



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:32 PM UTC

PDB ID : 6SEM / pdb_00006sem
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

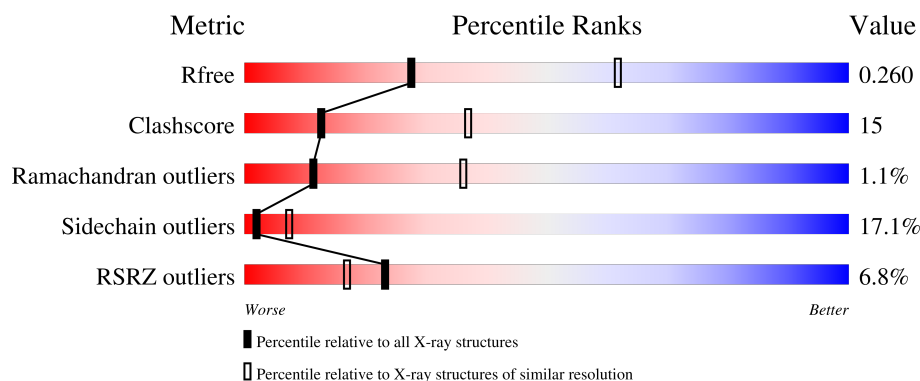
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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	5% 60% 29% 7%
1	B	535	10% 59% 32% 8%
1	C	535	7% 60% 30% 6%
1	D	535	5% 61% 29% 6%

2 Entry composition i

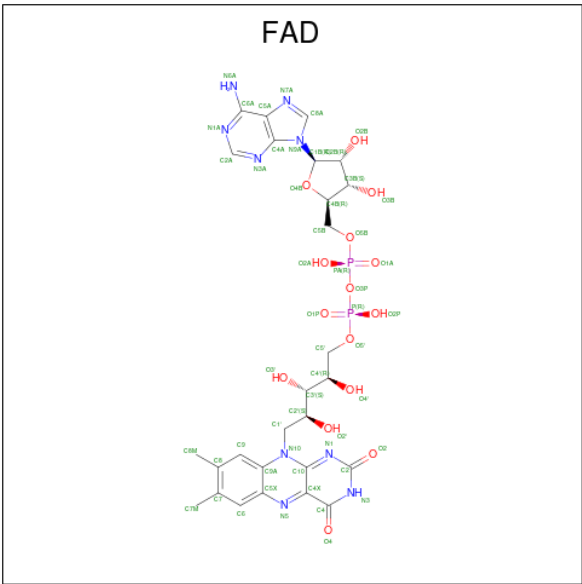
There are 3 unique types of molecules in this entry. The entry contains 16904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

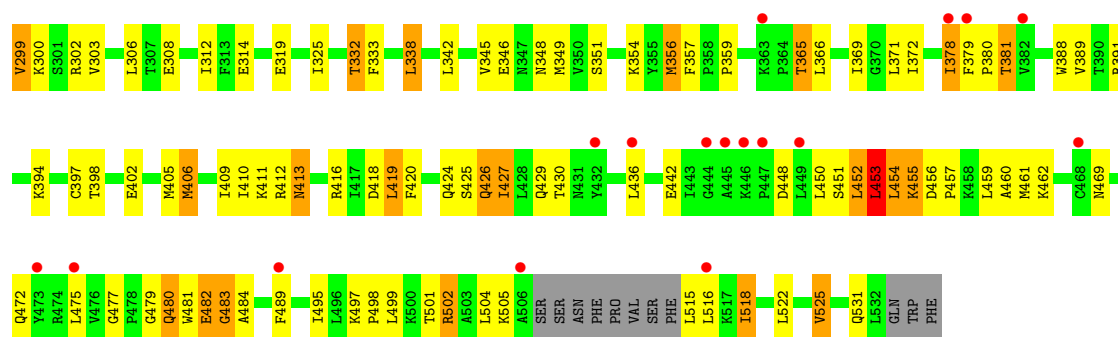


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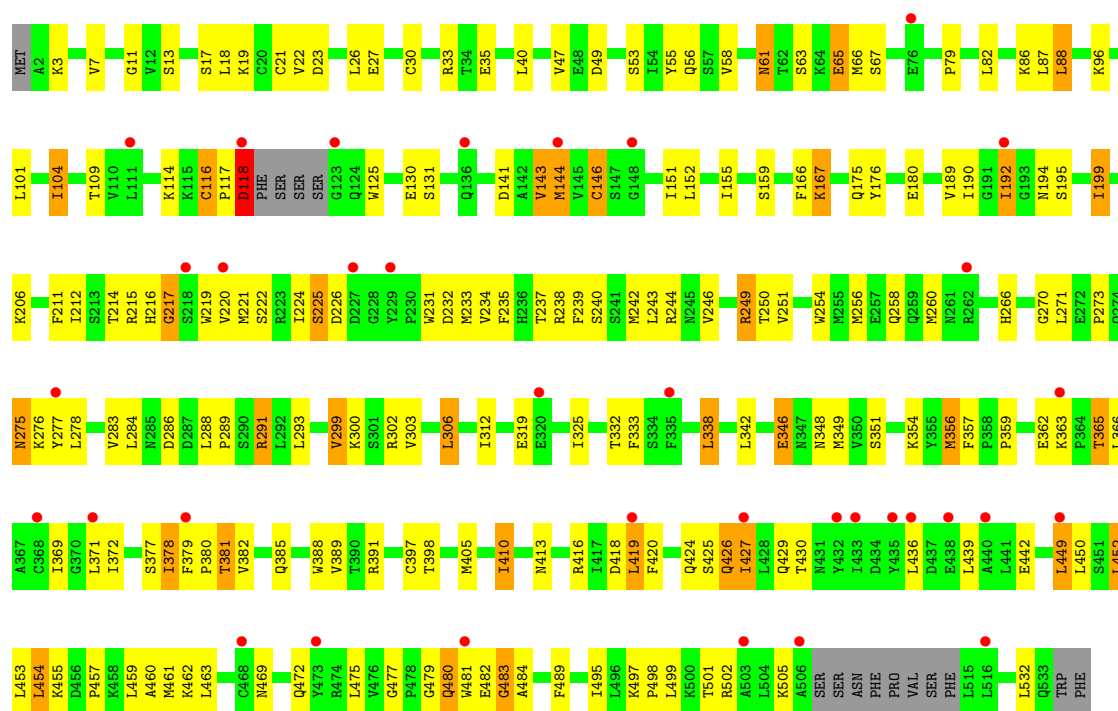
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is water.

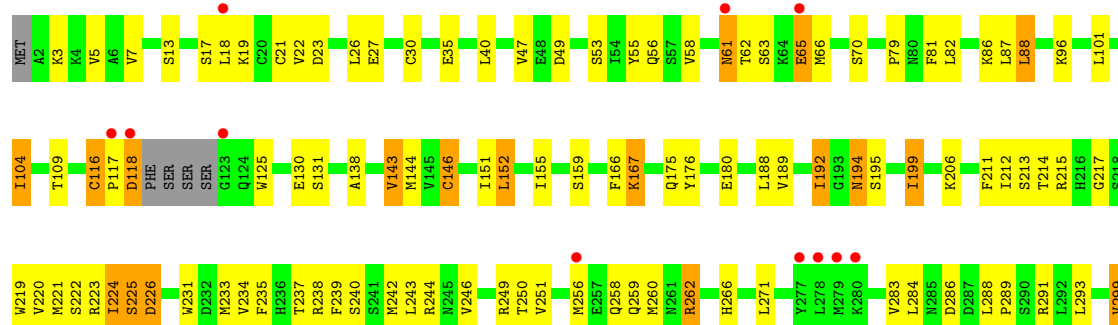
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	16	Total	O	0	0
			16	16		
3	A	10	Total	O	0	0
			10	10		
3	C	15	Total	O	0	0
			15	15		
3	D	12	Total	O	0	0
			12	12		



• 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 48.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	58.3 (48.40-2.80) 61.0 (48.40-2.80)	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	2375 reflections (4.83%)	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)	0.28 , 47.3	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

