



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:09 PM UTC

PDB ID : 4BCA / pdb_00004bca
Title : MAMMALIAN ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE: Tyr578Phe mutant
Authors : Nenci, S.; Piano, V.; Rosati, S.; Aliverti, A.; Pandini, V.; Fraaije, M.W.; Heck, A.J.R.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2012-10-01
Resolution : 2.40 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

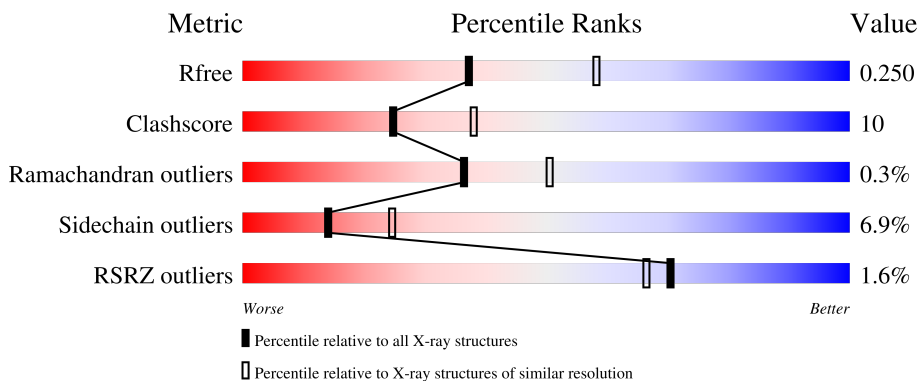
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	658	
1	B	658	
1	C	658	
1	D	658	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1659	-	-	X	-
4	SO4	B	1660	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18202 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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	4393	2789	762	818	24	0	0	0
1	B	543	4300	2732	747	797	24	0	0	0
1	C	557	4412	2799	766	822	25	0	2	0
1	D	550	4354	2761	757	811	25	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	578	PHE	TYR	engineered mutation	UNP P97275
B	578	PHE	TYR	engineered mutation	UNP P97275
C	578	PHE	TYR	engineered mutation	UNP P97275
D	578	PHE	TYR	engineered mutation	UNP P97275

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

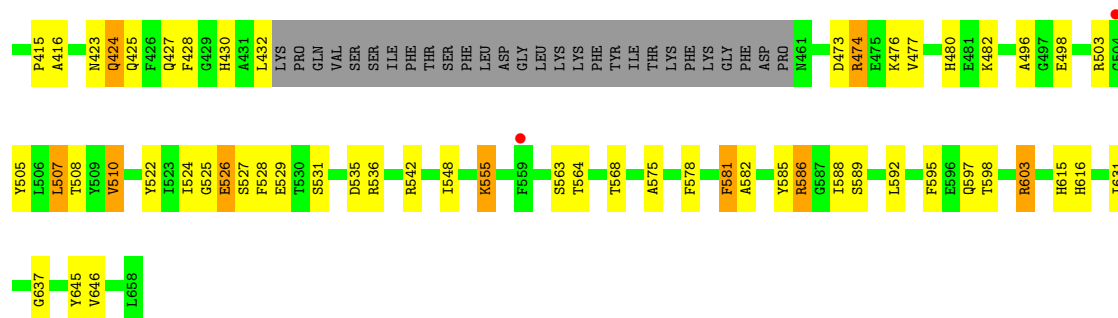
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	142	Total	O	0	0
			142	142		
5	B	95	Total	O	0	0
			95	95		
5	C	143	Total	O	0	0
			143	143		
5	D	112	Total	O	0	0
			112	112		



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.68Å 99.32Å 107.98Å 90.43° 92.12° 95.20°	Depositor
Resolution (Å)	47.58 – 2.40 47.58 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.58-2.40) 98.6 (47.58-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.187 , 0.252 0.190 , 0.250	Depositor DCC
R_{free} test set	1091 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtrriage
Anisotropy	0.075	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18202	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: CL, FAD, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.13	2/4492 (0.0%)	1.16	9/6071 (0.1%)
1	B	1.07	1/4397 (0.0%)	1.14	13/5942 (0.2%)
1	C	1.16	8/4518 (0.2%)	1.16	10/6107 (0.2%)
1	D	1.12	5/4454 (0.1%)	1.14	13/6020 (0.2%)
All	All	1.12	16/17861 (0.1%)	1.15	45/24140 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	335	HIS	CG-ND1	-7.14	1.30	1.38
1	C	508	THR	CA-CB	7.07	1.65	1.53
1	C	335	HIS	CD2-NE2	-7.03	1.30	1.37
1	C	616	HIS	C-O	-6.72	1.17	1.24
1	C	507	LEU	C-O	-5.95	1.19	1.23
1	C	337	LYS	C-O	-5.75	1.17	1.24
1	D	372	GLY	C-O	5.73	1.30	1.23
1	C	205	ILE	C-O	-5.55	1.20	1.24
1	C	364	ILE	C-O	5.33	1.29	1.23
1	D	631	ILE	CA-CB	5.33	1.60	1.54
