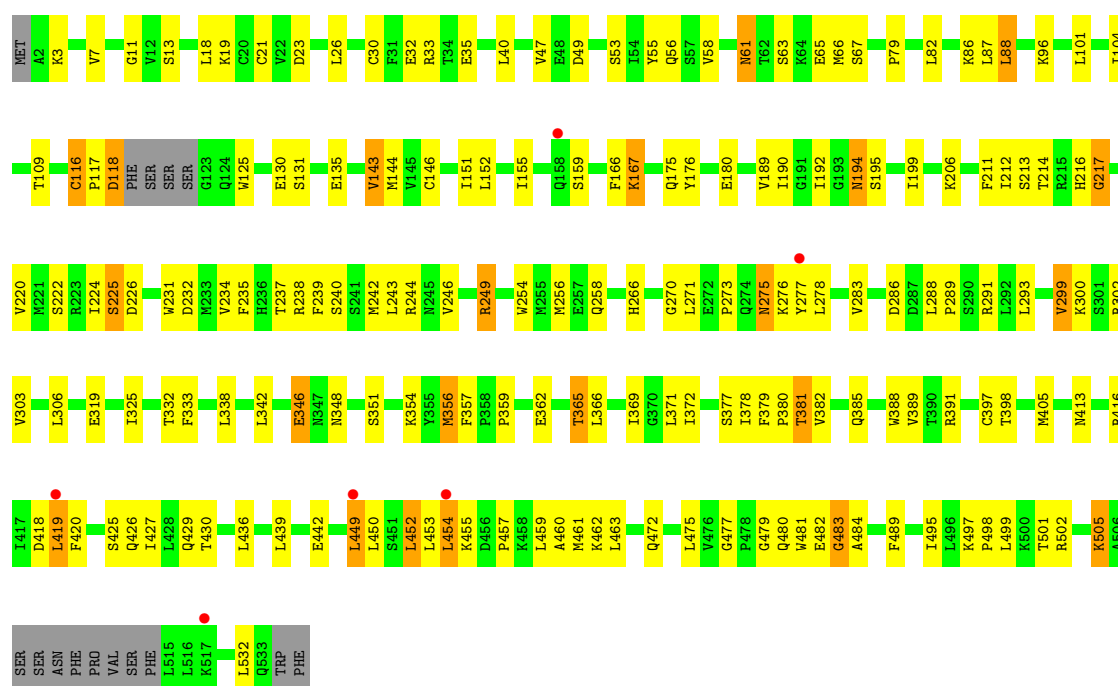


• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 2

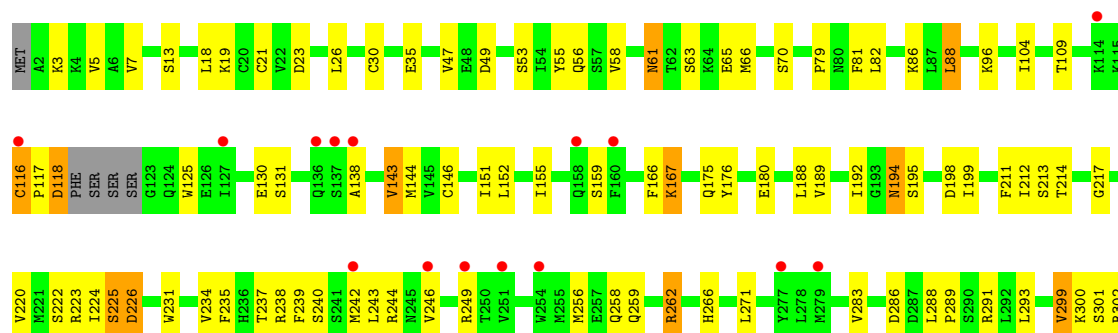


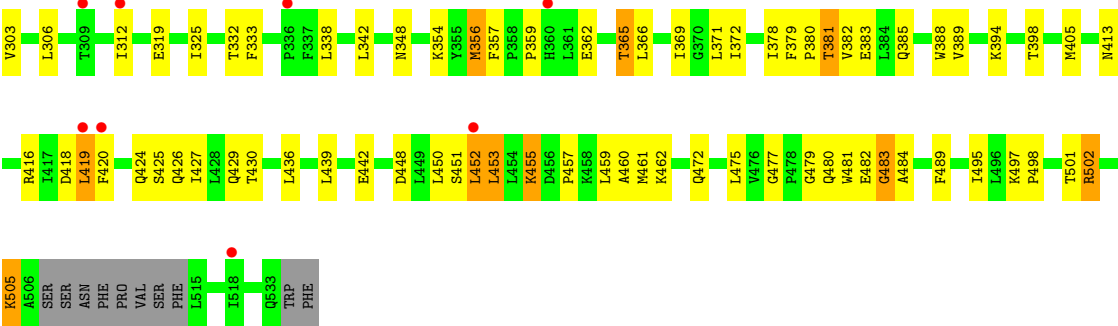


• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 2



• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.96Å 147.78Å 144.93Å 90.00° 96.91° 90.00°	Depositor
Resolution (Å)	48.40 – 2.80 48.39 – 2.75	Depositor EDS
% Data completeness (in resolution range)	58.3 (48.40-2.80) 58.3 (48.39-2.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.210 , 0.256 0.216 , 0.260	Depositor DCC
R_{free} test set	2346 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	82.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16904	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.46	0/4235	0.69	0/5725
1	B	0.47	0/4364	0.69	0/5902
1	C	0.47	0/4225	0.69	0/5712
1	D	0.47	0/4213	0.69	0/5697
All	All	0.47	0/17037	0.69	0/23036

There are no bond length outliers.