5.1 Standard geometry

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	0.70	0/4235	1.07	3/5725 (0.1%)
1	B	0.70	0/4364	1.06	7/5902 (0.1%)
1	C	0.71	0/4225	1.07	2/5712 (0.0%)
1	D	0.71	0/4213	1.06	5/5697 (0.1%)
All	All	0.71	0/17037	1.07	17/23036 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ASP	CA-CB-CG	9.60	122.19	112.60
1	A	118	ASP	CA-CB-CG	8.52	121.12	112.60
1	B	118	ASP	CA-CB-CG	8.44	121.03	112.60
1	C	118	ASP	CA-CB-CG	8.16	120.76	112.60
1	B	340	ASP	CA-CB-CG	8.13	120.73	112.60
1	B	529	PHE	CA-CB-CG	7.09	120.89	113.80
1	D	453	LEU	N-CA-C	-6.91	104.49	113.12
1	D	363	LYS	CB-CA-C	6.15	116.72	109.47
1	B	363	LYS	CB-CA-C	5.90	116.43	109.47
1	C	363	LYS	CB-CA-C	5.86	116.38	109.47
1	B	530	PHE	CA-CB-CG	5.77	119.57	113.80
1	B	453	LEU	N-CA-C	-5.51	107.20	114.04
1	D	62	THR	CA-C-N	5.47	130.12	120.87
1	D	62	THR	C-N-CA	5.47	130.12	120.87
1	A	453	LEU	N-CA-C	-5.37	105.54	112.68
1	A	456	ASP	CB-CA-C	-5.30	107.44	111.20
1	B	501	THR	CB-CA-C	5.07	118.81	109.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4138	0	4142	152	0
1	B	4257	0	4262	134	0
1	C	4128	0	4104	127	0
1	D	4116	0	4068	129	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	10	0	0	0	0
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	511	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 15.

All (511) 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:349:MET:HE1	1:A:410:ILE:HA	1.40	1.03
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:349:MET:CE	1:A:410:ILE:HA	2.13	0.78
1:A:502:ARG:HG3	1:D:300:LYS:C	2.11	0.76
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:453:LEU:HD22	1:D:453:LEU:C	2.21	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
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:A:502:ARG:CG	1:D:300:LYS:C	2.71	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:B:219:TRP:HB3	1:B:260:MET:HE2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:47:VAL:HG23	1:B:47:VAL:O	2.00	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:C:219:TRP:HB3	1:C:260:MET:HE2	1.84	0.59
1:B:512:VAL:HG21	1:C:276:LYS:HZ2	1.68	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
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:A:221:MET:HB2	1:A:260:MET:HE1	1.84	0.58
1:B:249:ARG:HH12	1:B:419:LEU:HG	1.69	0.58
1:B:221:MET:HB2	1:B:260:MET:HE1	1.86	0.58
1:A:505:LYS:O	1:A:505:LYS:HG2	2.03	0.58
1:C:221:MET:HB2	1:C:260:MET:HE1	1.86	0.57
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:453:LEU:HD22	1:A:453:LEU:C	2.30	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:219:TRP:HB3	1:A:260:MET:HE2	1.85	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:D:221:MET:HB2	1:D:260:MET:HE1	1.87	0.57
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:512:VAL:HG21	1:C:276:LYS:NZ	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:H	1:B:266:HIS:HE1	1.51	0.56
1:B:233:MET:HE1	1:B:495:ILE:CD1	2.36	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:A:349:MET:HE2	1:A:409:ILE:HG22	1.88	0.56
1:B:65:GLU:OE1	1:B:65:GLU:HA	2.05	0.56
1:D:233:MET:HE1	1:D:495:ILE:CD1	2.36	0.55
1:C:231:TRP:O	1:C:234:VAL:HG22	2.07	0.55
1:A:349:MET:HE3	1:A:413:ASN:HB3	1.87	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:C:233:MET:HE1	1:C:495:ILE:CD1	2.36	0.55
1:D:231:TRP:O	1:D:234:VAL:HG22	2.07	0.55
1:D:349:MET:HE1	1:D:410:ILE:HG13	1.89	0.55
1:B:349:MET:HE1	1:B:410:ILE:HG13	1.88	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:420:PHE:HB3	1:A:426:GLN:HG2	1.88	0.54
1:D:219:TRP:HB3	1:D:260:MET:HE2	1.90	0.54
1:A:143:VAL:HG13	1:A:366:LEU:HD12	1.90	0.54
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:21:CYS:SG	1:D:144:MET:HE3	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:C:359:PRO:HA	1:C:405:MET:HE1	1.92	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:C:349:MET:HE1	1:C:410:ILE:HG13	1.91	0.51
1:D:388:TRP:CE3	1:D:442:GLU:HB3	2.45	0.51
1:A:63:SER:O	1:A:67:SER:OG	2.24	0.51
1:C:388:TRP:CE3	1:C:442:GLU:HB3	2.45	0.51
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:D:176:TYR:CD2	1:D:199:ILE:HD13	2.46	0.51
1:B:359:PRO:HA	1:B:405:MET:HE1	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:332:THR:OG1	1:A:333:PHE:N	2.40	0.49
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:B:21:CYS:SG	1:B:144:MET:HE1	2.52	0.49
1:A:21:CYS:SG	1:A:144:MET:HE1	2.53	0.49
1:A:453:LEU:C	1:A:453:LEU:CD2	2.85	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:D:453:LEU:C	1:D:453:LEU:CD2	2.85	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:359:PRO:HA	1:D:405:MET:HE1	1.94	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:B:233:MET:HE1	1:B:495:ILE:HD11	1.95	0.48
1:A:359:PRO:HA	1:A:405:MET:HE1	1.95	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:D:225:SER:O	1:D:226:ASP:C	2.57	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:21:CYS:SG	1:C:144:MET:HE1	2.53	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:B:513:SER:C	1:B:516:LEU:HD13	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HH12	1:A:419:LEU:HG	1.80	0.47
1:C:225:SER:O	1:C:226:ASP:C	2.58	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:A:451:SER:C	1:A:453:LEU:H	2.24	0.46
1:D:495:ILE:O	1:D:498:PRO:HD2	2.15	0.46
1:A:215:ARG:HD2	1:A:314:GLU:CD	2.36	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:225:SER:O	1:B:226:ASP:C	2.59	0.46
1:A:225:SER:O	1:A:226:ASP:C	2.58	0.46
1:D:221:MET:HE2	1:D:284:LEU:HD11	1.98	0.46
1:B:451:SER:C	1:B:453:LEU:H	2.24	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: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:233:MET:HE1	1:C:495:ILE:HD11	1.98	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:D:233:MET:HE1	1:D:495:ILE:HD11	1.97	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:C:87:LEU:O	1:C:88:LEU:C	2.60	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:C:63:SER:O	1:C:67:SER:OG	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:87:LEU:O	1:A:88:LEU:C	2.61	0.44
1:D:21:CYS:SG	1:D:144:MET:HE1	2.56	0.44
1:D:87:LEU:O	1:D:88:LEU:C	2.61	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: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: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:87:LEU:O	1:B:88:LEU:C	2.61	0.43
1:B:220:VAL:H	1:B:266:HIS:CE1	2.34	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:A:45:GLU:H	1:A:45:GLU:CD	2.27	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:287:ASP:CG	1:C:291:ARG:HH22	2.25	0.43
1:A:426:GLN:O	1:A:427:ILE:C	2.61	0.43
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.85	0.43
1:B:283:VAL:C	1:B:284:LEU:HD12	2.44	0.43
1:B:354:LYS:O	1:B:356:MET:HB2	2.19	0.43
1:D:426:GLN:O	1:D:427:ILE:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:ARG:NH1	1:C:397:CYS:SG	2.92	0.43
1:B:221:MET:HE2	1:B:284:LEU:HD11	2.01	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:B:426:GLN:O	1:B:427:ILE:C	2.61	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
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:379:PHE:N	1:A:380:PRO:HD2	2.34	0.42
1:C:221:MET:HE2	1:C:284:LEU:HD11	2.00	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:C:426:GLN:O	1:C:427:ILE:C	2.62	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:283:VAL:C	1:C:284:LEU:HD12	2.45	0.42
1:D:354:LYS:O	1:D:356:MET:HE2	2.19	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:141:ASP:O	1:A:365:THR:OG1	2.37	0.42
1:C:141:ASP:O	1:C:365:THR:OG1	2.38	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
1:A:17:SER:O	1:A:18:LEU:C	2.63	0.41
1:A:215:ARG:HB2	1:A:302:ARG:HB2	2.01	0.41
1:A:283:VAL:C	1:A:284:LEU:HD12	2.45	0.41
1:C:482:GLU:O	1:C:484:ALA:N	2.50	0.41
1:B:63:SER:O	1:B:67:SER:OG	2.24	0.41
1:A:194:ASN:HD21	1:A:283:VAL:HA	1.85	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:C:354:LYS:O	1:C:356:MET:HE2	2.19	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:250:THR:O	1:B:251:VAL:C	2.63	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: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:A:221:MET:HE2	1:A:284:LEU:HD11	2.01	0.41
1:C:250:THR:O	1:C:251:VAL:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:VAL:C	1:D:284:LEU:HD12	2.46	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
1:D:437:ASP:O	1:D:438:GLU:C	2.64	0.41
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:17:SER:O	1:B:18:LEU:C	2.63	0.40
1:B:242:MET:O	1:B:246:VAL:HG13	2.20	0.40
1:B:294:TYR:OH	1:C:286:ASP:OD1	2.32	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:A:250:THR:O	1:A:251:VAL:C	2.63	0.40
1:D:17:SER:O	1:D:18:LEU:C	2.63	0.40
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.85	0.40
1:D:250:THR:O	1:D:251:VAL:C	2.64	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:A:354:LYS:O	1:A:356:MET:HE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:SER:O	1:C:18:LEU:C	2.63	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
1:D:423:SER:C	1:D:425:SER:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	12	38
1	B	526/535 (98%)	462 (88%)	57 (11%)	7 (1%)	9	31
1	C	514/535 (96%)	457 (89%)	52 (10%)	5 (1%)	12	38
1	D	514/535 (96%)	457 (89%)	51 (10%)	6 (1%)	10	34
All	All	2067/2140 (97%)	1832 (89%)	212 (10%)	23 (1%)	11	36