1	B	509	TYR	CA-C	5.25	1.60	1.52
1	D	159	ILE	CA-CB	5.24	1.59	1.53
1	A	241	VAL	CA-CB	5.13	1.61	1.54
1	D	581	PHE	CA-C	5.10	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	ALA	CA-CB	-5.08	1.44	1.53
1	D	510	VAL	CA-CB	-5.03	1.48	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ARG	N-CA-C	8.42	120.54	111.36
1	B	298	THR	N-CA-C	-7.74	104.37	113.88
1	A	314	ILE	N-CA-C	-7.59	103.05	110.72
1	B	233	ILE	CA-C-N	-7.07	112.71	119.85
1	B	233	ILE	C-N-CA	-7.07	112.71	119.85
1	A	631	ILE	N-CA-C	7.01	118.83	112.17
1	C	334	VAL	N-CA-C	-6.50	106.47	112.96
1	A	354	MET	N-CA-C	6.42	119.47	109.52
1	C	507	LEU	N-CA-C	-5.94	99.03	110.56
1	B	155	THR	CA-C-N	5.80	123.89	119.66
1	B	155	THR	C-N-CA	5.80	123.89	119.66
1	D	319	SER	CA-C-N	-5.77	116.98	121.82
1	D	319	SER	C-N-CA	-5.77	116.98	121.82
1	D	97	GLY	N-CA-C	5.64	122.51	112.02
1	B	118	TYR	CA-C-N	5.64	125.11	119.24
1	B	118	TYR	C-N-CA	5.64	125.11	119.24
1	D	125	LEU	CA-C-N	5.62	125.15	119.19
1	D	125	LEU	C-N-CA	5.62	125.15	119.19
1	C	484	VAL	N-CA-C	5.58	115.78	110.42
1	C	414	ALA	CA-C-N	-5.54	115.04	120.52
1	C	414	ALA	C-N-CA	-5.54	115.04	120.52
1	C	431	ALA	N-CA-C	-5.52	105.24	112.41
1	B	205	ILE	N-CA-C	-5.51	102.79	109.01
1	D	589	SER	N-CA-C	5.46	116.91	111.07
1	B	125	LEU	CA-C-N	5.42	125.76	119.47
1	B	125	LEU	C-N-CA	5.42	125.76	119.47
1	D	364	ILE	CB-CA-C	-5.40	106.12	111.30
1	C	590	ASP	CA-C-N	5.40	124.91	119.19
1	C	590	ASP	C-N-CA	5.40	124.91	119.19
1	A	180	ASP	N-CA-C	5.39	118.07	111.82
1	A	189	HIS	N-CA-C	5.31	119.36	111.87
1	C	547	ARG	N-CA-C	-5.30	105.58	111.36
1	A	433	LYS	CA-C-N	5.26	124.95	119.64
1	A	433	LYS	C-N-CA	5.26	124.95	119.64
1	D	93	TRP	N-CA-C	-5.21	106.87	113.18
1	B	310	VAL	N-CA-C	5.19	115.81	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	GLN	CA-C-N	5.17	128.44	121.05
1	B	462	GLN	C-N-CA	5.17	128.44	121.05
1	D	368	GLU	N-CA-C	5.14	118.49	111.39
1	D	603	ARG	CD-NE-CZ	5.13	131.59	124.40
1	D	522	TYR	CA-C-N	-5.12	116.84	123.19
1	D	522	TYR	C-N-CA	-5.12	116.84	123.19
1	A	368	GLU	N-CA-C	5.12	118.26	111.30
1	C	374	ILE	N-CA-C	-5.01	101.13	108.54
1	D	221	ILE	N-CA-C	5.01	115.23	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	460	PRO	Peptide
1	C	507	LEU	Peptide

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	4393	0	4328	91	0
1	B	4300	0	4242	80	1
1	C	4412	0	4356	108	1
1	D	4354	0	4300	68	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	1	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	1	0
4	A	10	0	0	1	0
4	B	10	0	0	2	0
4	C	5	0	0	1	0
4	D	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	142	0	0	12	0
5	B	95	0	0	4	0
5	C	143	0	0	5	0
5	D	112	0	0	4	0
All	All	18202	0	17350	345	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (345) 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:HIS:HB3	1:A:243:TYR:OH	1.37	1.25