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	4138	0	4142	139	0
1	B	4257	0	4262	124	0
1	C	4128	0	4104	116	0
1	D	4116	0	4068	115	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	0	0
3	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	0	3	0
3	C	15	0	0	3	0
3	D	12	0	0	1	0
All	All	16904	0	16700	462	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 (462) 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:A:192:ILE:HG13	1:A:214:THR:CG2	1.68	1.24
1:A:60:THR:HG21	1:A:82:LEU:HB2	1.18	1.14
1:A:60:THR:HG23	1:A:82:LEU:H	0.95	1.10
1:A:192:ILE:HG13	1:A:214:THR:HG21	1.22	1.09
1:A:60:THR:CG2	1:A:82:LEU:HB2	1.86	1.05
1:A:215:ARG:HD2	1:A:314:GLU:OE2	1.55	1.04
1:A:60:THR:HG23	1:A:82:LEU:N	1.78	0.98
1:A:60:THR:CG2	1:A:82:LEU:H	1.77	0.97
1:D:452:LEU:O	1:D:460:ALA:HB2	1.66	0.95
1:B:455:LYS:HE2	1:B:455:LYS:HA	1.46	0.95
1:B:502:ARG:HH21	1:C:217:GLY:HA3	1.34	0.92
1:B:452:LEU:O	1:B:460:ALA:HB2	1.69	0.92
1:A:452:LEU:O	1:A:460:ALA:HB2	1.69	0.92
1:A:192:ILE:HG13	1:A:214:THR:HG23	1.53	0.89
1:B:502:ARG:HG2	1:C:270:GLY:O	1.74	0.88
1:C:452:LEU:O	1:C:460:ALA:HB2	1.78	0.83
1:B:223:ARG:HD2	1:B:286:ASP:OD1	1.78	0.83
1:C:192:ILE:O	1:C:192:ILE:HG22	1.78	0.82
1:B:481:TRP:HD1	1:B:483:GLY:O	1.63	0.82
1:D:223:ARG:HG3	1:D:223:ARG:HH11	1.44	0.82
1:D:192:ILE:HG22	1:D:192:ILE:O	1.77	0.82
1:A:192:ILE:O	1:A:192:ILE:HG22	1.80	0.81
1:D:481:TRP:HD1	1:D:483:GLY:O	1.62	0.81
1:B:192:ILE:HG22	1:B:192:ILE:O	1.78	0.81
1:A:481:TRP:HD1	1:A:483:GLY:O	1.63	0.81
1:A:299:VAL:O	1:D:501:THR:HG23	1.80	0.81
1:C:481:TRP:HD1	1:C:483:GLY:O	1.63	0.80
1:A:60:THR:CG2	1:A:82:LEU:CB	2.58	0.80
1:B:520:GLY:HA2	3:B:707:HOH:O	1.82	0.79
1:A:192:ILE:CG1	1:A:214:THR:HG21	2.09	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:MET:CE	1:A:410:ILE:HA	2.13	0.78
1:B:453:LEU:O	1:B:453:LEU:HD22	1.85	0.76
1:A:270:GLY:O	1:D:502:ARG:HG2	1.86	0.75
1:A:502:ARG:HG3	1:D:300:LYS:CA	2.16	0.75
1:A:349:MET:HE1	1:A:410:ILE:HA	1.67	0.74
1:A:192:ILE:CG1	1:A:214:THR:CG2	2.60	0.73
1:B:47:VAL:HG21	1:B:175:GLN:HE21	1.53	0.73
1:A:60:THR:CG2	1:A:82:LEU:N	2.45	0.73
1:C:481:TRP:CD1	1:C:483:GLY:O	2.41	0.73
1:B:455:LYS:HE2	1:B:455:LYS:CA	2.19	0.73
1:B:481:TRP:CD1	1:B:483:GLY:O	2.41	0.73
1:B:501:THR:HG23	1:C:299:VAL:O	1.89	0.73
1:D:481:TRP:CD1	1:D:483:GLY:O	2.41	0.73
1:A:481:TRP:CD1	1:A:483:GLY:O	2.42	0.73
1:A:60:THR:HG22	1:A:82:LEU:O	1.90	0.72
1:B:462:LYS:HE2	1:B:489:PHE:HA	1.71	0.71
1:B:513:SER:HB2	1:B:516:LEU:HD22	1.70	0.71
1:A:502:ARG:HG3	1:D:300:LYS:C	2.11	0.70
1:C:306:LEU:HD21	1:C:325:ILE:CD1	2.21	0.70
1:C:152:LEU:HD22	1:C:332:THR:HG23	1.72	0.70
1:C:454:LEU:N	1:C:454:LEU:HD23	2.07	0.70
1:A:165:ARG:NH1	1:A:308:GLU:OE2	2.24	0.69
1:A:388:TRP:CZ3	1:A:442:GLU:HB3	2.28	0.69
1:D:388:TRP:CZ3	1:D:442:GLU:HB3	2.28	0.69
1:B:388:TRP:CZ3	1:B:442:GLU:HB3	2.28	0.68
1:D:453:LEU:O	1:D:453:LEU:HD22	1.93	0.68
1:A:501:THR:HG23	1:D:299:VAL:O	1.93	0.68
1:C:388:TRP:CZ3	1:C:442:GLU:HB3	2.28	0.68
1:A:293:LEU:HD12	1:D:224:ILE:HD13	1.75	0.68
1:B:55:TYR:CE2	1:B:58:VAL:HG22	2.29	0.68
1:C:55:TYR:CE2	1:C:58:VAL:HG22	2.28	0.68
1:A:55:TYR:CE2	1:A:58:VAL:HG22	2.30	0.67
1:D:152:LEU:HD22	1:D:332:THR:HG23	1.74	0.67
1:C:47:VAL:HG21	1:C:175:GLN:NE2	2.09	0.67
1:D:462:LYS:HE2	1:D:489:PHE:HA	1.76	0.66
1:A:402:GLU:O	1:A:406:MET:HG2	1.96	0.66
1:D:55:TYR:CE2	1:D:58:VAL:HG22	2.31	0.66
1:B:152:LEU:HD22	1:B:332:THR:HG23	1.78	0.65
1:D:125:TRP:HE1	1:D:365:THR:HG23	1.62	0.65
1:A:47:VAL:HG21	1:A:175:GLN:NE2	2.12	0.65
1:B:299:VAL:O	1:C:501:THR:HG23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:CYS:SG	1:B:144:MET:CE	2.85	0.64
1:A:238:ARG:NH1	1:A:472:GLN:OE1	2.31	0.64
1:C:125:TRP:HE1	1:C:365:THR:HG23	1.63	0.64
1:C:21:CYS:SG	1:C:144:MET:CE	2.86	0.64
1:A:152:LEU:HD22	1:A:332:THR:HG23	1.80	0.64
1:C:192:ILE:O	1:C:192:ILE:CG2	2.46	0.64
1:D:448:ASP:OD2	1:D:451:SER:HB3	1.98	0.64
1:D:238:ARG:NH1	1:D:472:GLN:OE1	2.31	0.63
1:B:125:TRP:HE1	1:B:365:THR:HG23	1.64	0.63
1:A:21:CYS:SG	1:A:144:MET:CE	2.86	0.63
1:C:238:ARG:NH1	1:C:472:GLN:OE1	2.31	0.63
1:A:452:LEU:O	1:A:452:LEU:HD12	1.99	0.63
1:B:457:PRO:O	1:B:461:MET:HG2	1.98	0.62
1:A:47:VAL:O	1:A:47:VAL:HG23	2.00	0.62
1:B:238:ARG:NH1	1:B:472:GLN:OE1	2.32	0.62
1:A:11:GLY:HA3	2:A:601:FAD:O1P	2.00	0.62
1:B:452:LEU:O	1:B:452:LEU:HD12	2.00	0.62
1:A:192:ILE:O	1:A:192:ILE:CG2	2.48	0.61
1:D:21:CYS:SG	1:D:144:MET:CE	2.88	0.61
1:B:527:ALA:HA	1:B:530:PHE:CZ	2.35	0.61
1:C:47:VAL:HG23	1:C:47:VAL:O	2.01	0.61
1:B:300:LYS:HE3	1:B:319:GLU:OE1	2.01	0.61
1:C:505:LYS:HG2	1:C:505:LYS:O	2.00	0.61
1:D:453:LEU:HD22	1:D:453:LEU:C	2.21	0.61
1:B:47:VAL:HG23	1:B:47:VAL:O	2.00	0.61
1:A:125:TRP:HE1	1:A:365:THR:HG23	1.65	0.61
1:B:192:ILE:O	1:B:192:ILE:CG2	2.47	0.60
1:B:217:GLY:HA3	1:C:502:ARG:HH22	1.65	0.60
1:D:300:LYS:HE3	1:D:319:GLU:OE1	2.01	0.60
1:B:55:TYR:CD2	1:B:58:VAL:HG22	2.36	0.60
1:A:300:LYS:HE3	1:A:319:GLU:OE1	2.01	0.60
1:C:450:LEU:O	1:C:453:LEU:HB2	2.01	0.60
1:A:477:GLY:O	1:A:480:GLN:NE2	2.35	0.60
1:C:300:LYS:HE3	1:C:319:GLU:OE1	2.02	0.60
1:A:502:ARG:CG	1:D:300:LYS:C	2.71	0.59
1:B:477:GLY:O	1:B:480:GLN:NE2	2.36	0.59
1:D:505:LYS:O	1:D:505:LYS:HG2	2.02	0.59
1:B:505:LYS:O	1:B:505:LYS:HG2	2.01	0.59
1:A:55:TYR:CD2	1:A:58:VAL:HG22	2.38	0.59
1:C:220:VAL:H	1:C:266:HIS:HE1	1.51	0.59
1:A:60:THR:CG2	1:A:82:LEU:CA	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:TYR:CD2	1:D:58:VAL:HG22	2.37	0.59
1:C:55:TYR:CD2	1:C:58:VAL:HG22	2.38	0.58
1:C:454:LEU:HD23	1:C:454:LEU:H	1.67	0.58
1:C:477:GLY:O	1:C:480:GLN:NE2	2.36	0.58
1:B:249:ARG:HH12	1:B:419:LEU:HG	1.69	0.58
1:A:505:LYS:O	1:A:505:LYS:HG2	2.03	0.58
1:D:47:VAL:HG23	1:D:47:VAL:O	2.03	0.57
1:A:359:PRO:HA	1:A:405:MET:CE	2.35	0.57
1:A:502:ARG:HB2	1:D:299:VAL:HG23	1.86	0.57
1:D:477:GLY:O	1:D:480:GLN:NE2	2.35	0.57
1:A:216:HIS:N	1:A:216:HIS:CD2	2.72	0.57
1:C:359:PRO:HA	1:C:405:MET:CE	2.34	0.57
1:A:220:VAL:H	1:A:266:HIS:HE1	1.52	0.57
1:D:192:ILE:O	1:D:192:ILE:CG2	2.47	0.57
1:B:512:VAL:HG21	1:C:276:LYS:NZ	2.19	0.56
1:D:65:GLU:HA	1:D:65:GLU:OE1	2.05	0.56
1:D:359:PRO:HA	1:D:405:MET:CE	2.35	0.56
1:B:220:VAL:H	1:B:266:HIS:HE1	1.51	0.56
1:C:65:GLU:OE1	1:C:65:GLU:HA	2.06	0.56
1:A:146:CYS:SG	1:A:369:ILE:HD11	2.46	0.56
1:B:65:GLU:OE1	1:B:65:GLU:HA	2.05	0.56
1:C:231:TRP:O	1:C:234:VAL:HG22	2.07	0.55
1:D:47:VAL:HG21	1:D:175:GLN:NE2	2.22	0.55
1:D:220:VAL:H	1:D:266:HIS:HE1	1.53	0.55
1:B:359:PRO:HA	1:B:405:MET:CE	2.37	0.55
1:D:81:PHE:CD2	1:D:223:ARG:HD3	2.42	0.55
1:B:231:TRP:O	1:B:234:VAL:HG22	2.06	0.55
1:A:192:ILE:CG1	1:A:214:THR:HG23	2.32	0.55
1:D:231:TRP:O	1:D:234:VAL:HG22	2.07	0.55
1:A:65:GLU:HA	1:A:65:GLU:OE1	2.07	0.55
1:C:332:THR:OG1	1:C:333:PHE:N	2.40	0.55
1:B:143:VAL:HG13	1:B:366:LEU:HD12	1.89	0.54
1:B:47:VAL:CG2	1:B:175:GLN:HE21	2.20	0.54
1:D:167:LYS:HE2	1:D:167:LYS:HA	1.89	0.54
1:A:349:MET:HE3	1:A:410:ILE:HA	1.90	0.54
1:A:420:PHE:HB3	1:A:426:GLN:HG2	1.88	0.54
1:A:143:VAL:HG13	1:A:366:LEU:HD12	1.90	0.54
1:A:332:THR:OG1	1:A:333:PHE:N	2.40	0.53
1:A:502:ARG:HG3	1:D:300:LYS:HA	1.87	0.53