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

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Mol	Chain	Res	Type
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%)	373 (82%)	80 (18%)	2	6
1	B	469/477 (98%)	387 (82%)	82 (18%)	2	7
1	C	448/477 (94%)	372 (83%)	76 (17%)	2	7
1	D	444/477 (93%)	372 (84%)	72 (16%)	2	8
All	All	1814/1908 (95%)	1504 (83%)	310 (17%)	2	7

All (310) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	LYS
1	B	22	VAL
1	B	27	GLU
1	B	35	GLU
1	B	40	LEU
1	B	49	ASP
1	B	53	SER
1	B	56	GLN
1	B	65	GLU

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Mol	Chain	Res	Type
1	B	86	LYS
1	B	88	LEU
1	B	96	LYS
1	B	101	LEU
1	B	104	ILE
1	B	109	THR
1	B	116	CYS
1	B	143	VAL
1	B	144	MET
1	B	146	CYS
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	192	ILE
1	B	194	ASN
1	B	199	ILE
1	B	206	LYS
1	B	214	THR
1	B	222	SER
1	B	224	ILE
1	B	225	SER
1	B	237	THR
1	B	256	MET
1	B	258	GLN
1	B	271	LEU
1	B	275	ASN
1	B	283	VAL
1	B	291	ARG
1	B	299	VAL
1	B	307	THR
1	B	308	GLU
1	B	312	ILE
1	B	338	LEU
1	B	340	ASP
1	B	351	SER
1	B	356	MET
1	B	362	GLU
1	B	371	LEU
1	B	378	ILE

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Mol	Chain	Res	Type
1	B	381	THR
1	B	398	THR
1	B	410	ILE
1	B	413	ASN
1	B	417	ILE
1	B	418	ASP
1	B	419	LEU
1	B	424	GLN
1	B	426	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	480	GLN
1	B	502	ARG
1	B	505	LYS
1	B	510	PHE
1	B	513	SER
1	B	517	LYS
1	B	522	LEU
1	B	525	VAL
1	B	530	PHE
1	B	531	GLN
1	B	533	GLN
1	B	535	PHE
1	A	3	LYS
1	A	27	GLU
1	A	35	GLU
1	A	40	LEU
1	A	53	SER
1	A	56	GLN
1	A	60	THR
1	A	65	GLU
1	A	86	LYS
1	A	88	LEU
1	A	96	LYS

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Mol	Chain	Res	Type
1	A	104	ILE
1	A	109	THR
1	A	114	LYS
1	A	116	CYS
1	A	118	ASP
1	A	135	GLU
1	A	143	VAL
1	A	144	MET
1	A	146	CYS
1	A	151	ILE
1	A	152	LEU
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	199	ILE
1	A	206	LYS
1	A	213	SER
1	A	214	THR
1	A	216	HIS
1	A	222	SER
1	A	223	ARG
1	A	224	ILE
1	A	225	SER
1	A	237	THR
1	A	256	MET
1	A	258	GLN
1	A	271	LEU
1	A	283	VAL
1	A	291	ARG
1	A	299	VAL
1	A	312	ILE
1	A	332	THR
1	A	338	LEU
1	A	346	GLU
1	A	351	SER
1	A	356	MET
1	A	365	THR
1	A	371	LEU
1	A	378	ILE

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Mol	Chain	Res	Type
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	426	GLN
1	A	427	ILE
1	A	429	GLN
1	A	436	LEU
1	A	452	LEU
1	A	453	LEU
1	A	454	LEU
1	A	455	LYS
1	A	459	LEU
1	A	469	ASN
1	A	475	LEU
1	A	480	GLN
1	A	482	GLU
1	A	502	ARG
1	A	516	LEU
1	A	518	ILE
1	A	525	VAL
1	A	531	GLN
1	C	3	LYS
1	C	22	VAL
1	C	26	LEU
1	C	27	GLU
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	65	GLU
1	C	86	LYS
1	C	88	LEU
1	C	96	LYS
1	C	101	LEU

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Mol	Chain	Res	Type
1	C	104	ILE
1	C	109	THR
1	C	114	LYS
1	C	116	CYS
1	C	118	ASP
1	C	143	VAL
1	C	144	MET
1	C	146	CYS
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	192	ILE
1	C	199	ILE
1	C	206	LYS
1	C	214	THR
1	C	215	ARG
1	C	222	SER
1	C	225	SER
1	C	237	THR
1	C	249	ARG
1	C	256	MET
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	306	LEU
1	C	312	ILE
1	C	338	LEU
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	378	ILE
1	C	381	THR
1	C	398	THR

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Mol	Chain	Res	Type
1	C	410	ILE
1	C	413	ASN
1	C	418	ASP
1	C	419	LEU
1	C	424	GLN
1	C	425	SER
1	C	426	GLN
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	469	ASN
1	C	475	LEU
1	C	480	GLN
1	C	532	LEU
1	D	3	LYS
1	D	22	VAL
1	D	27	GLU
1	D	35	GLU
1	D	40	LEU
1	D	49	ASP
1	D	53	SER
1	D	56	GLN
1	D	61	ASN
1	D	65	GLU
1	D	86	LYS
1	D	88	LEU
1	D	96	LYS
1	D	101	LEU
1	D	104	ILE
1	D	109	THR
1	D	116	CYS
1	D	143	VAL
1	D	146	CYS
1	D	151	ILE
1	D	152	LEU
1	D	155	ILE
1	D	167	LYS