1:C:508:THR:HA	1:C:511:ILE:CD1	1.65	1.24
1:A:421:MET:CG	5:A:2099:HOH:O	1.93	1.15
1:C:507:LEU:HD11	1:C:511:ILE:CG1	1.77	1.14
1:C:508:THR:HA	1:C:511:ILE:HD11	1.28	1.13
1:A:192:HIS:HB3	1:A:243:TYR:HH	0.98	1.07
1:C:508:THR:HA	1:C:511:ILE:HD12	1.42	1.02
1:D:192:HIS:HB3	1:D:243:TYR:OH	1.60	1.00
1:B:140:LEU:HB2	5:B:2014:HOH:O	1.62	1.00
1:D:386:GLU:HB2	5:D:2084:HOH:O	1.59	1.00
1:A:615:HIS:HD2	1:A:616:HIS:CD2	1.80	0.99
1:A:615:HIS:HD2	1:A:616:HIS:HD2	1.01	0.93
1:A:192:HIS:CB	1:A:243:TYR:OH	2.18	0.92
1:C:507:LEU:HD11	1:C:511:ILE:HG12	1.48	0.92
1:C:507:LEU:CD1	1:C:511:ILE:HG13	2.00	0.91
1:C:507:LEU:CD1	1:C:511:ILE:CG1	2.49	0.91
1:C:459:ASP:HB2	5:C:2111:HOH:O	1.71	0.89
1:A:439:ILE:HG13	1:D:535:ASP:HB2	1.55	0.88
1:A:421:MET:HG3	5:A:2099:HOH:O	1.60	0.88
1:B:192:HIS:CB	1:B:243:TYR:OH	2.21	0.88
1:B:140:LEU:CB	5:B:2014:HOH:O	2.21	0.88
1:C:192:HIS:HB3	1:C:243:TYR:OH	1.74	0.88
1:C:508:THR:CA	1:C:511:ILE:CD1	2.52	0.87
1:C:635:GLY:HA2	1:C:638:MET:HE3	1.55	0.87
1:A:615:HIS:CD2	1:A:616:HIS:HD2	1.91	0.87
1:A:439:ILE:HG13	1:D:535:ASP:CB	2.07	0.83
1:C:507:LEU:HD11	1:C:511:ILE:HG13	1.55	0.83
1:C:508:THR:CA	1:C:511:ILE:HD11	2.09	0.82
1:B:192:HIS:HB3	1:B:243:TYR:OH	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:TYR:OH	1:A:615:HIS:HE1	1.67	0.77
1:C:115:GLY:O	1:C:116:LYS:HD3	1.87	0.75
1:A:526:GLU:HB3	1:A:595:PHE:HZ	1.50	0.75
1:D:423:ASN:HD21	1:D:427:GLN:NE2	1.85	0.75
1:C:508:THR:CA	1:C:511:ILE:HD12	2.16	0.73
1:A:507:LEU:O	1:A:511:ILE:HD12	1.89	0.73
1:A:119:PRO:HG2	1:A:506:LEU:HD22	1.71	0.72
1:A:106:ASN:HD21	1:A:110:GLN:HE21	1.37	0.72
1:B:526:GLU:HB3	1:B:595:PHE:HZ	1.54	0.72
1:D:142:HIS:CE1	1:D:586:ARG:NH2	2.58	0.72
1:A:625:GLN:OE1	5:A:2132:HOH:O	2.07	0.71
1:A:421:MET:HG2	5:A:2099:HOH:O	1.75	0.71
1:B:555:LYS:NZ	1:B:597:GLN:HE21	1.88	0.70
1:D:425:GLN:HG3	1:D:564:THR:OG1	1.91	0.70
1:D:192:HIS:CB	1:D:243:TYR:OH	2.37	0.70
1:C:161:ASN:OD1	1:C:163:ASP:N	2.25	0.70
1:D:423:ASN:HD21	1:D:427:GLN:HE21	1.38	0.70
1:C:507:LEU:HD12	1:C:507:LEU:C	2.18	0.69
1:B:425:GLN:OE1	1:B:566:ARG:HD3	1.93	0.68
1:B:298:THR:CG2	1:B:300:HIS:H	2.06	0.67
1:A:213:THR:O	5:A:2032:HOH:O	2.13	0.67
2:A:999:FAD:N5	3:A:1659:CL:CL	2.65	0.66
1:B:505:TYR:HA	1:B:508:THR:OG1	1.96	0.66
1:A:615:HIS:CD2	1:A:616:HIS:CD2	2.73	0.65
1:C:461:ASN:CG	5:C:2112:HOH:O	2.39	0.65
1:B:195:PHE:O	1:B:196:LEU:C	2.40	0.65
1:D:424:GLN:NE2	1:D:563:SER:O	2.30	0.65
1:B:415:PRO:HA	4:B:1660:SO4:O1	1.97	0.65
1:B:503:ARG:O	1:B:505:TYR:N	2.30	0.65
1:C:480:HIS:ND1	4:C:1660:SO4:O3	2.29	0.64
1:A:155:THR:HG22	1:A:201:MET:HE3	1.79	0.64
1:D:151:ASN:C	1:D:151:ASN:HD22	2.06	0.64
1:A:439:ILE:CG1	1:D:535:ASP:HB2	2.28	0.64