1:D:338:LEU:HG	1:D:342:LEU:HD23	1.90	0.53
1:A:502:ARG:HD2	1:D:301:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:THR:OG1	1:D:333:PHE:N	2.42	0.53
1:B:195:SER:O	1:B:199:ILE:HG12	2.09	0.53
1:B:388:TRP:CE3	1:B:442:GLU:HB3	2.43	0.53
1:B:235:PHE:O	1:B:244:ARG:NH2	2.42	0.53
1:A:55:TYR:O	1:A:58:VAL:HG23	2.09	0.53
1:A:231:TRP:O	1:A:234:VAL:HG22	2.08	0.53
1:C:449:LEU:CD1	1:C:463:LEU:HB2	2.39	0.53
1:B:275:ASN:HB2	1:B:278:LEU:HD13	1.91	0.53
1:A:195:SER:O	1:A:199:ILE:HG12	2.09	0.53
1:D:61:ASN:OD1	1:D:61:ASN:N	2.42	0.53
1:B:338:LEU:HG	1:B:342:LEU:HD23	1.91	0.53
1:A:453:LEU:HD22	1:A:453:LEU:C	2.30	0.53
1:D:457:PRO:O	1:D:461:MET:HG2	2.09	0.53
1:B:26:LEU:HD12	1:B:26:LEU:N	2.24	0.52
1:C:146:CYS:SG	1:C:369:ILE:HD11	2.49	0.52
1:C:167:LYS:HE2	1:C:167:LYS:HA	1.91	0.52
1:C:249:ARG:HH12	1:C:419:LEU:HG	1.73	0.52
1:B:123:GLY:N	3:B:701:HOH:O	2.41	0.52
1:C:235:PHE:O	1:C:244:ARG:NH2	2.42	0.52
1:C:449:LEU:N	1:C:449:LEU:CD2	2.72	0.52
1:C:55:TYR:O	1:C:58:VAL:HG23	2.09	0.52
1:C:143:VAL:HG13	1:C:366:LEU:HD12	1.90	0.52
1:D:21:CYS:SG	1:D:144:MET:HE1	2.50	0.52
1:D:143:VAL:HG13	1:D:366:LEU:HD12	1.91	0.52
1:C:249:ARG:HH22	1:C:419:LEU:HA	1.74	0.52
1:C:338:LEU:HG	1:C:342:LEU:HD23	1.91	0.52
1:A:21:CYS:SG	1:A:144:MET:HE1	2.50	0.52
1:B:32:GLU:HG3	1:B:34:THR:O	2.10	0.52
1:B:254:TRP:HB3	3:B:708:HOH:O	2.09	0.52
1:A:235:PHE:O	1:A:244:ARG:NH2	2.42	0.52
1:D:26:LEU:HD12	1:D:26:LEU:N	2.25	0.52
1:A:26:LEU:HD11	1:A:394:LYS:HD2	1.92	0.52
1:A:457:PRO:O	1:A:461:MET:HG2	2.10	0.52
1:C:450:LEU:HD12	1:C:450:LEU:H	1.74	0.52
1:D:348:ASN:HD21	1:D:416:ARG:HH12	1.58	0.52
1:A:462:LYS:HE2	1:A:489:PHE:HA	1.91	0.52
1:B:55:TYR:O	1:B:58:VAL:HG23	2.10	0.52
1:D:146:CYS:SG	1:D:369:ILE:HD11	2.49	0.52
1:A:338:LEU:HG	1:A:342:LEU:HD23	1.93	0.51
1:D:388:TRP:CE3	1:D:442:GLU:HB3	2.45	0.51
1:C:388:TRP:CE3	1:C:442:GLU:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:LEU:HD11	1:C:463:LEU:CB	2.40	0.51
1:B:146:CYS:SG	1:B:369:ILE:HD11	2.49	0.51
1:C:359:PRO:HA	1:C:405:MET:HE1	1.93	0.51
1:D:176:TYR:CD2	1:D:199:ILE:HD13	2.46	0.51
1:C:457:PRO:O	1:C:461:MET:HG2	2.11	0.51
1:C:346:GLU:HB3	3:C:713:HOH:O	2.11	0.51
1:A:388:TRP:CE3	1:A:442:GLU:HB3	2.44	0.51
1:C:275:ASN:HB2	1:C:278:LEU:HD13	1.93	0.51
1:B:359:PRO:HA	1:B:405:MET:HE1	1.92	0.50
1:C:420:PHE:HB3	1:C:426:GLN:HG2	1.92	0.50
1:C:462:LYS:HE2	1:C:489:PHE:HA	1.94	0.50
1:D:55:TYR:O	1:D:58:VAL:HG23	2.11	0.50
1:B:526:VAL:HA	1:B:529:PHE:HB2	1.93	0.50
1:B:26:LEU:HD11	1:B:394:LYS:HD2	1.93	0.50
1:B:249:ARG:HH22	1:B:419:LEU:HA	1.76	0.50
1:D:249:ARG:HH12	1:D:419:LEU:HG	1.76	0.50
1:C:497:LYS:N	1:C:498:PRO:HD2	2.27	0.50
1:D:223:ARG:NH1	1:D:223:ARG:CG	2.73	0.50
1:B:63:SER:HB3	1:B:66:MET:HB2	1.93	0.50
1:B:11:GLY:HA3	2:B:601:FAD:O1P	2.11	0.50
1:D:420:PHE:HB3	1:D:426:GLN:HG2	1.94	0.50
1:B:348:ASN:HD21	1:B:416:ARG:HH12	1.60	0.49
1:A:239:PHE:O	1:A:243:LEU:HD13	2.12	0.49
1:D:223:ARG:HG3	1:D:223:ARG:NH1	2.21	0.49
1:D:223:ARG:NH1	1:D:286:ASP:OD1	2.45	0.49
1:D:63:SER:HB3	1:D:66:MET:HB2	1.95	0.49
1:B:293:LEU:HD12	1:C:224:ILE:HD13	1.95	0.49
1:A:26:LEU:N	1:A:26:LEU:HD12	2.26	0.49
1:A:357:PHE:CZ	1:A:389:VAL:HG22	2.48	0.49
1:D:194:ASN:ND2	1:D:283:VAL:HA	2.28	0.49
1:D:249:ARG:HH22	1:D:419:LEU:HA	1.78	0.49
1:A:288:LEU:HB3	1:A:289:PRO:HD3	1.94	0.49
1:A:348:ASN:HD21	1:A:416:ARG:HH12	1.61	0.49
1:C:357:PHE:CZ	1:C:389:VAL:HG22	2.48	0.49
1:C:449:LEU:N	1:C:449:LEU:HD23	2.28	0.49
1:D:235:PHE:O	1:D:244:ARG:NH2	2.43	0.49
1:C:61:ASN:N	1:C:61:ASN:ND2	2.61	0.49
1:B:194:ASN:ND2	1:B:283:VAL:HA	2.28	0.49
1:C:21:CYS:SG	1:C:144:MET:HE1	2.52	0.49
1:C:348:ASN:HD21	1:C:416:ARG:HH12	1.60	0.49
1:D:357:PHE:CZ	1:D:389:VAL:HG22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PHE:CZ	1:B:389:VAL:HG22	2.48	0.48
1:B:526:VAL:O	1:B:530:PHE:CD2	2.65	0.48
1:A:402:GLU:O	1:A:406:MET:CG	2.61	0.48
1:C:239:PHE:O	1:C:243:LEU:HD13	2.13	0.48
1:D:159:SER:HB2	1:D:302:ARG:NH2	2.28	0.48
1:B:21:CYS:SG	1:B:144:MET:HE1	2.52	0.48
1:A:167:LYS:HE2	1:A:167:LYS:HA	1.94	0.48
1:A:270:GLY:O	1:D:502:ARG:CG	2.60	0.48
1:C:63:SER:HB3	1:C:66:MET:HB2	1.96	0.48
1:C:195:SER:O	1:C:199:ILE:HG12	2.12	0.48
1:D:288:LEU:HB3	1:D:289:PRO:HD3	1.95	0.48
1:B:502:ARG:NH2	1:C:217:GLY:HA3	2.16	0.48
1:A:448:ASP:O	1:A:452:LEU:HB2	2.13	0.48
1:B:420:PHE:HB3	1:B:426:GLN:HG2	1.94	0.48
1:C:33:ARG:CB	3:C:714:HOH:O	2.60	0.48
1:D:223:ARG:HH11	1:D:223:ARG:CG	2.13	0.48
1:B:448:ASP:O	1:B:452:LEU:HB2	2.13	0.48
1:A:216:HIS:CD2	1:A:216:HIS:H	2.30	0.48
1:D:138:ALA:HB1	3:D:702:HOH:O	2.13	0.48
1:D:239:PHE:O	1:D:243:LEU:HD13	2.13	0.48
1:C:449:LEU:HD11	1:C:463:LEU:HB3	1.95	0.48
1:D:497:LYS:N	1:D:498:PRO:HD2	2.28	0.48
1:A:194:ASN:ND2	1:A:283:VAL:HA	2.29	0.48
1:A:495:ILE:O	1:A:498:PRO:HD2	2.13	0.48
1:B:217:GLY:HA3	1:C:502:ARG:NH2	2.28	0.48
1:A:63:SER:HB3	1:A:66:MET:HB2	1.96	0.48
1:C:194:ASN:ND2	1:C:283:VAL:HA	2.29	0.47
1:A:60:THR:HG22	1:A:82:LEU:CB	2.43	0.47
1:C:176:TYR:CD2	1:C:199:ILE:HD13	2.49	0.47
1:A:497:LYS:N	1:A:498:PRO:HD2	2.29	0.47
1:C:159:SER:HB2	1:C:302:ARG:NH2	2.29	0.47
1:C:495:ILE:O	1:C:498:PRO:HD2	2.14	0.47
1:B:32:GLU:HB3	1:B:106:PHE:HA	1.96	0.47
1:C:454:LEU:H	1:C:454:LEU:CD2	2.22	0.47
1:B:159:SER:HB2	1:B:302:ARG:NH2	2.29	0.47
1:A:502:ARG:CG	1:D:301:SER:N	2.77	0.47
1:B:495:ILE:O	1:B:498:PRO:HD2	2.15	0.47
1:B:497:LYS:N	1:B:498:PRO:HD2	2.29	0.47
1:A:249:ARG:HH22	1:A:419:LEU:HA	1.78	0.47
1:A:372:ILE:HD11	1:A:430:THR:HG21	1.96	0.47
1:D:26:LEU:HD11	1:D:394:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:SER:OG	1:D:383:GLU:OE2	2.23	0.47
1:A:159:SER:HB2	1:A:302:ARG:NH2	2.30	0.47
1:A:249:ARG:HH12	1:A:419:LEU:HG	1.80	0.47
1:C:372:ILE:HD11	1:C:430:THR:HG21	1.97	0.47
1:C:449:LEU:HD23	1:C:449:LEU:H	1.80	0.47
1:B:239:PHE:O	1:B:243:LEU:HD13	2.15	0.46
1:D:495:ILE:O	1:D:498:PRO:HD2	2.15	0.46
1:A:499:LEU:HD21	1:D:293:LEU:HD23	1.98	0.46
1:C:30:CYS:HB3	1:C:104:ILE:HA	1.97	0.46
1:B:294:TYR:OH	1:C:286:ASP:OD1	2.32	0.46
1:A:359:PRO:HA	1:A:405:MET:HE1	1.97	0.46
1:C:453:LEU:HD23	1:C:453:LEU:HA	1.77	0.46
1:C:220:VAL:H	1:C:266:HIS:CE1	2.33	0.46
1:C:288:LEU:HB3	1:C:289:PRO:HD3	1.97	0.46
1:D:359:PRO:HA	1:D:405:MET:HE1	1.96	0.46
1:B:30:CYS:HB3	1:B:104:ILE:HA	1.98	0.46
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.81	0.46
1:B:272:GLU:O	1:C:502:ARG:NH1	2.49	0.46
1:A:60:THR:CG2	1:A:82:LEU:O	2.63	0.46
1:C:306:LEU:HD21	1:C:325:ILE:HD12	1.95	0.46
1:D:354:LYS:NZ	1:D:442:GLU:OE1	2.48	0.46
1:B:510:PHE:CD2	1:B:511:PRO:HD3	2.51	0.45
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.85	0.45
1:B:176:TYR:CD2	1:B:199:ILE:HD13	2.50	0.45
1:B:508:SER:HB2	1:B:512:VAL:O	2.16	0.45
1:A:450:LEU:HD12	1:A:450:LEU:HA	1.82	0.45
1:B:354:LYS:NZ	1:B:442:GLU:OE1	2.49	0.45
1:A:7:VAL:HG21	1:A:18:LEU:HD13	1.98	0.45
1:A:30:CYS:HB3	1:A:104:ILE:HA	1.99	0.45
1:C:457:PRO:HD2	3:C:704:HOH:O	2.16	0.45
1:D:47:VAL:O	1:D:47:VAL:CG2	2.65	0.45
1:D:30:CYS:HB3	1:D:104:ILE:HA	1.98	0.45
1:B:288:LEU:HB3	1:B:289:PRO:HD3	1.98	0.45
1:B:372:ILE:HD11	1:B:430:THR:HG21	1.99	0.45