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Mol	Chain	Res	Type
1	D	180	GLU
1	D	189	VAL
1	D	192	ILE
1	D	194	ASN
1	D	199	ILE
1	D	206	LYS
1	D	213	SER
1	D	214	THR
1	D	215	ARG
1	D	222	SER
1	D	224	ILE
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	307	THR
1	D	312	ILE
1	D	338	LEU
1	D	351	SER
1	D	356	MET
1	D	362	GLU
1	D	365	THR
1	D	371	LEU
1	D	378	ILE
1	D	381	THR
1	D	398	THR
1	D	410	ILE
1	D	413	ASN
1	D	418	ASP
1	D	419	LEU
1	D	424	GLN
1	D	425	SER
1	D	426	GLN
1	D	427	ILE
1	D	429	GLN
1	D	436	LEU
1	D	450	LEU
1	D	452	LEU

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Mol	Chain	Res	Type
1	D	453	LEU
1	D	455	LYS
1	D	459	LEU
1	D	469	ASN
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 (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	124	GLN
1	B	169	GLN
1	B	175	GLN
1	B	216	HIS
1	B	258	GLN
1	B	259	GLN
1	B	266	HIS
1	B	274	GLN
1	B	347	ASN
1	B	424	GLN
1	B	429	GLN
1	B	469	ASN
1	B	480	GLN
1	B	531	GLN
1	A	124	GLN
1	A	169	GLN
1	A	216	HIS
1	A	258	GLN
1	A	259	GLN
1	A	266	HIS
1	A	274	GLN
1	A	347	ASN
1	A	424	GLN
1	A	429	GLN
1	A	469	ASN
1	A	480	GLN
1	C	124	GLN
1	C	169	GLN
1	C	175	GLN
1	C	259	GLN
1	C	266	HIS

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Mol	Chain	Res	Type
1	C	274	GLN
1	C	347	ASN
1	C	424	GLN
1	C	429	GLN
1	C	469	ASN
1	C	480	GLN
1	D	124	GLN
1	D	169	GLN
1	D	175	GLN
1	D	216	HIS
1	D	259	GLN
1	D	266	HIS
1	D	274	GLN
1	D	347	ASN
1	D	424	GLN
1	D	429	GLN
1	D	469	ASN
1	D	480	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	A	601	-	58,58,58	1.90	11 (18%)	85,89,89	1.87	22 (25%)
2	FAD	B	601	-	58,58,58	1.56	12 (20%)	85,89,89	1.84	26 (30%)
2	FAD	C	601	-	58,58,58	1.87	13 (22%)	85,89,89	1.80	22 (25%)
2	FAD	D	601	-	58,58,58	1.79	15 (25%)	85,89,89	1.94	23 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	-	8/34/50/50	0/6/6/6
2	FAD	B	601	-	-	7/34/50/50	0/6/6/6
2	FAD	C	601	-	-	11/34/50/50	0/6/6/6
2	FAD	D	601	-	-	11/34/50/50	0/6/6/6

All (51) 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
2	C	601	FAD	C5A-C4A	5.09	1.48	1.39
2	A	601	FAD	C5A-C4A	4.22	1.46	1.39
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	C5A-C4A	3.78	1.45	1.39
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	C5A-C4A	3.48	1.45	1.39
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	P-O3P	3.02	1.62	1.59
2	A	601	FAD	C8A-N7A	3.00	1.37	1.31
2	D	601	FAD	C4-N3	-2.99	1.33	1.38
2	A	601	FAD	C5A-N7A	-2.96	1.33	1.39
2	B	601	FAD	C8-C7	2.94	1.48	1.40
2	C	601	FAD	C8A-N7A	2.90	1.37	1.31
2	A	601	FAD	C10-N10	2.86	1.43	1.37
2	C	601	FAD	C5A-C6A	2.72	1.48	1.41
2	C	601	FAD	C2'-C3'	-2.72	1.48	1.53
2	D	601	FAD	C5A-C6A	2.66	1.48	1.41
2	C	601	FAD	C10-N10	2.65	1.43	1.37
2	B	601	FAD	C5A-N7A	-2.64	1.34	1.39
2	B	601	FAD	C4A-N9A	-2.63	1.32	1.37
2	A	601	FAD	C5A-C6A	2.60	1.48	1.41
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	C8A-N9A	-2.45	1.33	1.37
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	D	601	FAD	C8A-N7A	2.37	1.36	1.31
2	C	601	FAD	C4A-N9A	-2.33	1.32	1.37
2	D	601	FAD	C4A-N9A	-2.33	1.32	1.37
2	D	601	FAD	C5A-N7A	-2.32	1.34	1.39
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	C8A-N7A	2.22	1.35	1.31
2	B	601	FAD	C5X-N5	-2.16	1.35	1.39
2	C	601	FAD	C5A-N7A	-2.07	1.35	1.39
2	B	601	FAD	C4X-N5	2.05	1.35	1.30
2	A	601	FAD	C9A-N10	2.02	1.44	1.41
2	B	601	FAD	C5A-C6A	2.02	1.46	1.41

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C5A-C4A-N3A	-6.13	118.28	126.72
2	D	601	FAD	C5A-C4A-N3A	-5.85	118.66	126.72
2	C	601	FAD	C4'-C3'-C2'	-5.07	105.14	113.57
2	A	601	FAD	N3A-C2A-N1A	-5.04	120.96	128.58
2	B	601	FAD	C5'-C4'-C3'	4.86	121.39	112.22
2	D	601	FAD	N3A-C4A-N9A	4.78	135.30	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C5A-C4A-N3A	-4.72	120.21	126.72
2	B	601	FAD	N3A-C2A-N1A	-4.54	121.72	128.58
2	A	601	FAD	N3A-C4A-N9A	4.50	134.81	127.17
2	D	601	FAD	C4A-N9A-C8A	4.45	110.41	105.74
2	A	601	FAD	C2A-N3A-C4A	4.31	122.37	111.83
2	D	601	FAD	N3A-C2A-N1A	-4.21	122.21	128.58
2	D	601	FAD	C2A-N3A-C4A	4.16	121.99	111.83
2	C	601	FAD	N3A-C2A-N1A	-4.15	122.31	128.58
2	B	601	FAD	C4A-N9A-C8A	4.09	110.03	105.74
2	A	601	FAD	C4A-C5A-N7A	-4.09	105.91	110.58
2	D	601	FAD	C4A-C5A-N7A	-4.08	105.92	110.58
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	C	601	FAD	N3A-C4A-N9A	3.74	133.53	127.17
2	B	601	FAD	C5A-C4A-N3A	-3.55	121.83	126.72
2	C	601	FAD	C2A-N3A-C4A	3.55	120.50	111.83
2	D	601	FAD	N9A-C8A-N7A	-3.46	109.03	113.94
2	B	601	FAD	N3A-C4A-N9A	3.41	132.96	127.17
2	B	601	FAD	O2P-P-O3P	-3.37	98.16	107.27
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	B	601	FAD	C2A-N1A-C6A	3.32	124.18	118.73
2	D	601	FAD	C4X-C10-N10	3.32	121.23	116.48
2	C	601	FAD	C4A-C5A-N7A	-3.31	106.79	110.58
2	D	601	FAD	C5A-N7A-C8A	3.28	108.61	103.45
2	A	601	FAD	C5A-N7A-C8A	3.28	108.60	103.45
2	D	601	FAD	C10-N1-C2	3.24	123.87	116.85
2	A	601	FAD	C2A-N1A-C6A	3.21	124.01	118.73
2	D	601	FAD	C4-C4X-N5	3.21	122.64	118.21
2	B	601	FAD	C2A-N3A-C4A	3.16	119.56	111.83
2	D	601	FAD	O2P-P-O1P	3.11	126.89	112.44
2	C	601	FAD	C4A-N9A-C8A	3.08	108.97	105.74
2	B	601	FAD	O2A-PA-O1A	3.06	126.70	112.44
2	C	601	FAD	C2A-N1A-C6A	3.06	123.76	118.73
2	B	601	FAD	O4B-C1B-N9A	3.04	113.93	108.09
2	D	601	FAD	C5X-N5-C4X	2.96	122.88	118.09
2	A	601	FAD	N9A-C8A-N7A	-2.93	109.78	113.94
2	A	601	FAD	C4A-N9A-C8A	2.89	108.78	105.74
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	B	601	FAD	N9A-C8A-N7A	-2.79	109.97	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C6A-C5A-N7A	2.78	137.45	132.09
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	C	601	FAD	C2B-C1B-N9A	2.66	119.91	113.30
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	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	D	601	FAD	C6A-C5A-N7A	2.43	136.77	132.09
2	B	601	FAD	C4A-N9A-C1B	-2.42	120.97	126.63
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	C2A-N1A-C6A	2.37	122.62	118.73
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	A	601	FAD	C6A-C5A-N7A	2.27	136.47	132.09
2	B	601	FAD	N3-C2-N1	2.26	124.30	119.50
2	B	601	FAD	C6A-C5A-N7A	2.24	136.41	132.09
2	A	601	FAD	C2B-C1B-N9A	2.23	118.85	113.30
2	B	601	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
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
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	B	601	FAD	C5A-N7A-C8A	2.10	106.75	103.45
2	D	601	FAD	O2P-P-O5'	-2.09	98.08	107.57
2	C	601	FAD	C5A-N7A-C8A	2.04	106.66	103.45
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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'