1:C:144:THR:HG22	1:C:520:GLU:HA	1.78	0.64
1:B:98:TYR:CD2	1:B:117:ARG:HD3	2.32	0.64
2:D:999:FAD:N5	3:D:1659:CL:CL	2.68	0.64
1:D:526:GLU:HB3	1:D:595:PHE:HZ	1.63	0.63
1:C:423:ASN:HD21	1:C:427:GLN:NE2	1.96	0.63
1:C:526:GLU:HG3	1:C:527:SER:H	1.63	0.63
1:A:432:LEU:HD13	1:A:507:LEU:HD11	1.80	0.63
1:C:507:LEU:CD1	1:C:511:ILE:HD11	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:ARG:HG2	1:D:474:ARG:HH11	1.62	0.63
1:D:83:ILE:HG23	1:D:91:MET:HE1	1.81	0.62
1:C:526:GLU:HB3	1:C:595:PHE:HZ	1.63	0.62
1:C:139:ASN:HB2	1:C:141:ASP:OD1	2.00	0.62
1:A:349:CYS:SG	1:A:354:MET:HE1	2.40	0.61
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.81	0.61
1:A:215:HIS:HD2	1:A:375:THR:OG1	1.83	0.61
1:C:432:LEU:HD21	1:C:514:MET:HE1	1.83	0.61
1:B:167:GLU:HA	1:B:170:LYS:HE3	1.81	0.60
1:C:508:THR:C	1:C:511:ILE:HD12	2.26	0.60
1:C:331:ASP:O	1:C:380:LYS:HE3	2.02	0.60
1:C:128:PHE:CZ	1:C:514:MET:HE2	2.37	0.59
1:C:507:LEU:CD1	1:C:511:ILE:CD1	2.80	0.59
1:B:128:PHE:CD1	1:B:432:LEU:HD11	2.37	0.59
1:A:342:ARG:HD2	1:A:645:TYR:CZ	2.38	0.59
1:B:139:ASN:O	1:B:140:LEU:CB	2.51	0.59
1:C:192:HIS:HB3	1:C:243:TYR:HH	1.67	0.59
1:C:144:THR:HG21	1:C:519:LEU:O	2.02	0.58
1:B:192:HIS:HB2	1:B:243:TYR:OH	1.99	0.58
2:C:999:FAD:N5	3:C:1659:CL:CL	2.73	0.58
1:A:189:HIS:HE1	5:A:2027:HOH:O	1.86	0.58
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.83	0.58
1:A:190:CYS:HB2	1:A:193:GLU:OE1	2.04	0.58
1:B:288:GLU:OE1	1:B:298:THR:HB	2.03	0.58
1:C:508:THR:OG1	1:C:511:ILE:CD1	2.51	0.57
1:D:423:ASN:ND2	1:D:427:GLN:NE2	2.52	0.57
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.85	0.57
1:C:507:LEU:HD12	1:C:511:ILE:HG13	1.86	0.57
1:B:230:LEU:HD22	1:B:254:THR:HB	1.87	0.57
1:B:390:TYR:CE1	1:B:505:TYR:HB2	2.40	0.57
1:D:192:HIS:CE1	1:D:592:LEU:HD13	2.40	0.57
1:B:298:THR:HG23	1:B:300:HIS:H	1.70	0.57
1:B:421:MET:HG2	1:B:425:GLN:HB3	1.86	0.56
1:C:419:ARG:O	1:C:466:ALA:HA	2.06	0.56
1:D:392:SER:OG	1:D:496:ALA:HB3	2.05	0.56
1:B:432:LEU:HD23	1:B:507:LEU:HD21	1.88	0.56
1:D:151:ASN:HD22	1:D:152:PRO:N	2.04	0.56
1:B:139:ASN:O	1:B:140:LEU:HB2	2.05	0.56
1:C:246:MET:HE2	1:C:621:LYS:HE3	1.87	0.56
1:A:428:PHE:HD1	1:A:428:PHE:C	2.14	0.56
1:A:428:PHE:C	1:A:428:PHE:CD1	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ARG:O	1:B:466:ALA:HA	2.06	0.56
1:C:526:GLU:HG3	1:C:527:SER:N	2.20	0.56
1:B:298:THR:HG22	1:B:300:HIS:H	1.70	0.55
1:C:150:LEU:HD12	1:C:180:ASP:HB3	1.87	0.55
1:C:551:GLU:O	1:C:555:LYS:HD3	2.06	0.55
1:A:571:TYR:OH	1:A:615:HIS:CE1	2.56	0.55
1:B:423:ASN:HD21	1:B:427:GLN:NE2	2.05	0.55
1:B:390:TYR:HE1	1:B:505:TYR:HB2	1.72	0.55
1:D:528:PHE:HZ	1:D:548:ILE:HD11	1.71	0.55
1:D:139:ASN:HB2	1:D:141:ASP:OD1	2.07	0.55