1:B:70:SER:OG	1:B:383:GLU:OE2	2.23	0.44
1:D:7:VAL:HG21	1:D:18:LEU:HD13	1.99	0.44
1:C:293:LEU:HD23	1:C:293:LEU:HA	1.83	0.44
1:D:5:VAL:HG21	1:D:26:LEU:HD23	1.98	0.44
1:D:195:SER:O	1:D:199:ILE:HG12	2.18	0.44
1:B:47:VAL:HG21	1:B:175:GLN:NE2	2.28	0.44
1:B:512:VAL:HG11	1:C:276:LYS:HZ2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ARG:HE	1:A:502:ARG:HB3	1.39	0.44
1:C:11:GLY:HA3	2:C:601:FAD:O1P	2.18	0.44
1:D:88:LEU:HD23	1:D:88:LEU:HA	1.86	0.44
1:B:512:VAL:HG21	1:C:276:LYS:HZ2	1.82	0.44
1:A:303:VAL:HG11	1:A:306:LEU:HD13	2.00	0.44
1:B:527:ALA:HA	1:B:530:PHE:CE2	2.53	0.44
1:C:7:VAL:HG21	1:C:18:LEU:HD13	1.99	0.44
1:D:303:VAL:HG11	1:D:306:LEU:HD13	1.99	0.44
1:B:514:PHE:HE1	1:C:254:TRP:CE3	2.36	0.43
1:A:81:PHE:CE2	1:A:223:ARG:HG2	2.52	0.43
1:D:455:LYS:HA	1:D:455:LYS:HD3	1.33	0.43
1:B:220:VAL:H	1:B:266:HIS:CE1	2.34	0.43
1:D:21:CYS:SG	1:D:144:MET:HE3	2.57	0.43
1:D:453:LEU:HA	1:D:460:ALA:CB	2.48	0.43
1:B:514:PHE:CZ	1:C:254:TRP:HB3	2.53	0.43
1:B:517:LYS:HB2	1:B:517:LYS:NZ	2.33	0.43
1:C:13:SER:HB2	1:C:146:CYS:HB3	1.99	0.43
1:D:448:ASP:O	1:D:452:LEU:HB2	2.19	0.43
1:B:7:VAL:HG21	1:B:18:LEU:HD13	2.01	0.43
1:A:453:LEU:HD22	1:A:453:LEU:O	2.17	0.43
1:D:79:PRO:HG2	1:D:82:LEU:HD12	2.00	0.43
1:B:293:LEU:HD23	1:C:499:LEU:HD21	2.00	0.43
1:C:302:ARG:HG2	1:C:303:VAL:O	2.18	0.43
1:D:47:VAL:HG21	1:D:175:GLN:HE22	1.82	0.43
1:B:220:VAL:HA	1:B:283:VAL:HG22	2.00	0.43
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.85	0.43
1:B:354:LYS:O	1:B:356:MET:HB2	2.19	0.43
1:D:225:SER:O	1:D:226:ASP:C	2.57	0.43
1:A:302:ARG:HG2	1:A:303:VAL:O	2.18	0.43
1:C:354:LYS:O	1:C:356:MET:HB2	2.19	0.43
1:C:391:ARG:NH1	1:C:397:CYS:SG	2.92	0.43
1:D:453:LEU:C	1:D:453:LEU:CD2	2.85	0.43
1:B:391:ARG:NH1	1:B:397:CYS:SG	2.92	0.43
1:A:455:LYS:HA	1:A:455:LYS:HD3	1.76	0.43
1:D:452:LEU:O	1:D:452:LEU:HD12	2.19	0.43
1:C:242:MET:O	1:C:246:VAL:HG13	2.19	0.43
1:C:303:VAL:HG11	1:C:306:LEU:HD13	2.00	0.43
1:A:354:LYS:HE2	1:A:412:ARG:HH12	1.83	0.42
1:C:211:PHE:CE1	1:C:319:GLU:HG2	2.53	0.42
1:D:19:LYS:HD3	1:D:23:ASP:OD2	2.19	0.42
1:A:166:PHE:CD2	1:A:167:LYS:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TYR:CD2	1:A:199:ILE:HD13	2.54	0.42
1:A:220:VAL:HA	1:A:283:VAL:HG22	2.01	0.42
1:A:349:MET:HE1	1:A:410:ILE:CA	2.44	0.42
1:A:379:PHE:N	1:A:380:PRO:HD2	2.34	0.42
1:D:354:LYS:O	1:D:356:MET:HB2	2.18	0.42
1:D:385:GLN:N	1:D:439:LEU:HD23	2.34	0.42
1:B:385:GLN:N	1:B:439:LEU:HD23	2.34	0.42
1:A:453:LEU:C	1:A:453:LEU:CD2	2.85	0.42
1:D:242:MET:O	1:D:246:VAL:HG13	2.19	0.42
1:D:259:GLN:O	1:D:262:ARG:HB2	2.19	0.42
1:A:47:VAL:HG21	1:A:175:GLN:HE22	1.84	0.42
1:A:220:VAL:H	1:A:266:HIS:CE1	2.34	0.42
1:A:515:LEU:HA	1:A:518:ILE:HB	2.01	0.42
1:C:32:GLU:OE2	2:C:601:FAD:O2B	2.32	0.42
1:D:482:GLU:O	1:D:484:ALA:N	2.51	0.42
1:B:19:LYS:HD3	1:B:23:ASP:OD2	2.19	0.42
1:B:513:SER:C	1:B:516:LEU:HD13	2.40	0.42
1:B:515:LEU:HA	1:B:518:ILE:HB	2.00	0.42
1:B:5:VAL:HG21	1:B:26:LEU:HD23	2.00	0.42
1:A:13:SER:HB2	1:A:146:CYS:HB3	2.02	0.42
1:C:159:SER:HB2	1:C:302:ARG:HH22	1.85	0.42
1:D:159:SER:HB2	1:D:302:ARG:HH22	1.84	0.42
1:A:391:ARG:NH1	1:A:397:CYS:SG	2.92	0.42
1:A:502:ARG:HB2	1:D:299:VAL:CG2	2.48	0.42
1:D:302:ARG:HG2	1:D:303:VAL:O	2.19	0.42
1:A:482:GLU:O	1:A:484:ALA:N	2.50	0.42
1:C:225:SER:O	1:C:226:ASP:C	2.58	0.42
1:D:13:SER:HB2	1:D:146:CYS:HB3	2.02	0.42
1:D:166:PHE:CD2	1:D:167:LYS:O	2.73	0.42
1:D:372:ILE:HD11	1:D:430:THR:HG21	2.01	0.42
1:B:302:ARG:HG2	1:B:303:VAL:O	2.20	0.42
1:B:378:ILE:HA	1:B:381:THR:OG1	2.20	0.42
1:A:451:SER:C	1:A:453:LEU:H	2.24	0.42
1:D:379:PHE:N	1:D:380:PRO:HD2	2.35	0.42
1:B:47:VAL:O	1:B:47:VAL:CG2	2.67	0.42
1:A:242:MET:O	1:A:246:VAL:HG13	2.19	0.42
1:A:454:LEU:H	1:A:454:LEU:HG	1.60	0.42
1:C:67:SER:HB2	1:C:377:SER:OG	2.20	0.42
1:D:116:CYS:O	1:D:118:ASP:N	2.53	0.42
1:B:159:SER:HB2	1:B:302:ARG:HH22	1.84	0.41
1:B:303:VAL:HG11	1:B:306:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HB2	1:A:302:ARG:HB2	2.01	0.41
1:C:482:GLU:O	1:C:484:ALA:N	2.50	0.41
1:B:225:SER:O	1:B:226:ASP:C	2.59	0.41
1:A:194:ASN:HD21	1:A:283:VAL:HA	1.85	0.41
1:A:225:SER:O	1:A:226:ASP:C	2.58	0.41
1:A:240:SER:HB3	1:A:244:ARG:HH21	1.85	0.41
1:C:216:HIS:O	1:C:273:PRO:HA	2.20	0.41
1:B:451:SER:C	1:B:453:LEU:H	2.24	0.41
1:A:280:LYS:HG3	1:A:426:GLN:NE2	2.36	0.41
1:A:504:LEU:O	1:A:505:LYS:HG2	2.20	0.41
1:B:382:VAL:HA	1:B:385:GLN:HB2	2.02	0.41
1:B:116:CYS:O	1:B:118:ASP:N	2.53	0.41
1:B:532:LEU:O	1:B:532:LEU:HD23	2.19	0.41
1:A:47:VAL:O	1:A:47:VAL:CG2	2.67	0.41
1:C:47:VAL:O	1:C:47:VAL:CG2	2.68	0.41
1:B:63:SER:O	1:B:67:SER:OG	2.24	0.41
1:B:211:PHE:CE1	1:B:319:GLU:HG2	2.55	0.41
1:A:354:LYS:O	1:A:356:MET:HB2	2.20	0.41
1:D:130:GLU:OE1	1:D:131:SER:O	2.39	0.41
1:B:47:VAL:HG11	1:B:175:GLN:HA	2.03	0.41
1:B:482:GLU:O	1:B:484:ALA:N	2.50	0.41
1:C:240:SER:HB3	1:C:244:ARG:HH21	1.86	0.41
1:C:385:GLN:N	1:C:439:LEU:HD23	2.36	0.41
1:D:188:LEU:O	1:D:325:ILE:HA	2.21	0.41
1:D:382:VAL:HA	1:D:385:GLN:HB2	2.02	0.41
1:B:79:PRO:HG2	1:B:82:LEU:HD12	2.03	0.41
1:B:512:VAL:HG21	1:C:276:LYS:HZ3	1.85	0.41
1:B:166:PHE:CD2	1:B:167:LYS:O	2.73	0.41
1:A:19:LYS:HD3	1:A:23:ASP:OD2	2.21	0.41
1:A:54:ILE:HB	1:A:58:VAL:HG21	2.02	0.41
1:A:188:LEU:O	1:A:325:ILE:HA	2.21	0.41
1:A:345:VAL:HG13	1:A:345:VAL:O	2.21	0.41
1:A:378:ILE:HA	1:A:381:THR:OG1	2.21	0.41
1:A:502:ARG:HG2	1:D:301:SER:N	2.36	0.41
1:C:19:LYS:HD3	1:C:23:ASP:OD2	2.21	0.41
1:C:63:SER:N	1:C:232:ASP:OD2	2.53	0.41
1:C:79:PRO:HG2	1:C:82:LEU:HD12	2.02	0.41
1:C:382:VAL:HA	1:C:385:GLN:HB2	2.03	0.41
1:C:497:LYS:N	1:C:498:PRO:CD	2.84	0.41
1:D:211:PHE:CE1	1:D:319:GLU:HG2	2.56	0.41
1:D:220:VAL:H	1:D:266:HIS:CE1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:TRP:CH2	1:A:289:PRO:HG2	2.56	0.41
1:C:130:GLU:OE1	1:C:131:SER:O	2.39	0.41
1:C:166:PHE:CD2	1:C:167:LYS:O	2.74	0.41
1:B:242:MET:O	1:B:246:VAL:HG13	2.20	0.40
1:A:522:LEU:HA	1:A:525:VAL:HG12	2.02	0.40
1:C:379:PHE:N	1:C:380:PRO:HD2	2.37	0.40
1:D:312:ILE:HD13	1:D:312:ILE:N	2.37	0.40
1:C:378:ILE:HA	1:C:381:THR:OG1	2.21	0.40
1:D:240:SER:HB3	1:D:244:ARG:HH21	1.86	0.40
1:A:159:SER:HB2	1:A:302:ARG:HH22	1.85	0.40
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.85	0.40
1:D:378:ILE:HA	1:D:381:THR:OG1	2.22	0.40
1:B:13:SER:HB2	1:B:146:CYS:HB3	2.03	0.40
1:B:101:LEU:HD12	1:B:101:LEU:HA	1.99	0.40
1:B:240:SER:HB3	1:B:244:ARG:HH21	1.86	0.40
1:B:379:PHE:N	1:B:380:PRO:HD2	2.36	0.40
1:A:79:PRO:HG2	1:A:82:LEU:HD12	2.03	0.40
1:A:116:CYS:O	1:A:118:ASP:N	2.55	0.40
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.90	0.40
1:C:87:LEU:O	1:C:88:LEU:C	2.60	0.40
1:C:116:CYS:O	1:C:118:ASP:N	2.55	0.40
1:D:378:ILE:HG22	1:D:379:PHE:CD1	2.56	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	513/535 (96%)	456 (89%)	52 (10%)	5 (1%)	15	44
1	B	526/535 (98%)	462 (88%)	57 (11%)	7 (1%)	12	36
1	C	514/535 (96%)	457 (89%)	52 (10%)	5 (1%)	15	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	514/535 (96%)	457 (89%)	51 (10%)	6 (1%)	13	39
All	All	2067/2140 (97%)	1832 (89%)	212 (10%)	23 (1%)	14	41