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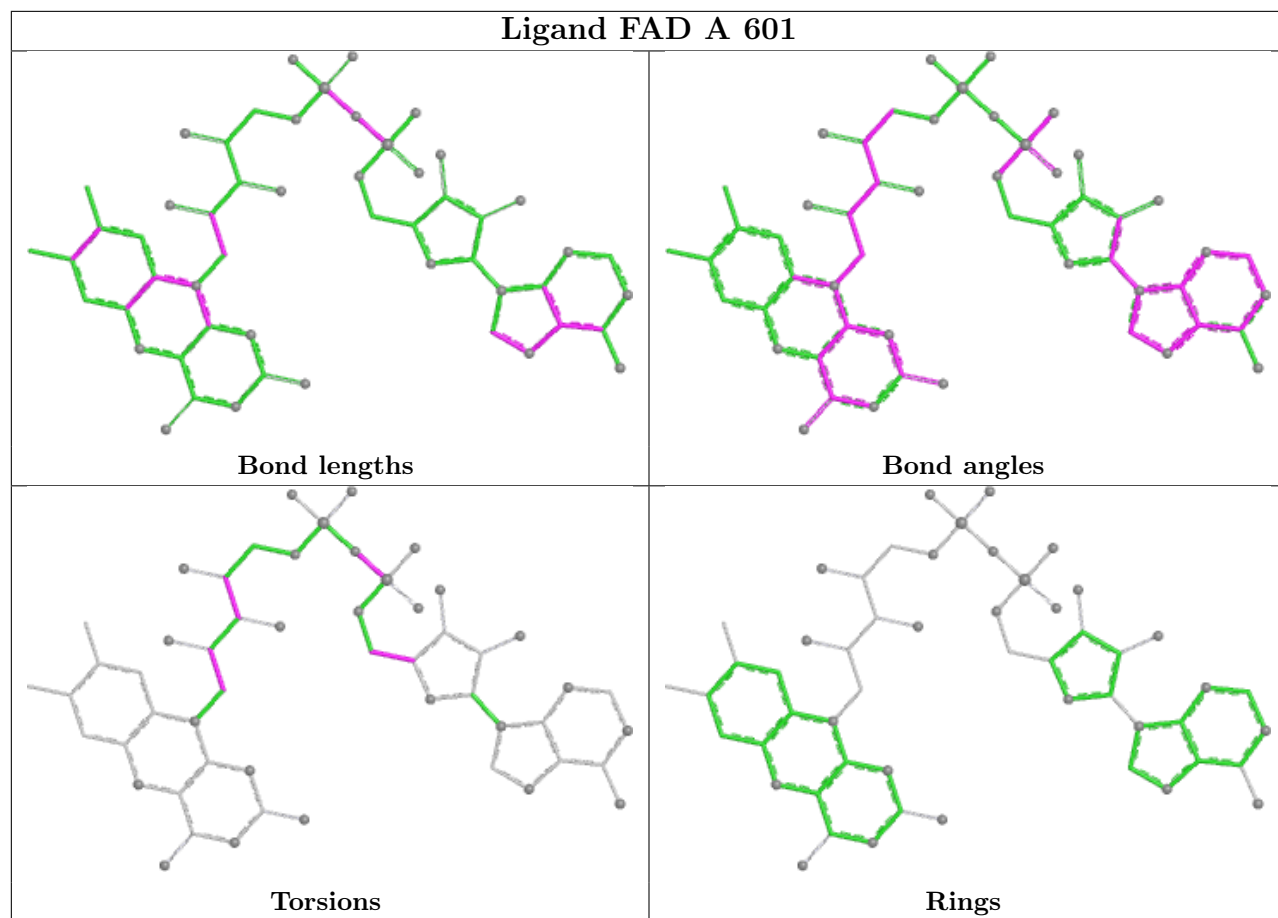
Mol	Chain	Res	Type	Atoms
2	C	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	O4B-C4B-C5B-O5B

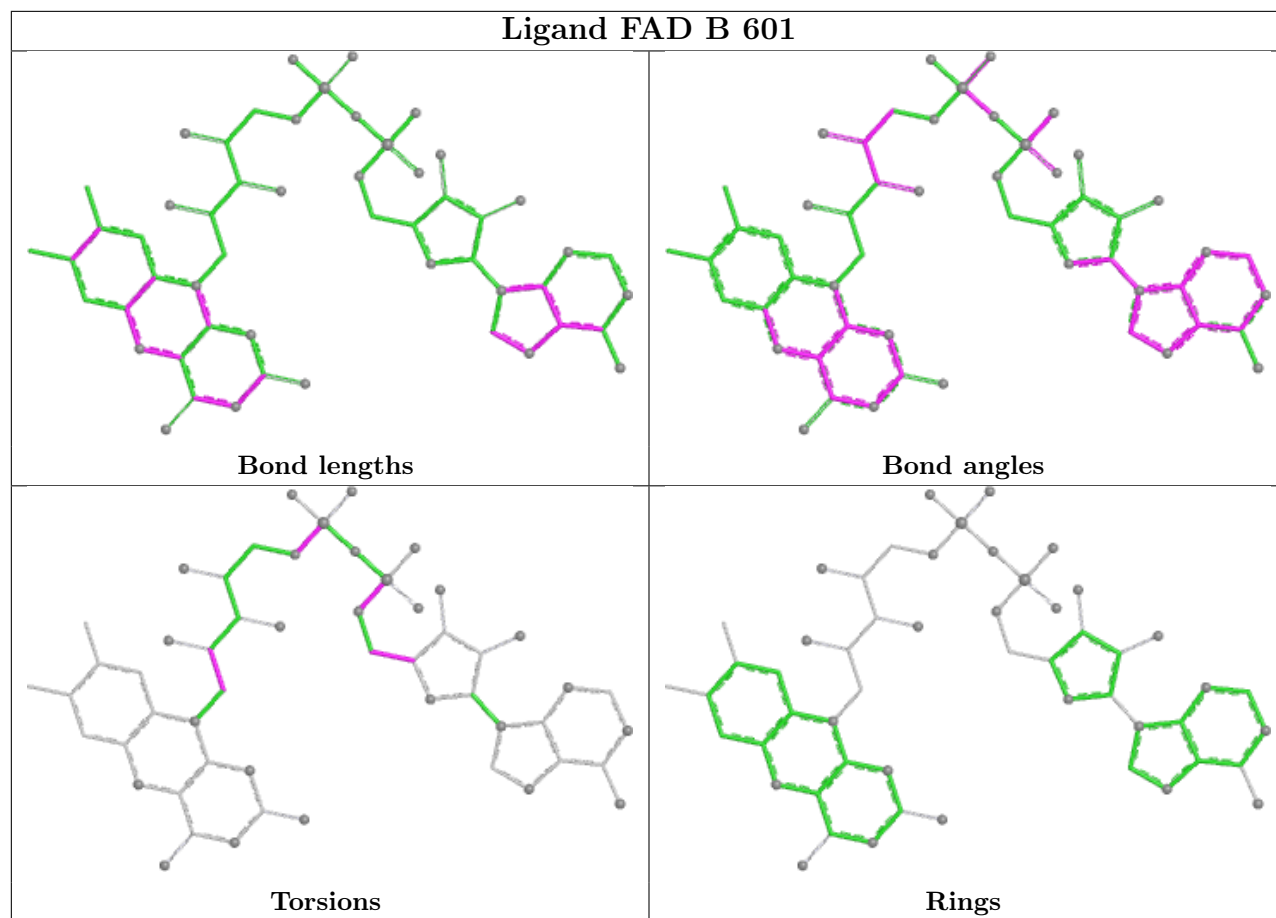
There are no ring outliers.