1:C:342:ARG:HD2	1:C:645:TYR:CZ	2.41	0.55
1:A:480:HIS:CE1	4:A:1661:SO4:O4	2.60	0.55
1:A:192:HIS:CG	1:A:243:TYR:OH	2.60	0.54
1:A:189:HIS:CE1	5:A:2027:HOH:O	2.59	0.54
1:A:419:ARG:O	1:A:466:ALA:HA	2.07	0.54
1:D:139:ASN:O	1:D:140:LEU:HB2	2.07	0.54
1:A:192:HIS:CD2	1:A:243:TYR:OH	2.61	0.54
1:A:277:HIS:HE1	1:A:376:GLU:OE1	1.89	0.54
1:D:505:TYR:HA	1:D:508:THR:OG1	2.08	0.54
1:A:210:LEU:HD13	1:A:256:ILE:HG23	1.90	0.54
1:A:389:LYS:HD3	1:A:481:GLU:OE1	2.08	0.54
1:C:505:TYR:O	1:C:508:THR:N	2.41	0.54
1:C:508:THR:O	1:C:511:ILE:HD12	2.07	0.54
1:C:507:LEU:HD11	1:C:511:ILE:CD1	2.37	0.54
1:B:555:LYS:HZ1	1:B:597:GLN:HE21	1.56	0.53
1:B:94:ASN:HA	1:B:197:LEU:HD13	1.90	0.53
1:B:399:GLU:CD	1:B:399:GLU:H	2.16	0.53
1:C:141:ASP:OD1	1:C:141:ASP:N	2.41	0.53
1:A:479:GLN:HE22	1:B:479:GLN:HE22	1.55	0.53
1:C:161:ASN:OD1	1:C:161:ASN:C	2.51	0.53
1:A:423:ASN:HD21	1:A:427:GLN:NE2	2.07	0.52
1:C:515:ARG:NH2	5:C:2117:HOH:O	2.30	0.52
1:A:528:PHE:HZ	1:A:548:ILE:HD11	1.74	0.52
1:B:390:TYR:CD1	1:B:502:GLN:HA	2.45	0.52
1:D:161:ASN:OD1	1:D:163:ASP:N	2.42	0.52
1:C:129:LYS:O	1:C:133:GLN:HG3	2.09	0.52
1:C:300:HIS:HB2	1:C:332:LEU:CD1	2.40	0.52
1:A:613:LEU:HD21	1:A:626:TRP:HB2	1.91	0.52
1:D:399:GLU:CD	1:D:399:GLU:H	2.18	0.52
1:C:643:LYS:NZ	1:C:650:ASN:HD22	2.08	0.52
1:C:481:GLU:HG2	1:C:485:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ILE:O	1:B:198:ARG:HD3	2.09	0.51
1:D:480:HIS:ND1	4:D:1660:SO4:O2	2.43	0.51
1:D:108:LYS:HB2	1:D:110:GLN:HG3	1.92	0.51
1:D:474:ARG:HH11	1:D:474:ARG:CG	2.24	0.51
1:C:220:LYS:O	1:C:224:LEU:HD22	2.10	0.51
1:D:133:GLN:HG2	1:D:138:ILE:O	2.11	0.51
1:D:423:ASN:ND2	1:D:427:GLN:HE21	2.08	0.51
1:D:529:GLU:OE1	1:D:615:HIS:HB3	2.11	0.51
1:B:524:ILE:O	1:B:582:ALA:HA	2.10	0.50
1:A:238:GLY:HA2	1:A:245:LEU:HD11	1.93	0.50
1:A:268:TRP:CZ2	1:A:277:HIS:HB2	2.47	0.50
1:A:540:LEU:O	1:A:544:VAL:HG23	2.12	0.50
1:B:585:TYR:HA	1:B:588:ILE:HD13	1.93	0.50
2:B:999:FAD:N5	3:B:1659:CL:CL	2.82	0.50
1:D:415:PRO:O	1:D:416:ALA:C	2.55	0.50
1:A:432:LEU:CD1	1:A:507:LEU:HD11	2.41	0.50
1:C:303:ASP:OD1	1:C:508:THR:HG23	2.11	0.50
1:A:399:GLU:OE2	5:A:2094:HOH:O	2.19	0.50
1:B:140:LEU:HB3	5:B:2014:HOH:O	2.00	0.49
1:B:423:ASN:ND2	1:B:427:GLN:NE2	2.60	0.49
1:C:144:THR:CG2	1:C:520:GLU:HA	2.42	0.49
1:D:480:HIS:HB2	5:D:2093:HOH:O	2.12	0.49
1:C:323:LYS:HD2	1:C:323:LYS:C	2.37	0.49
1:D:527:SER:HB2	1:D:578:PHE:CE1	2.46	0.49
1:B:372:GLY:HA2	1:B:652:PHE:CZ	2.48	0.49
1:B:527:SER:HB3	1:B:580:TYR:CE1	2.48	0.49
1:D:161:ASN:OD1	1:D:161:ASN:C	2.55	0.49
1:A:242:SER:O	1:A:243:TYR:HB2	2.12	0.49
1:A:442:SER:HB3	1:D:542:ARG:NH1	2.26	0.49
1:C:425:GLN:HG3	1:C:564:THR:OG1	2.12	0.49
1:C:508:THR:OG1	1:C:511:ILE:HD13	2.11	0.49
1:B:244:GLY:HA2	1:B:656:ASN:HD21	1.78	0.49