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	117	PRO
1	B	217	GLY
1	B	479	GLY
1	B	512	VAL
1	A	479	GLY
1	C	217	GLY
1	C	479	GLY
1	D	479	GLY
1	A	117	PRO
1	A	483	GLY
1	C	117	PRO
1	C	483	GLY
1	D	217	GLY
1	B	514	PHE
1	A	226	ASP
1	D	117	PRO
1	D	483	GLY
1	D	226	ASP
1	B	483	GLY
1	C	212	ILE
1	D	212	ILE
1	B	212	ILE
1	A	212	ILE

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	453/477 (95%)	391 (86%)	62 (14%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	469/477 (98%)	404 (86%)	65 (14%)	3	11
1	C	448/477 (94%)	387 (86%)	61 (14%)	3	11
1	D	444/477 (93%)	391 (88%)	53 (12%)	5	16
All	All	1814/1908 (95%)	1573 (87%)	241 (13%)	4	12

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	49	ASP
1	B	53	SER
1	B	56	GLN
1	B	86	LYS
1	B	88	LEU
1	B	96	LYS
1	B	101	LEU
1	B	109	THR
1	B	116	CYS
1	B	118	ASP
1	B	143	VAL
1	B	151	ILE
1	B	155	ILE
1	B	167	LYS
1	B	175	GLN
1	B	180	GLU
1	B	189	VAL
1	B	194	ASN
1	B	198	ASP
1	B	213	SER
1	B	214	THR
1	B	222	SER
1	B	225	SER
1	B	237	THR
1	B	249	ARG
1	B	256	MET
1	B	258	GLN
1	B	271	LEU
1	B	275	ASN
1	B	277	TYR
1	B	291	ARG
1	B	299	VAL
1	B	308	GLU

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Mol	Chain	Res	Type
1	B	340	ASP
1	B	351	SER
1	B	356	MET
1	B	362	GLU
1	B	371	LEU
1	B	381	THR
1	B	398	THR
1	B	413	ASN
1	B	418	ASP
1	B	419	LEU
1	B	424	GLN
1	B	427	ILE
1	B	429	GLN
1	B	436	LEU
1	B	450	LEU
1	B	452	LEU
1	B	453	LEU
1	B	455	LYS
1	B	456	ASP
1	B	459	LEU
1	B	475	LEU
1	B	502	ARG
1	B	505	LYS
1	B	510	PHE
1	B	513	SER
1	B	514	PHE
1	B	517	LYS
1	B	522	LEU
1	B	530	PHE
1	B	531	GLN
1	B	533	GLN
1	B	535	PHE
1	A	3	LYS
1	A	35	GLU
1	A	53	SER
1	A	56	GLN
1	A	60	THR
1	A	86	LYS
1	A	88	LEU
1	A	109	THR
1	A	114	LYS
1	A	116	CYS

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Mol	Chain	Res	Type
1	A	118	ASP
1	A	135	GLU
1	A	143	VAL
1	A	151	ILE
1	A	155	ILE
1	A	167	LYS
1	A	180	GLU
1	A	189	VAL
1	A	192	ILE
1	A	194	ASN
1	A	198	ASP
1	A	206	LYS
1	A	213	SER
1	A	214	THR
1	A	222	SER
1	A	223	ARG
1	A	225	SER
1	A	237	THR
1	A	249	ARG
1	A	256	MET
1	A	258	GLN
1	A	271	LEU
1	A	291	ARG
1	A	299	VAL
1	A	332	THR
1	A	346	GLU
1	A	351	SER
1	A	356	MET
1	A	365	THR
1	A	371	LEU
1	A	381	THR
1	A	398	THR
1	A	406	MET
1	A	411	LYS
1	A	413	ASN
1	A	418	ASP
1	A	419	LEU
1	A	424	GLN
1	A	425	SER
1	A	427	ILE
1	A	429	GLN
1	A	436	LEU

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Mol	Chain	Res	Type
1	A	452	LEU
1	A	453	LEU
1	A	454	LEU
1	A	459	LEU
1	A	475	LEU
1	A	482	GLU
1	A	502	ARG
1	A	516	LEU
1	A	525	VAL
1	A	531	GLN
1	C	3	LYS
1	C	26	LEU
1	C	35	GLU
1	C	40	LEU
1	C	49	ASP
1	C	53	SER
1	C	56	GLN
1	C	61	ASN
1	C	86	LYS
1	C	88	LEU
1	C	96	LYS
1	C	101	LEU
1	C	109	THR
1	C	116	CYS
1	C	118	ASP
1	C	135	GLU
1	C	143	VAL
1	C	151	ILE
1	C	155	ILE
1	C	167	LYS
1	C	180	GLU
1	C	189	VAL
1	C	190	ILE
1	C	194	ASN
1	C	206	LYS
1	C	213	SER
1	C	214	THR
1	C	222	SER
1	C	225	SER
1	C	237	THR
1	C	249	ARG
1	C	256	MET

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Mol	Chain	Res	Type
1	C	258	GLN
1	C	271	LEU
1	C	275	ASN
1	C	277	TYR
1	C	291	ARG
1	C	299	VAL
1	C	346	GLU
1	C	351	SER
1	C	356	MET
1	C	362	GLU
1	C	365	THR
1	C	371	LEU
1	C	381	THR
1	C	398	THR
1	C	413	ASN
1	C	418	ASP
1	C	419	LEU
1	C	425	SER
1	C	427	ILE
1	C	429	GLN
1	C	436	LEU
1	C	449	LEU
1	C	452	LEU
1	C	454	LEU
1	C	455	LYS
1	C	459	LEU
1	C	475	LEU
1	C	505	LYS
1	C	532	LEU
1	D	3	LYS
1	D	35	GLU
1	D	49	ASP
1	D	53	SER
1	D	56	GLN
1	D	61	ASN
1	D	86	LYS
1	D	88	LEU
1	D	96	LYS
1	D	109	THR
1	D	116	CYS
1	D	118	ASP
1	D	143	VAL

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Mol	Chain	Res	Type
1	D	151	ILE
1	D	155	ILE
1	D	167	LYS
1	D	180	GLU
1	D	189	VAL
1	D	194	ASN
1	D	198	ASP
1	D	213	SER
1	D	214	THR
1	D	222	SER
1	D	225	SER
1	D	237	THR
1	D	256	MET
1	D	258	GLN
1	D	262	ARG
1	D	271	LEU
1	D	291	ARG
1	D	299	VAL
1	D	356	MET
1	D	362	GLU
1	D	365	THR
1	D	371	LEU
1	D	381	THR
1	D	398	THR
1	D	413	ASN
1	D	418	ASP
1	D	419	LEU
1	D	424	GLN
1	D	425	SER
1	D	427	ILE
1	D	429	GLN
1	D	436	LEU
1	D	450	LEU
1	D	452	LEU
1	D	453	LEU
1	D	455	LYS
1	D	459	LEU
1	D	475	LEU
1	D	502	ARG
1	D	505	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	124	GLN
1	B	175	GLN
1	B	216	HIS
1	B	266	HIS
1	B	274	GLN
1	B	347	ASN
1	B	424	GLN
1	B	469	ASN
1	B	480	GLN
1	B	533	GLN
1	A	124	GLN
1	A	175	GLN
1	A	216	HIS
1	A	266	HIS
1	A	274	GLN
1	A	424	GLN
1	A	469	ASN
1	A	480	GLN
1	C	124	GLN
1	C	175	GLN
1	C	266	HIS
1	C	274	GLN
1	C	424	GLN
1	C	469	ASN
1	C	480	GLN
1	D	124	GLN
1	D	175	GLN
1	D	216	HIS
1	D	266	HIS
1	D	274	GLN
1	D	424	GLN
1	D	469	ASN
1	D	480	GLN

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 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	B	601	-	54,58,58	1.41	7 (12%)	71,89,89	1.80	18 (25%)
2	FAD	D	601	-	54,58,58	1.67	9 (16%)	71,89,89	1.64	15 (21%)
2	FAD	C	601	-	54,58,58	1.71	8 (14%)	71,89,89	1.71	17 (23%)
2	FAD	A	601	-	54,58,58	1.79	9 (16%)	71,89,89	1.57	13 (18%)