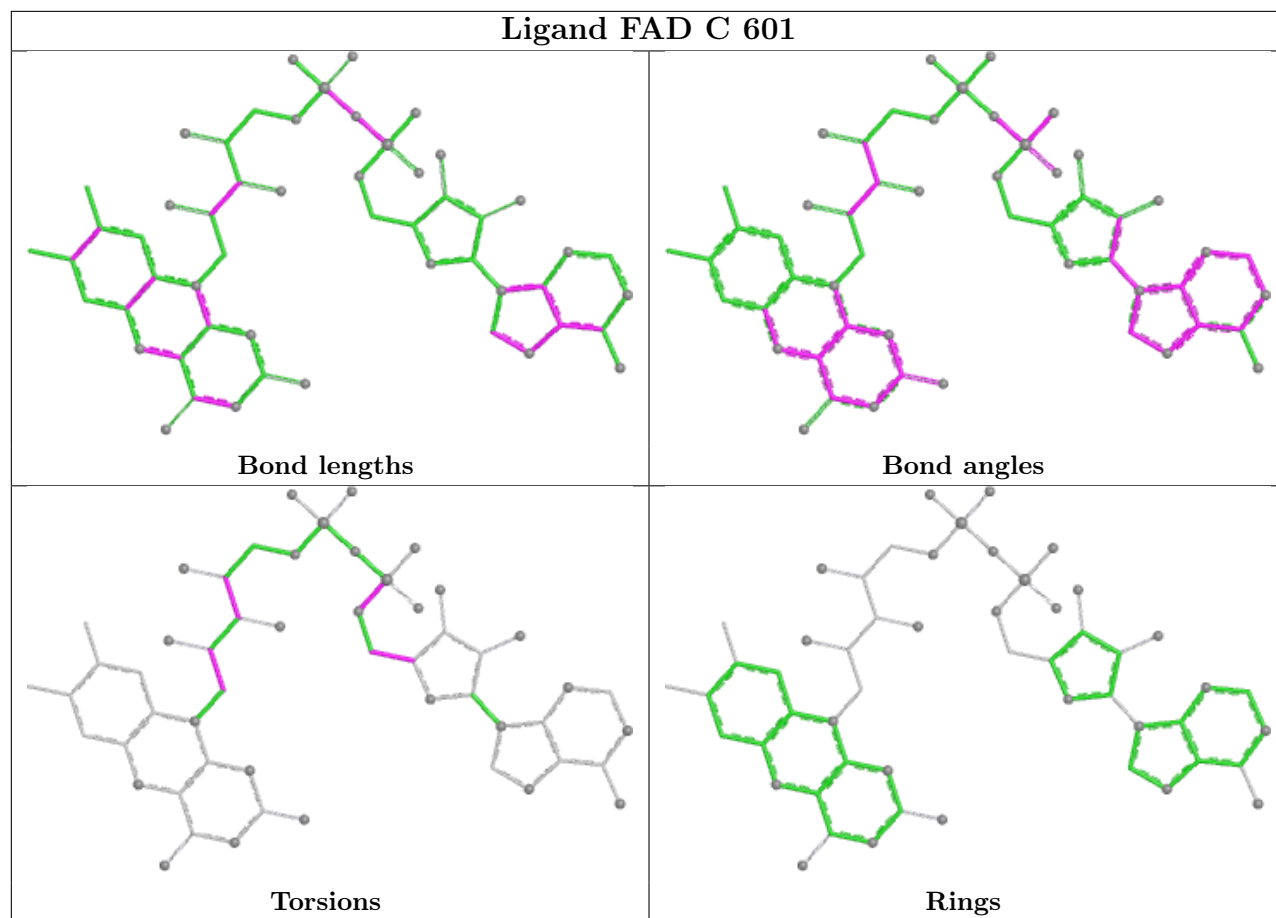
3 monomers are involved in 3 short contacts:

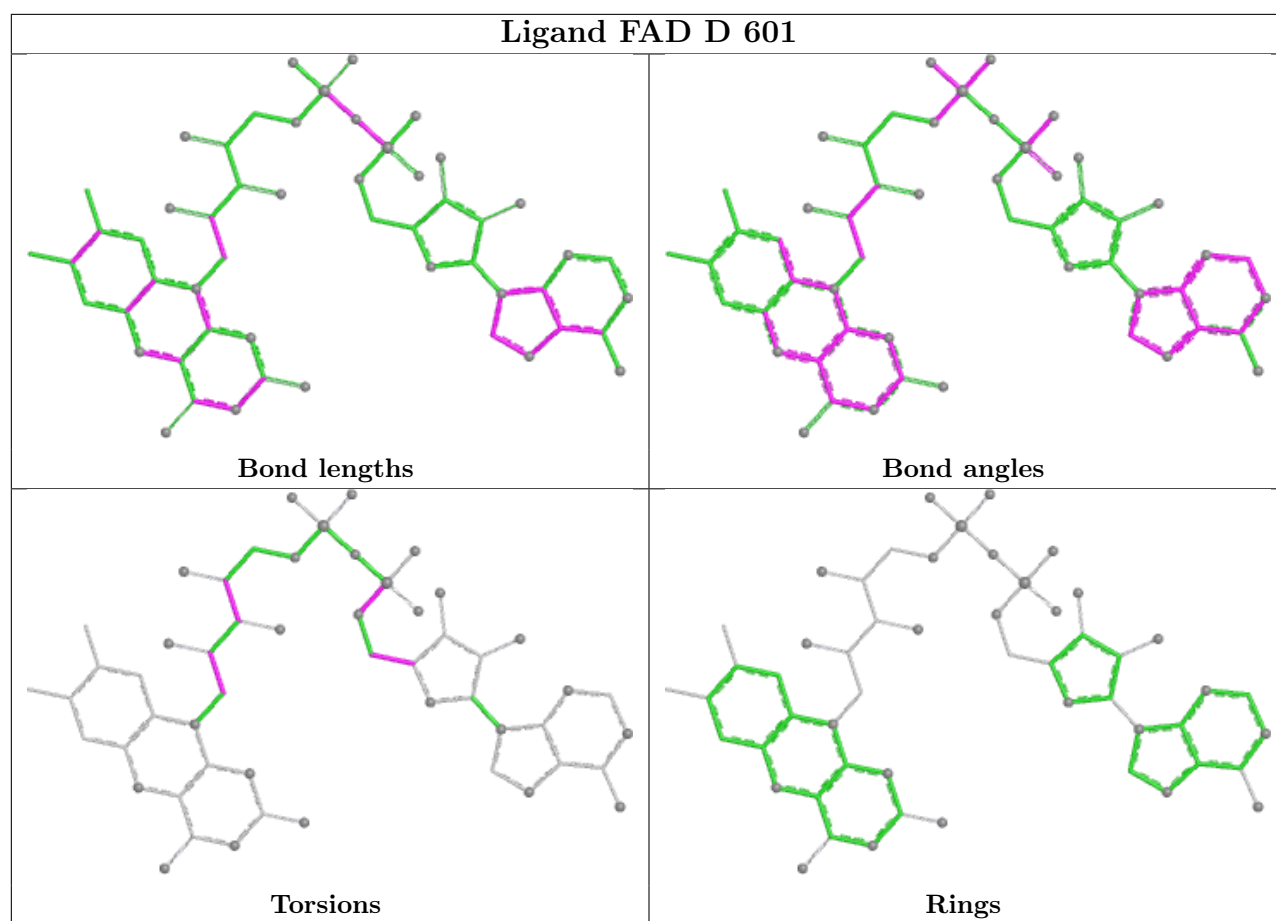
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	1	0
2	B	601	FAD	1	0
2	C	601	FAD	1	0