1:B:246:MET:HB3	1:B:621:LYS:HE2	1.95	0.49
1:D:555:LYS:NZ	1:D:597:GLN:HE21	2.10	0.49
1:B:187:HIS:NE2	1:B:197:LEU:HD11	2.28	0.49
1:D:154:ASP:O	1:D:201:MET:HG2	2.13	0.48
1:B:83:ILE:HG23	1:B:91:MET:HE1	1.95	0.48
1:A:349:CYS:SG	1:A:354:MET:CE	3.01	0.48
1:D:503:ARG:O	1:D:507:LEU:HB2	2.13	0.48
1:D:507:LEU:O	1:D:510:VAL:HG22	2.13	0.48
1:B:387:TYR:O	1:B:471:GLU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ILE:HG13	1:B:468:LEU:HD23	1.94	0.48
1:B:526:GLU:HB3	1:B:595:PHE:CZ	2.43	0.48
1:A:342:ARG:HG3	1:A:342:ARG:O	2.13	0.47
1:B:390:TYR:HE1	1:B:505:TYR:CB	2.27	0.47
1:C:635:GLY:HA2	1:C:638:MET:CE	2.38	0.47
1:C:564:THR:CG2	1:C:580:TYR:HB2	2.44	0.47
1:D:524:ILE:HG12	1:D:585:TYR:HD2	1.79	0.47
1:A:432:LEU:HD13	1:A:507:LEU:CD1	2.43	0.47
1:D:142:HIS:CE1	1:D:586:ARG:HH22	2.33	0.47
1:A:246:MET:HE2	1:A:621:LYS:HE3	1.96	0.47
1:B:185:ARG:HG2	1:B:235:ILE:HD13	1.95	0.47
1:C:355:SER:HB2	1:D:616:HIS:HA	1.96	0.47
1:C:643:LYS:HZ2	1:C:650:ASN:HD22	1.63	0.47
1:A:129:LYS:HD2	1:A:140:LEU:HD23	1.96	0.47
1:B:230:LEU:HD13	1:B:256:ILE:HD11	1.96	0.47
1:C:501:GLY:C	1:C:503:ARG:H	2.23	0.47
1:D:581:PHE:CZ	1:D:598:THR:HG21	2.49	0.47
1:A:400:GLN:HA	1:A:400:GLN:NE2	2.30	0.47
1:D:171:THR:OG1	1:D:173:ILE:HD12	2.15	0.46
1:A:524:ILE:HD12	1:A:595:PHE:HB2	1.98	0.46
1:C:419:ARG:HH12	1:C:508:THR:HG21	1.80	0.46
1:D:525:GLY:HA2	1:D:581:PHE:O	2.15	0.46
1:C:645:TYR:CZ	1:D:637:GLY:HA3	2.51	0.46
1:B:196:LEU:O	1:B:197:LEU:C	2.57	0.46
1:D:473:ASP:O	1:D:477:VAL:HG23	2.16	0.46
1:C:637:GLY:HA3	1:D:645:TYR:CZ	2.50	0.46
1:A:475:GLU:HA	1:A:475:GLU:OE1	2.15	0.46
1:A:643:LYS:NZ	1:A:650:ASN:HD22	2.14	0.46
1:C:300:HIS:HB2	1:C:332:LEU:HD11	1.98	0.46
1:C:507:LEU:HD12	1:C:511:ILE:HD11	1.98	0.46
1:B:138:ILE:HD12	1:B:140:LEU:HD23	1.96	0.46
1:B:524:ILE:HD11	1:B:583:PHE:CZ	2.50	0.46
1:B:529:GLU:OE1	1:B:615:HIS:HB3	2.16	0.45
1:C:360:ILE:HG12	5:C:2088:HOH:O	2.16	0.45
1:A:516:ASP:O	1:A:520:GLU:HG2	2.17	0.45
1:C:433:LYS:HD3	1:C:503:ARG:NH1	2.31	0.45
1:A:388:GLN:NE2	5:A:2064:HOH:O	2.48	0.45
1:A:506:LEU:HA	1:A:506:LEU:HD23	1.69	0.45
1:B:161:ASN:HB3	1:B:164:PHE:HB3	1.99	0.45
1:C:144:THR:HG22	1:C:520:GLU:CA	2.45	0.45
1:C:209:VAL:C	1:C:210:LEU:HD12	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:TYR:C	1:C:507:LEU:N	2.75	0.45
1:C:528:PHE:HZ	1:C:548:ILE:HD11	1.81	0.45
1:A:277:HIS:CE1	1:A:376:GLU:OE1	2.69	0.45
1:A:564:THR:HG22	1:A:580:TYR:HB3	1.98	0.45
1:C:116:LYS:HD2	1:C:116:LYS:HA	1.60	0.45
1:C:184:PHE:O	1:C:184:PHE:CD1	2.70	0.45
1:C:507:LEU:HD12	1:C:511:ILE:CD1	2.46	0.45
1:B:551:GLU:HB2	1:B:598:THR:HG23	1.99	0.45
1:C:423:ASN:HD21	1:C:427:GLN:HE21	1.62	0.45
1:A:243:TYR:HD2	1:A:622:LEU:HB2	1.82	0.44
1:D:428:PHE:CD1	1:D:428:PHE:C	2.95	0.44