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	B	601	-	-	7/30/50/50	0/6/6/6
2	FAD	D	601	-	-	11/30/50/50	0/6/6/6
2	FAD	C	601	-	-	11/30/50/50	0/6/6/6
2	FAD	A	601	-	-	8/30/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C9A-C5X	7.05	1.52	1.41
2	D	601	FAD	C9A-C5X	6.32	1.51	1.41
2	B	601	FAD	C9A-C5X	5.81	1.50	1.41
2	C	601	FAD	C9A-C5X	5.43	1.49	1.41
2	C	601	FAD	PA-O3P	5.42	1.65	1.59
2	C	601	FAD	P-O3P	5.12	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C1'-C2'	4.10	1.58	1.52
2	A	601	FAD	C8-C7	4.01	1.50	1.40
2	A	601	FAD	P-O3P	3.86	1.63	1.59
2	D	601	FAD	C10-N10	3.57	1.45	1.37
2	A	601	FAD	PA-O3P	3.53	1.63	1.59
2	D	601	FAD	C8-C7	3.51	1.49	1.40
2	B	601	FAD	C10-N10	3.24	1.44	1.37
2	C	601	FAD	C8-C7	3.11	1.48	1.40
2	D	601	FAD	PA-O3P	3.03	1.62	1.59
2	D	601	FAD	P-O3P	3.02	1.62	1.59
2	D	601	FAD	C4-N3	-2.99	1.33	1.38
2	B	601	FAD	C8-C7	2.94	1.48	1.40
2	A	601	FAD	C10-N10	2.86	1.43	1.37
2	C	601	FAD	C2'-C3'	-2.72	1.48	1.53
2	C	601	FAD	C10-N10	2.65	1.43	1.37
2	B	601	FAD	C4-N3	-2.56	1.34	1.38
2	D	601	FAD	C4X-N5	2.51	1.36	1.30
2	D	601	FAD	C1'-C2'	2.40	1.56	1.52
2	C	601	FAD	C4-N3	-2.38	1.34	1.38
2	C	601	FAD	C4X-N5	2.32	1.35	1.30
2	B	601	FAD	C2-N3	-2.31	1.33	1.39
2	D	601	FAD	C2-N3	-2.26	1.34	1.39
2	B	601	FAD	C5X-N5	-2.16	1.35	1.39
2	A	601	FAD	O4B-C1B	2.15	1.43	1.40
2	B	601	FAD	C4X-N5	2.05	1.35	1.30
2	A	601	FAD	C2A-N3A	2.03	1.35	1.32
2	A	601	FAD	C9A-N10	2.02	1.44	1.41

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	N3A-C2A-N1A	-5.68	120.96	128.67
2	B	601	FAD	N3A-C2A-N1A	-5.12	121.72	128.67
2	C	601	FAD	C4'-C3'-C2'	-5.07	105.14	113.57
2	B	601	FAD	C5'-C4'-C3'	4.86	121.39	112.22
2	D	601	FAD	N3A-C2A-N1A	-4.76	122.21	128.67
2	C	601	FAD	N3A-C2A-N1A	-4.69	122.31	128.67
2	C	601	FAD	C4-C4X-N5	3.99	123.71	118.21
2	D	601	FAD	C4X-C10-N1	-3.93	114.96	124.59
2	B	601	FAD	O4B-C1B-N9A	3.91	113.93	108.75
2	C	601	FAD	O4B-C1B-N9A	-3.39	104.25	108.75
2	B	601	FAD	O2P-P-O3P	-3.37	98.16	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	O4-C4-C4X	-3.36	117.66	126.53
2	B	601	FAD	C4X-C10-N1	-3.36	116.35	124.59
2	D	601	FAD	C4X-C10-N10	3.32	121.23	116.48
2	A	601	FAD	C4A-C5A-N7A	-3.25	105.91	109.34
2	D	601	FAD	C10-N1-C2	3.24	123.87	116.85
2	B	601	FAD	C4B-O4B-C1B	-3.24	106.96	109.92
2	D	601	FAD	C4A-C5A-N7A	-3.24	105.92	109.34
2	B	601	FAD	C1B-N9A-C4A	-3.23	120.97	126.64
2	D	601	FAD	C4-C4X-N5	3.21	122.64	118.21
2	D	601	FAD	O2P-P-O1P	3.11	126.89	112.44
2	B	601	FAD	O2A-PA-O1A	3.06	126.70	112.44
2	C	601	FAD	C4B-O4B-C1B	-3.03	107.15	109.92
2	D	601	FAD	C5X-N5-C4X	2.96	122.88	118.09
2	D	601	FAD	C10-C4X-N5	-2.86	118.96	124.81
2	A	601	FAD	O2A-PA-O1A	2.80	125.46	112.44
2	B	601	FAD	O3'-C3'-C4'	2.80	115.28	108.93
2	A	601	FAD	O5B-PA-O1A	-2.78	97.93	108.94
2	C	601	FAD	O2-C2-N1	-2.68	117.35	121.80
2	C	601	FAD	O2A-PA-O1A	2.67	124.86	112.44
2	C	601	FAD	C4X-C10-N10	2.66	120.29	116.48
2	A	601	FAD	C4X-C10-N1	-2.65	118.09	124.59
2	B	601	FAD	O4'-C4'-C5'	-2.64	104.17	109.99
2	B	601	FAD	C4-N3-C2	-2.63	120.98	125.64
2	A	601	FAD	C9A-N10-C10	-2.62	116.76	120.75
2	C	601	FAD	C4X-C10-N1	-2.60	118.22	124.59
2	C	601	FAD	C1B-N9A-C4A	-2.59	122.09	126.64
2	B	601	FAD	C4-C4X-N5	2.57	121.75	118.21
2	C	601	FAD	C5X-N5-C4X	2.44	122.04	118.09
2	C	601	FAD	C10-C4X-N5	-2.43	119.85	124.81
2	C	601	FAD	C4A-C5A-N7A	-2.41	106.79	109.34
2	B	601	FAD	C4X-C10-N10	2.40	119.92	116.48
2	D	601	FAD	C1'-C2'-C3'	2.39	116.14	109.66
2	D	601	FAD	O2A-PA-O1A	2.36	123.41	112.44
2	B	601	FAD	C10-N1-C2	2.35	121.93	116.85
2	A	601	FAD	C1'-C2'-C3'	2.29	115.88	109.66
2	B	601	FAD	N3-C2-N1	2.26	124.30	119.50
2	D	601	FAD	C4-N3-C2	-2.23	121.69	125.64
2	C	601	FAD	O2A-PA-O3P	2.23	113.29	107.27
2	C	601	FAD	C10-N1-C2	2.21	121.63	116.85
2	B	601	FAD	C4X-C4-N3	2.20	118.86	113.25
2	A	601	FAD	C10-N1-C2	2.17	121.55	116.85
2	C	601	FAD	C4-N3-C2	-2.16	121.80	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4X-C4-N3	2.16	118.76	113.25
2	A	601	FAD	C2'-C1'-N10	2.13	120.28	110.20
2	A	601	FAD	O2-C2-N1	-2.11	118.29	121.80
2	B	601	FAD	C5X-N5-C4X	2.11	121.49	118.09
2	D	601	FAD	O2P-P-O5'	-2.09	98.08	107.57
2	D	601	FAD	C9-C9A-N10	2.04	124.60	121.85
2	A	601	FAD	C5'-C4'-C3'	2.04	116.07	112.22
2	B	601	FAD	C10-C4X-N5	-2.03	120.66	124.81
2	C	601	FAD	C4X-C4-N3	2.03	118.42	113.25
2	D	601	FAD	C4X-C4-N3	2.02	118.39	113.25

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	C5'-O5'-P-O2P
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	C	601	FAD	C5B-O5B-PA-O2A
2	C	601	FAD	C5B-O5B-PA-O3P
2	C	601	FAD	N10-C1'-C2'-O2'
2	C	601	FAD	N10-C1'-C2'-C3'
2	C	601	FAD	C2'-C3'-C4'-O4'
2	C	601	FAD	C2'-C3'-C4'-C5'
2	C	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	O3'-C3'-C4'-C5'
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O3P
2	D	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	N10-C1'-C2'-C3'
2	D	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B

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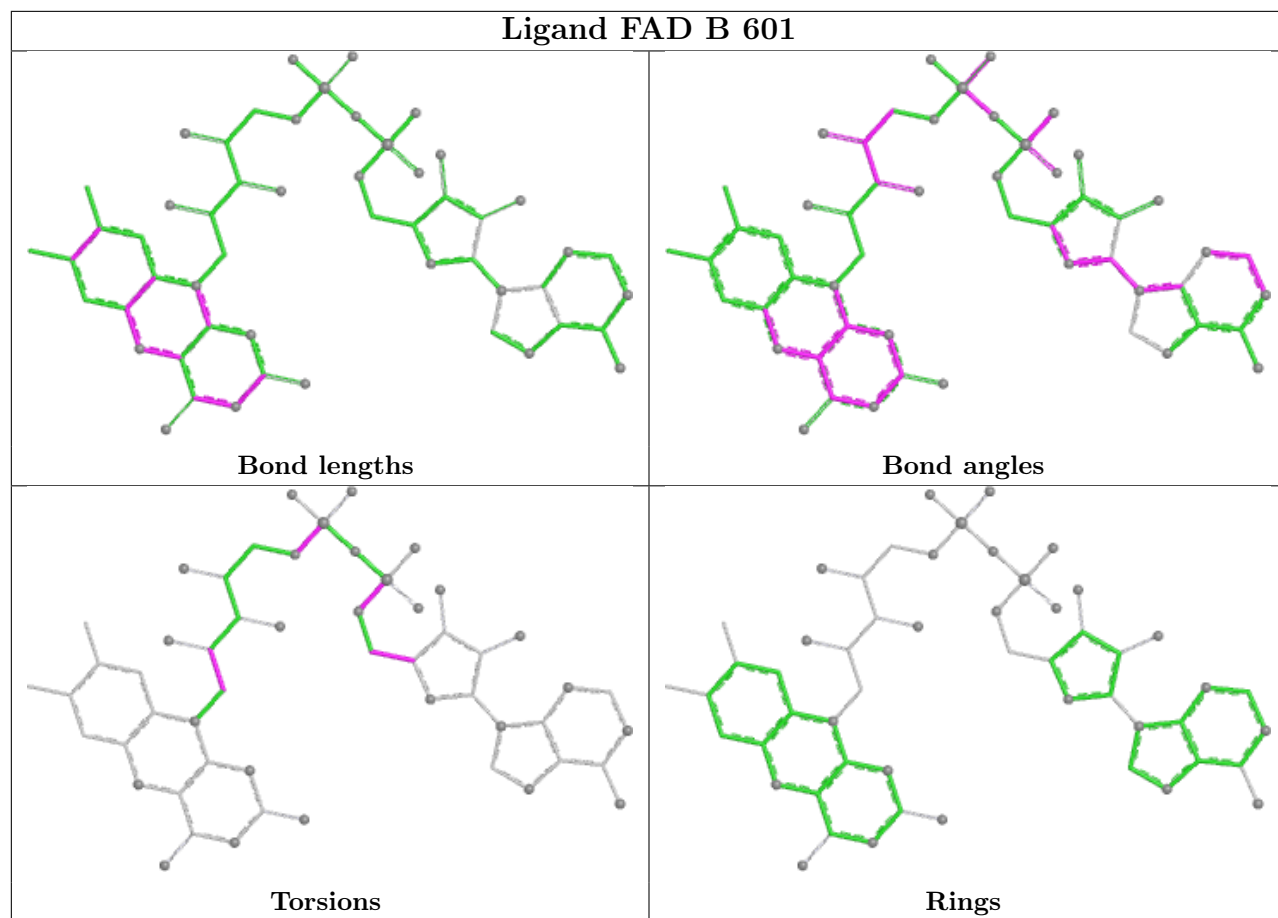
Mol	Chain	Res	Type	Atoms
2	D	601	FAD	C2'-C3'-C4'-C5'
2	D	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	P-O3P-PA-O5B
2	A	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	O4B-C4B-C5B-O5B