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%)	0.32	27 (5%) 33 25	46, 79, 129, 175	0
1	B	530/535 (99%)	0.61	55 (10%) 11 8	47, 84, 144, 219	0
1	C	520/535 (97%)	0.36	35 (6%) 24 17	50, 80, 133, 173	0
1	D	520/535 (97%)	0.40	26 (5%) 34 26	51, 83, 134, 190	0
All	All	2089/2140 (97%)	0.42	143 (6%) 23 17	46, 82, 133, 219	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	379	PHE	7.1
1	B	262	ARG	6.7
1	B	348	ASN	5.7
1	C	227	ASP	5.5
1	B	372	ILE	5.4
1	B	435	TYR	4.5
1	C	468	CYS	4.4
1	A	123	GLY	4.3
1	A	446	LYS	4.2
1	B	254	TRP	4.2
1	C	277	TYR	4.1
1	B	373	GLN	4.0
1	C	368	CYS	4.0
1	B	530	PHE	3.9
1	C	111	LEU	3.8
1	C	419	LEU	3.7
1	B	535	PHE	3.7
1	D	123	GLY	3.6
1	B	529	PHE	3.5
1	B	429	GLN	3.5
1	C	363	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	515	LEU	3.4
1	B	432	TYR	3.4
1	A	280	LYS	3.4
1	A	379	PHE	3.4
1	B	512	VAL	3.4
1	C	449	LEU	3.4
1	C	220	VAL	3.3
1	B	436	LEU	3.3
1	B	468	CYS	3.3
1	B	534	TRP	3.3
1	B	355	TYR	3.3
1	B	473	TYR	3.3
1	D	394	LYS	3.3
1	B	378	ILE	3.3
1	B	381	THR	3.2
1	B	380	PRO	3.2
1	B	376	GLY	3.2
1	D	479	GLY	3.2
1	D	336	PRO	3.1
1	C	481	TRP	3.1
1	C	118	ASP	3.1
1	B	533	GLN	3.1
1	B	192	ILE	3.1
1	B	388	TRP	3.1
1	C	435	TYR	3.1
1	A	382	VAL	3.1
1	C	433	ILE	3.1
1	B	45	GLU	3.0
1	D	18	LEU	3.0
1	C	379	PHE	3.0
1	A	436	LEU	3.0
1	C	440	ALA	3.0
1	C	148	GLY	2.9
1	D	117	PRO	2.9
1	C	438	GLU	2.9
1	C	229	TYR	2.9
1	B	241	SER	2.9
1	D	278	LEU	2.9
1	A	25	GLY	2.8
1	B	425	SER	2.8
1	B	117	PRO	2.8
1	C	436	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	377	SER	2.8
1	A	378	ILE	2.7
1	D	516	LEU	2.7
1	B	258	GLN	2.7
1	B	329	THR	2.7
1	B	426	GLN	2.7
1	D	391	ARG	2.7
1	B	424	GLN	2.7
1	B	438	GLU	2.7
1	D	277	TYR	2.6
1	D	363	LYS	2.6
1	B	522	LEU	2.6
1	B	242	MET	2.6
1	B	279	MET	2.6
1	C	218	SER	2.6
1	D	256	MET	2.5
1	D	279	MET	2.5
1	B	422	GLU	2.5
1	C	371	LEU	2.5
1	C	503	ALA	2.5
1	B	514	PHE	2.5
1	D	61	ASN	2.5
1	A	444	GLY	2.4
1	A	117	PRO	2.4
1	B	420	PHE	2.4
1	B	53	SER	2.4
1	A	236	HIS	2.4
1	B	428	LEU	2.4
1	A	516	LEU	2.4
1	C	427	ILE	2.4
1	D	118	ASP	2.3
1	D	423	SER	2.3
1	D	378	ILE	2.3
1	C	262	ARG	2.3
1	B	439	LEU	2.3
1	C	123	GLY	2.3
1	A	235	PHE	2.3
1	A	254	TRP	2.3
1	D	481	TRP	2.3
1	B	277	TYR	2.3
1	A	475	LEU	2.3
1	D	432	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	506	ALA	2.2
1	A	363	LYS	2.2
1	B	423	SER	2.2
1	A	447	PRO	2.2
1	D	335	PHE	2.2
1	C	192	ILE	2.2
1	A	489	PHE	2.2
1	D	280	LYS	2.2
1	A	449	LEU	2.2
1	B	29	THR	2.2
1	B	459	LEU	2.2
1	B	515	LEU	2.2
1	C	76	GLU	2.2
1	B	374	PRO	2.1
1	B	516	LEU	2.1
1	A	277	TYR	2.1
1	C	432	TYR	2.1
1	C	473	TYR	2.1
1	C	506	ALA	2.1
1	D	65	GLU	2.1
1	B	347	ASN	2.1
1	B	12	VAL	2.1
1	B	511	PRO	2.1
1	D	345	VAL	2.1
1	B	4	LYS	2.1
1	D	393	PHE	2.1
1	C	136	GLN	2.1
1	A	132	ASN	2.1
1	C	516	LEU	2.1
1	C	320	GLU	2.1
1	A	445	ALA	2.1
1	A	432	TYR	2.1
1	A	468	CYS	2.0
1	C	144	MET	2.0
1	A	296	ALA	2.0
1	C	335	PHE	2.0
1	D	506	ALA	2.0
1	A	473	TYR	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 [i](#)

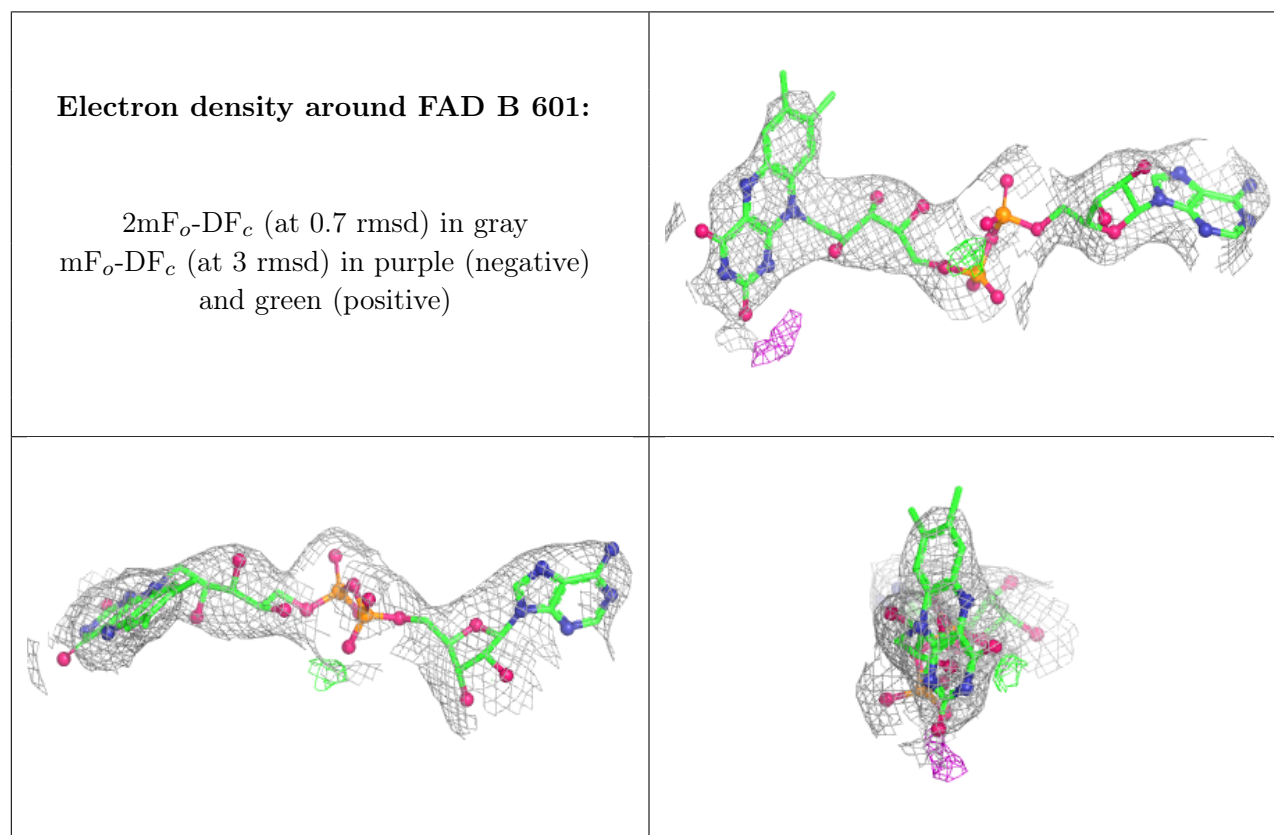
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