1:A:526:GLU:CB	1:A:595:PHE:HZ	2.24	0.44
1:B:480:HIS:CE1	4:B:1660:SO4:O1	2.69	0.44
1:C:195:PHE:CD1	1:C:592:LEU:HD11	2.53	0.44
1:D:526:GLU:HB3	1:D:595:PHE:CZ	2.49	0.44
1:B:139:ASN:O	1:B:140:LEU:HG	2.18	0.44
1:B:277:HIS:HE1	1:B:376:GLU:OE1	2.01	0.44
1:D:428:PHE:C	1:D:428:PHE:HD1	2.25	0.44
1:A:425:GLN:HE21	1:A:564:THR:HG23	1.82	0.44
1:A:568:THR:HG22	1:A:576:CYS:SG	2.58	0.44
1:A:425:GLN:OE1	1:A:566:ARG:HD3	2.18	0.44
1:B:619:VAL:HB	1:B:657:LEU:HD23	1.99	0.44
1:B:204:ARG:NH2	1:B:253:ARG:O	2.51	0.43
1:C:388:GLN:NE2	1:C:471:GLU:OE1	2.50	0.43
1:A:417:SER:HB3	1:A:469:LEU:HB3	1.99	0.43
1:C:585:TYR:HB2	1:C:591:PRO:HB3	2.01	0.43
1:B:432:LEU:N	1:B:432:LEU:CD1	2.81	0.43
1:C:143:LYS:HE3	1:C:143:LYS:HB3	1.83	0.43
1:C:383:PRO:O	1:C:384:THR:C	2.62	0.43
1:C:461:ASN:HB3	5:C:2110:HOH:O	2.18	0.43
1:D:387:TYR:CD2	1:D:474:ARG:HG3	2.54	0.43
1:A:167:GLU:OE2	1:A:227:LYS:NZ	2.51	0.43
1:C:94:ASN:HA	1:C:197:LEU:HD13	2.00	0.43
1:B:432:LEU:HD23	1:B:507:LEU:CD2	2.48	0.43
1:D:425:GLN:HG3	1:D:564:THR:HG1	1.84	0.43
1:B:503:ARG:C	1:B:505:TYR:H	2.25	0.43
1:D:524:ILE:O	1:D:582:ALA:HA	2.18	0.43
1:B:259:ASP:C	1:B:259:ASP:OD1	2.62	0.43
2:B:999:FAD:H1'2	2:B:999:FAD:H9	1.76	0.43
1:C:111:LEU:HD13	1:C:128:PHE:CD2	2.53	0.43
1:A:127:THR:O	1:A:127:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:HIS:CG	5:A:2110:HOH:O	2.72	0.42
1:B:268:TRP:CZ2	1:B:277:HIS:HB2	2.54	0.42
1:C:434:PRO:O	1:C:435:GLN:HB2	2.18	0.42
1:A:187:HIS:CE1	1:A:197:LEU:HD11	2.54	0.42
1:C:127:THR:O	1:C:127:THR:HG22	2.18	0.42
1:C:508:THR:CB	1:C:511:ILE:CD1	2.97	0.42
1:B:564:THR:CG2	1:B:580:TYR:HB2	2.49	0.42
1:C:342:ARG:HH11	1:C:342:ARG:HD3	1.63	0.42
1:C:507:LEU:CD1	1:C:507:LEU:C	2.87	0.42
1:C:621:LYS:HG3	1:C:656:ASN:HD22	1.83	0.42
1:A:201:MET:CG	1:A:202:PHE:N	2.82	0.42
1:B:196:LEU:O	1:B:199:GLU:N	2.45	0.42
1:C:150:LEU:HD12	1:C:180:ASP:CB	2.50	0.42
2:A:999:FAD:C4X	3:A:1659:CL:CL	3.04	0.42
1:B:209:VAL:C	1:B:210:LEU:HD12	2.43	0.42
1:C:81:GLY:HA3	1:C:286:GLU:OE1	2.19	0.42
1:C:325:ILE:CD1	1:C:416:ALA:HB2	2.49	0.42
1:C:505:TYR:C	1:C:507:LEU:H	2.27	0.42
1:A:433:LYS:HB3	1:A:434:PRO:HD2	2.00	0.42
1:A:372:GLY:HA2	1:A:652:PHE:CZ	2.54	0.42
1:A:476:LYS:O	1:A:480:HIS:HB2	2.19	0.42
1:D:83:ILE:HB	1:D:261:SER:HB2	2.02	0.42
1:D:212:PRO:HD2	1:D:259:ASP:O	2.20	0.42
1:C:417:SER:HB3	1:C:469:LEU:HB3	2.02	0.42
1:D:314:ILE:O	1:D:365:MET:HA	2.19	0.42
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.83	0.42
1:A:439:ILE:HD13	1:A:439:ILE:HA	1.88	0.42
1:A:215:HIS:HE1	5:A:2034:HOH:O	2.03	0.41
1:C:98:TYR:CD1	1:C:117:ARG:HD3	2.55	0.41
1:B:118:TYR:HB3	1:B:119:PRO:HD2	2.02	0.41
1:C:321:MET:HE1	1:C:469:LEU:HD22	2.02	0.41
1:C:612:SER:HB2	1:D:354[A]:MET:HG2	2.01	0.41
1:A:268:TRP:CE2	1:A:277:HIS:HB2	2.56	0.41