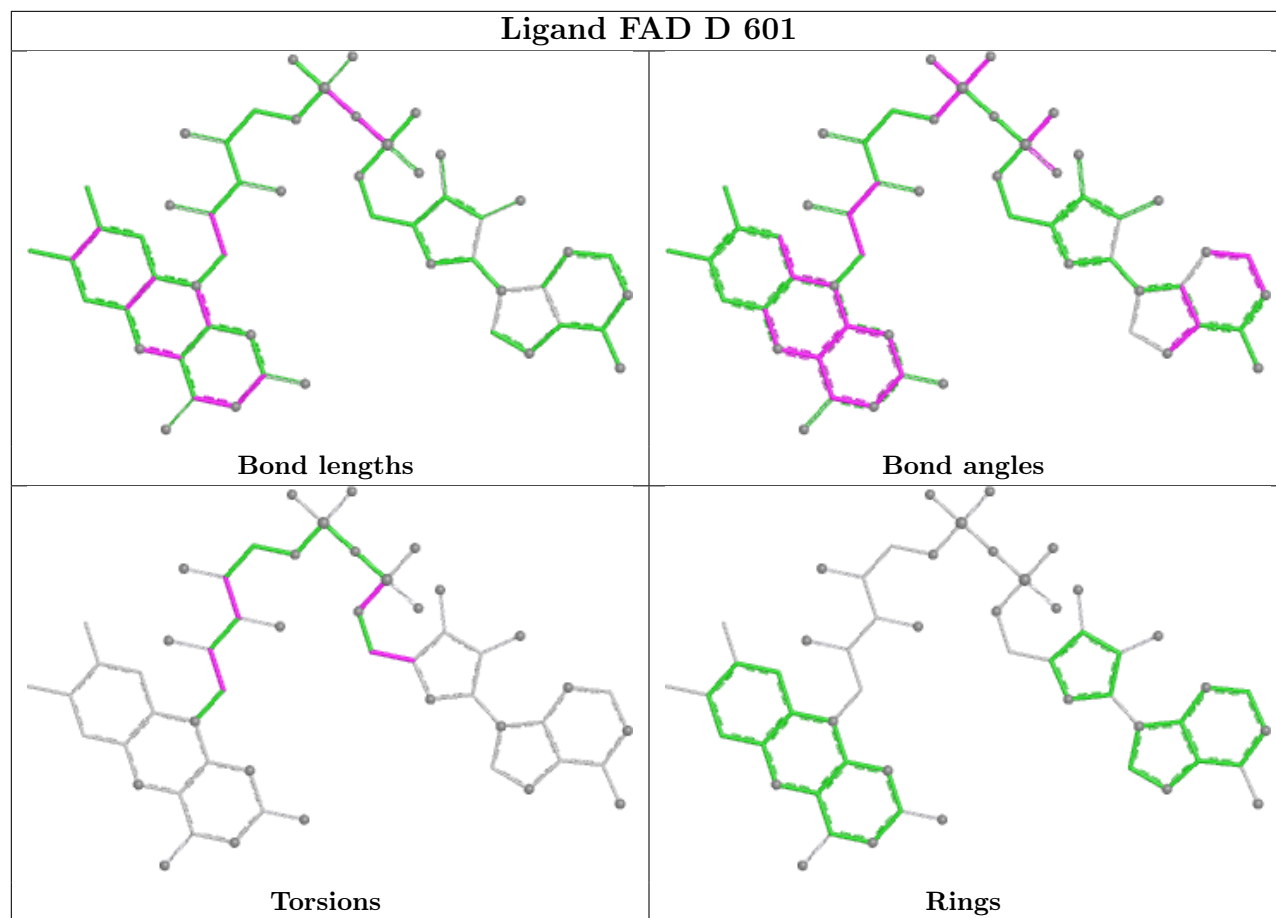
There are no ring outliers.

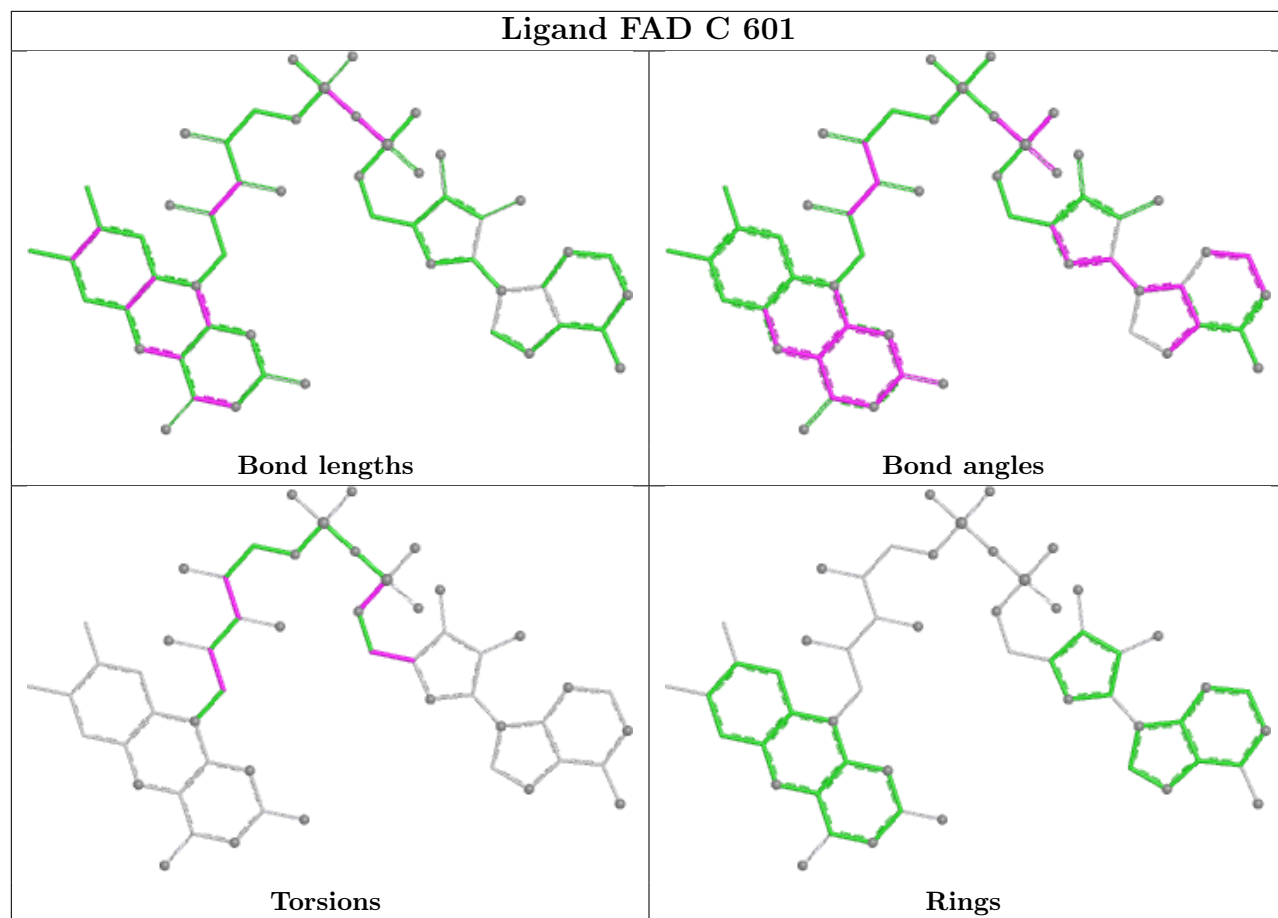
3 monomers are involved in 4 short contacts:

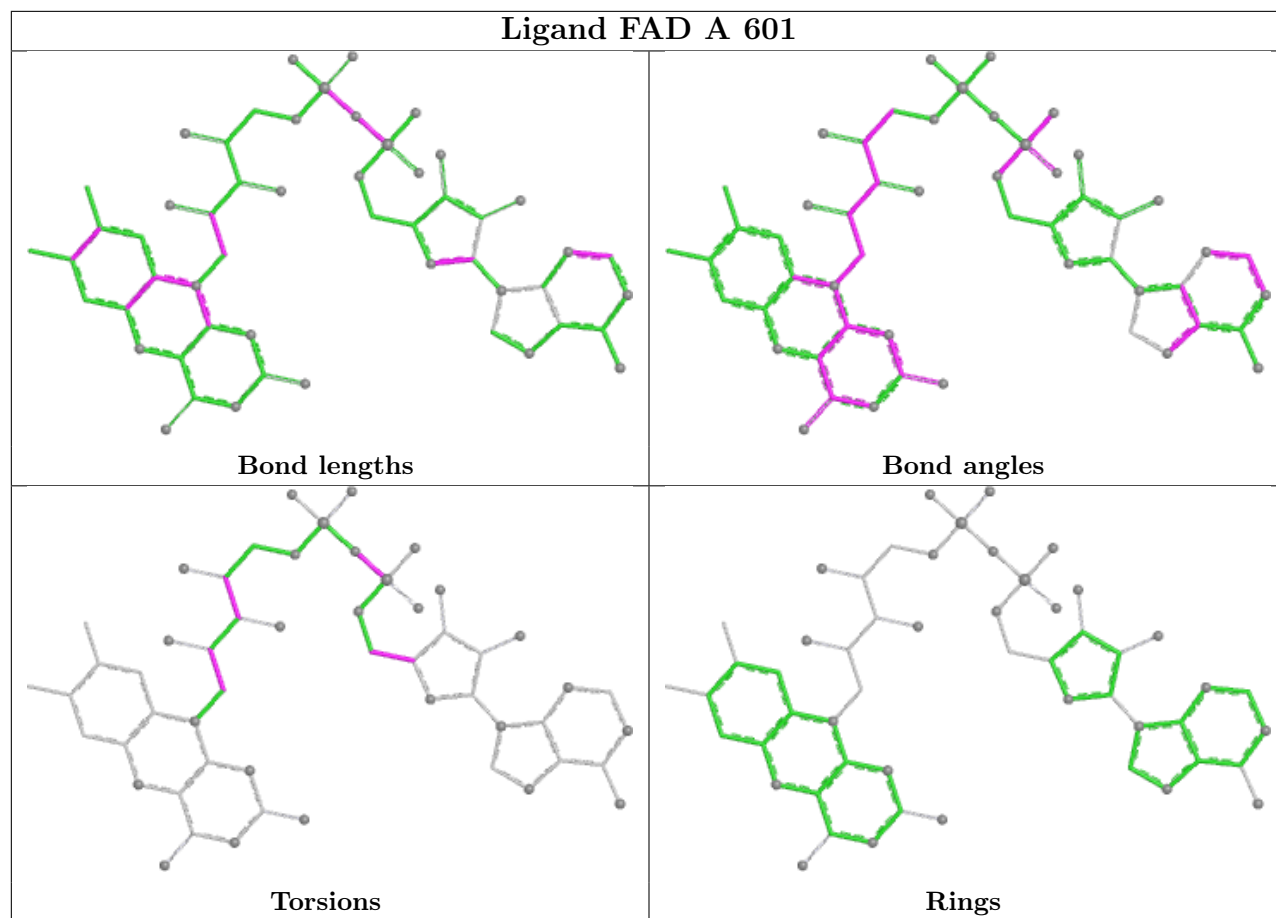
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	1	0
2	C	601	FAD	2	0
2	A	601	FAD	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	519/535 (97%)	-0.04	18 (3%) 44 34	46, 79, 129, 175	0
1	B	530/535 (99%)	0.08	27 (5%) 28 19	47, 84, 144, 219	0
1	C	520/535 (97%)	-0.08	6 (1%) 79 73	50, 80, 133, 173	0
1	D	520/535 (97%)	-0.01	23 (4%) 34 24	51, 83, 134, 190	0
All	All	2089/2140 (97%)	-0.01	74 (3%) 44 34	46, 82, 133, 219	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	277	TYR	9.1
1	D	279	MET	6.0
1	B	530	PHE	5.2
1	D	137	SER	4.8
1	D	136	GLN	4.5
1	A	449	LEU	4.4
1	B	519	LEU	4.3
1	C	517	LYS	4.2
1	D	309	THR	4.0
1	B	254	TRP	3.9
1	D	138	ALA	3.9
1	D	254	TRP	3.8
1	C	449	LEU	3.8
1	C	454	LEU	3.8
1	B	533	GLN	3.7
1	B	510	PHE	3.7
1	B	511	PRO	3.6
1	B	4	LYS	3.6
1	B	134	LYS	3.6
1	D	518	ILE	3.5
1	A	254	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	167	LYS	3.3
1	B	29	THR	3.3
1	A	518	ILE	3.2
1	C	419	LEU	3.2
1	A	132	ASN	3.2
1	D	277	TYR	3.2
1	A	517	LYS	3.1
1	B	170	TYR	3.1
1	B	348	ASN	3.0
1	B	130	GLU	3.0
1	B	168	GLY	3.0
1	B	111	LEU	2.9
1	D	452	LEU	2.8
1	B	507	SER	2.7
1	D	116	CYS	2.7
1	D	158	GLN	2.7
1	A	446	LYS	2.7
1	A	454	LEU	2.6
1	A	452	LEU	2.6
1	B	163	ILE	2.5
1	A	515	LEU	2.5
1	A	440	ALA	2.5
1	D	249	ARG	2.5
1	B	129	THR	2.5
1	A	450	LEU	2.4
1	D	420	PHE	2.4
1	B	6	ALA	2.4
1	B	454	LEU	2.4
1	A	485	ARG	2.4
1	B	521	LEU	2.4
1	C	158	GLN	2.4
1	B	327	PHE	2.3
1	D	242	MET	2.3
1	B	424	GLN	2.3
1	D	360	HIS	2.3
1	D	246	VAL	2.3
1	B	31	PHE	2.2
1	D	127	ILE	2.2
1	A	448	ASP	2.2
1	A	489	PHE	2.2
1	A	447	PRO	2.2
1	D	336	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	251	VAL	2.2
1	B	529	PHE	2.1
1	B	5	VAL	2.1
1	D	114	LYS	2.1
1	A	531	GLN	2.1
1	B	341	SER	2.1
1	D	160	PHE	2.1
1	B	512	VAL	2.0
1	D	312	ILE	2.0
1	A	475	LEU	2.0
1	D	419	LEU	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](#)

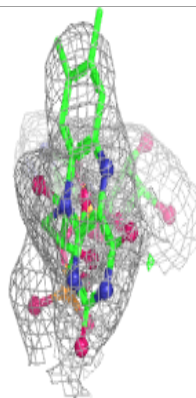
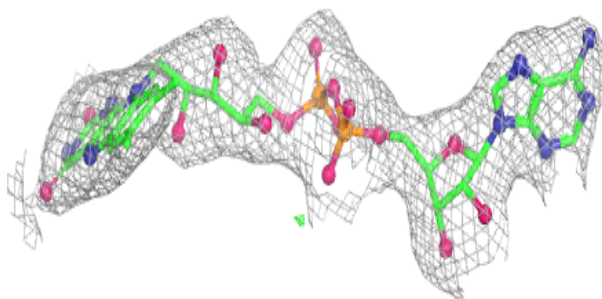
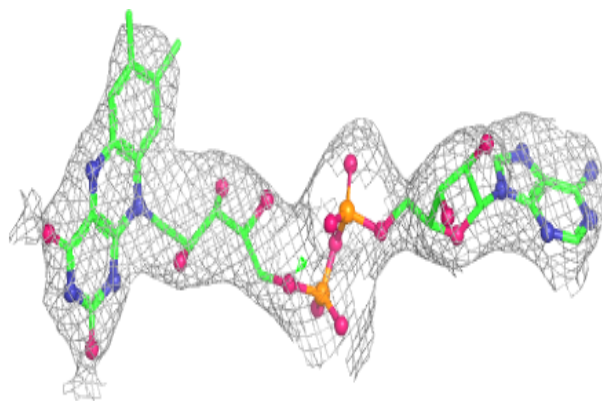
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	601	53/53	0.95	0.17	62,81,98,105	0
2	FAD	C	601	53/53	0.96	0.16	51,75,101,104	0
2	FAD	A	601	53/53	0.97	0.15	49,65,89,96	0
2	FAD	D	601	53/53	0.97	0.17	58,79,101,113	0

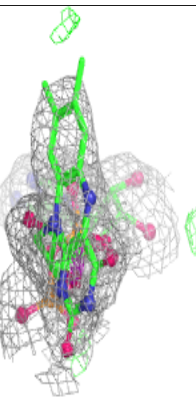
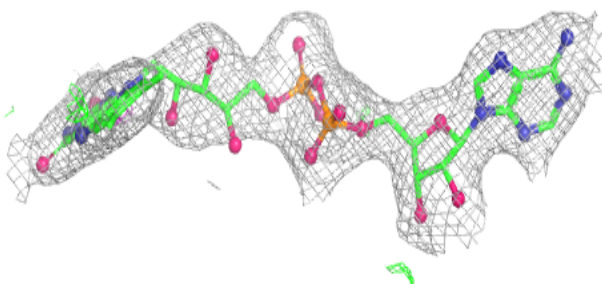
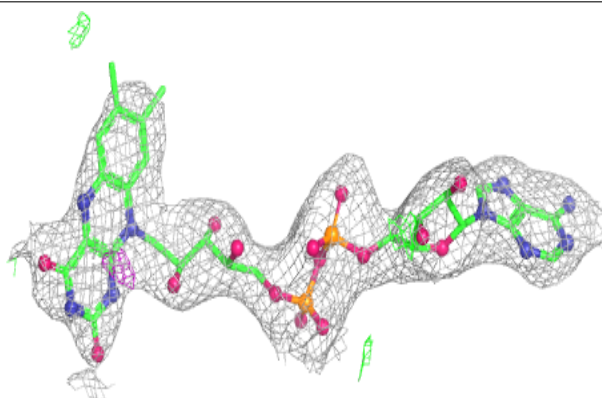
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 601:

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

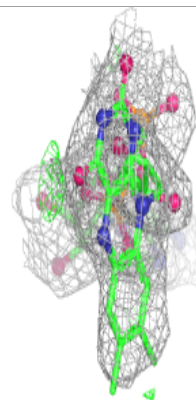
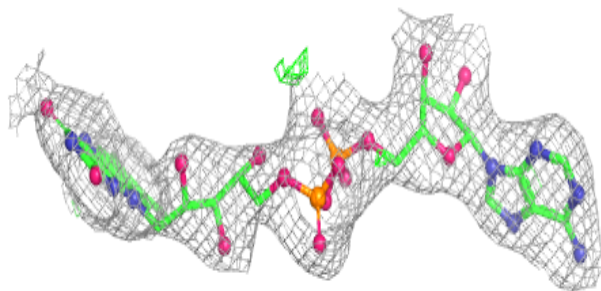
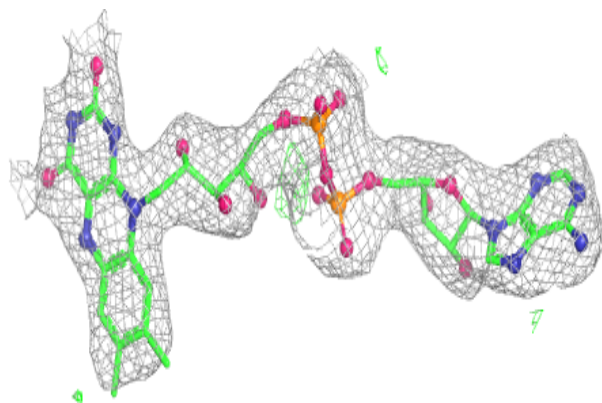
**Electron density around FAD C 601:**

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

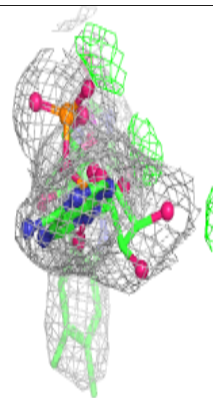
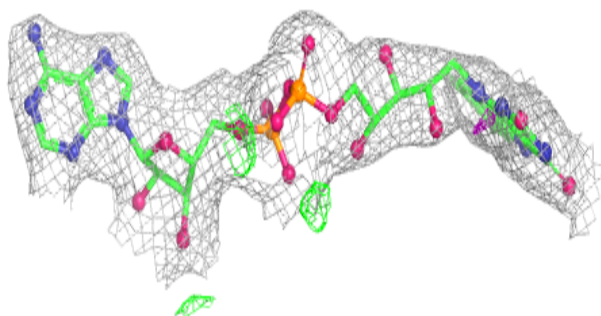
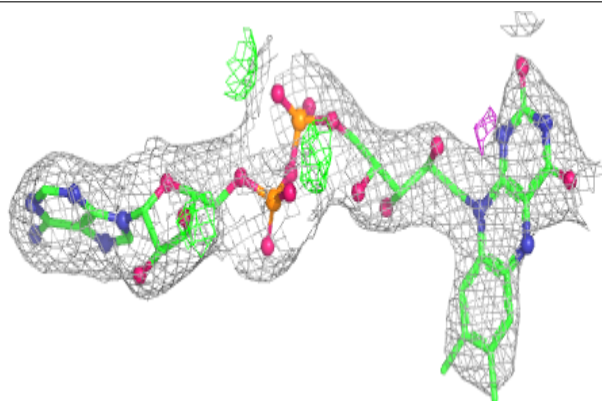


Electron density around FAD A 601:

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

**Electron density around FAD D 601:**

$2mF_o-DF_c$ (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.