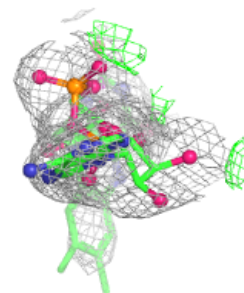
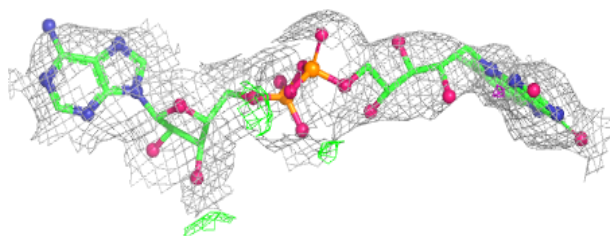
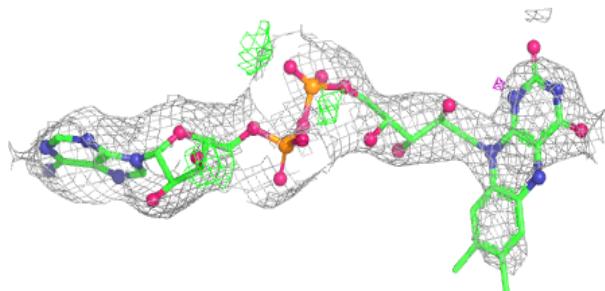
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	601	53/53	0.94	0.11	62,81,98,105	0
2	FAD	D	601	53/53	0.94	0.11	58,79,101,113	0
2	FAD	C	601	53/53	0.96	0.07	51,75,101,104	0
2	FAD	A	601	53/53	0.96	0.09	49,65,89,96	0

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

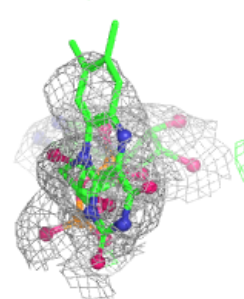
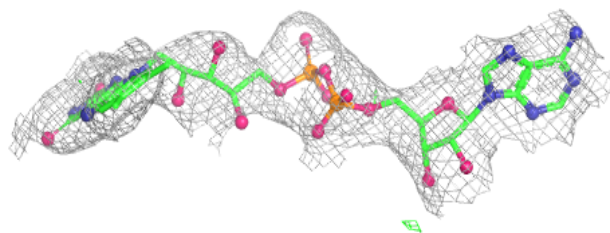
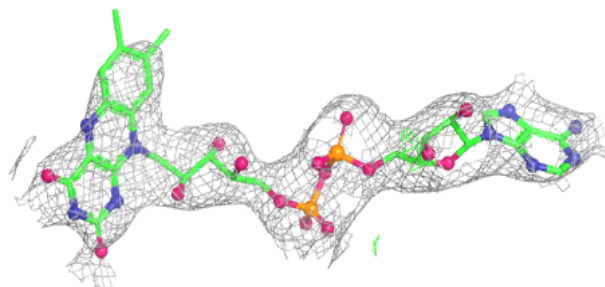


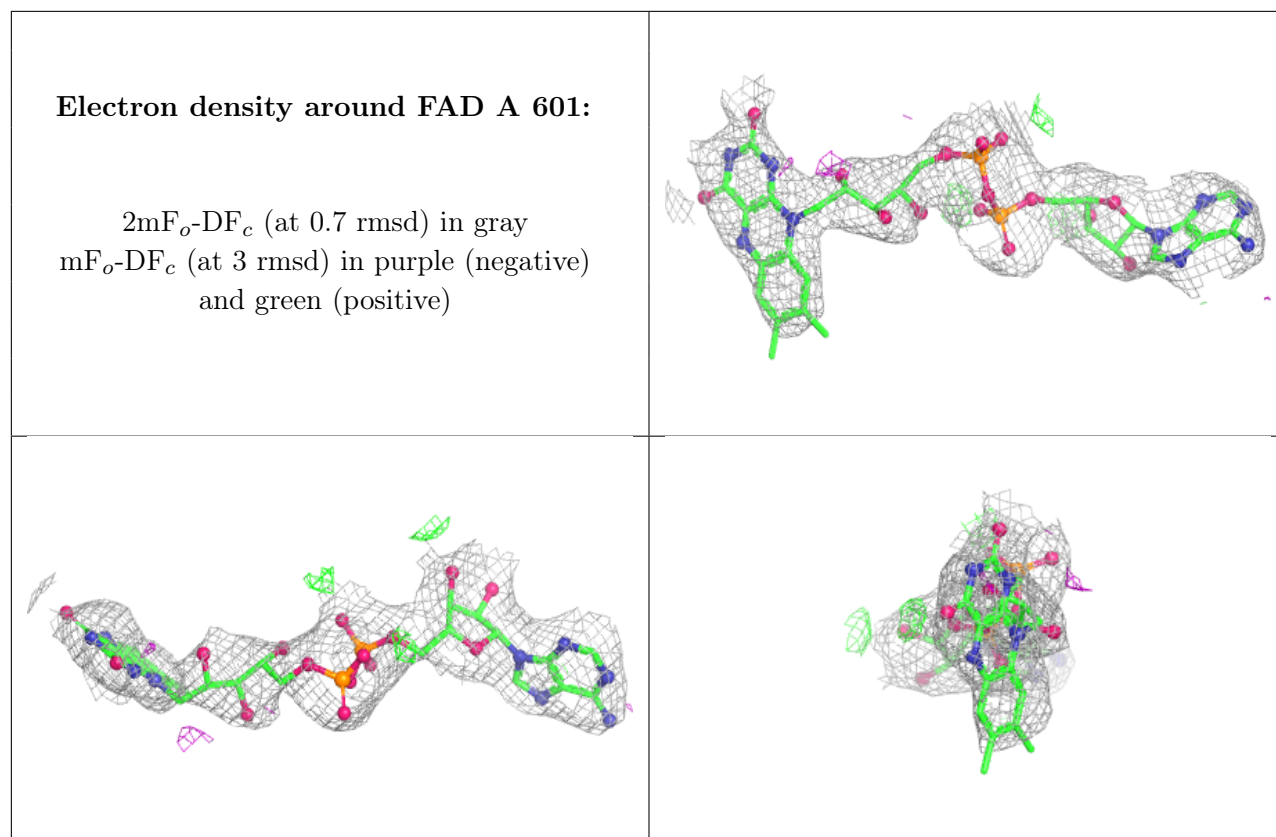
Electron density around FAD D 601:

$2mF_o - DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.