1:C:259:ASP:OD1	1:C:259:ASP:C	2.63	0.41
1:C:342:ARG:O	1:C:342:ARG:HG3	2.20	0.41
1:C:428:PHE:C	1:C:428:PHE:CD1	2.99	0.41
1:A:102:LYS:C	1:A:113:LEU:HD12	2.45	0.41
1:A:286:GLU:OE2	1:A:289:ARG:NH2	2.36	0.41
1:A:328:ASN:O	1:A:329:ILE:C	2.60	0.41
1:A:438:SER:HB3	1:A:441:THR:HG22	2.02	0.41
1:B:277:HIS:HD2	1:B:378:THR:OG1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:HIS:HA	1:A:592:LEU:HD21	2.02	0.41
1:C:83:ILE:HB	1:C:261:SER:HB2	2.03	0.41
1:D:585:TYR:CD1	1:D:585:TYR:C	2.99	0.41
1:B:243:TYR:HD2	1:B:622:LEU:HB2	1.85	0.41
1:B:354:MET:HE3	1:B:354:MET:HB2	1.79	0.41
1:B:555:LYS:HZ2	1:B:597:GLN:HE21	1.63	0.41
1:C:481:GLU:HG2	1:C:485:TYR:HE2	1.85	0.41
1:D:151:ASN:C	1:D:151:ASN:ND2	2.71	0.41
1:B:286:GLU:OE1	1:B:286:GLU:HA	2.20	0.41
1:B:555:LYS:NZ	1:B:597:GLN:NE2	2.64	0.41
1:B:568:THR:HG22	1:B:576:CYS:SG	2.61	0.41
1:C:325:ILE:HD11	1:C:416:ALA:HB2	2.02	0.41
1:C:621:LYS:NZ	1:C:654:ASN:O	2.54	0.41
1:D:161:ASN:OD1	1:D:162:GLU:N	2.54	0.41
1:D:342:ARG:NE	1:D:645:TYR:O	2.33	0.41
1:A:520:GLU:HG2	1:A:520:GLU:H	1.74	0.40
1:B:127:THR:HG22	1:B:127:THR:O	2.21	0.40
1:C:397:ASN:HA	1:C:462:GLN:O	2.21	0.40
1:D:480:HIS:CE1	5:D:2088:HOH:O	2.74	0.40
1:A:342:ARG:HD2	1:A:645:TYR:OH	2.21	0.40
1:C:433:LYS:HD2	1:C:434:PRO:HD2	2.03	0.40
1:A:340:THR:HB	1:A:646:VAL:HG13	2.03	0.40
1:D:192:HIS:ND1	1:D:592:LEU:HD13	2.35	0.40
1:D:531:SER:HA	1:D:575:ALA:O	2.22	0.40
4:D:1661:SO4:O4	5:D:2067:HOH:O	2.20	0.40
1:A:189:HIS:CD2	5:A:2113:HOH:O	2.74	0.40
1:A:372:GLY:O	2:A:999:FAD:H2A	2.21	0.40
1:B:305:LEU:HD22	5:B:2039:HOH:O	2.21	0.40
1:D:524:ILE:HG12	1:D:585:TYR:CD2	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ASN:ND2	1:C:536:ARG:NH2[1_546]	2.14	0.06

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	549/658 (83%)	534 (97%)	15 (3%)	0	100	100
1	B	537/658 (82%)	514 (96%)	18 (3%)	5 (1%)	14	22
1	C	555/658 (84%)	528 (95%)	26 (5%)	1 (0%)	43	58
1	D	547/658 (83%)	525 (96%)	21 (4%)	1 (0%)	43	58
All	All	2188/2632 (83%)	2101 (96%)	80 (4%)	7 (0%)	36	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	504	GLY
1	B	195	PHE
1	B	196	LEU
1	C	506	LEU
1	B	503	ARG
1	D	430	HIS
1	B	477	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	476/545 (87%)	437 (92%)	39 (8%)	10	18
1	B	464/545 (85%)	432 (93%)	32 (7%)	14	24
1	C	479/545 (88%)	454 (95%)	25 (5%)	21	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	472/545 (87%)	438 (93%)	34 (7%)	13	23
All	All	1891/2180 (87%)	1761 (93%)	130 (7%)	14	24

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ILE
1	A	90	LEU
1	A	105	LEU
1	A	107	LYS
1	A	108	LYS
1	A	116	LYS
1	A	120	LEU
1	A	162	GLU
1	A	165	LEU
1	A	174	SER
1	A	180	ASP
1	A	199	GLU
1	A	224	LEU
1	A	263	MET
1	A	342	ARG
1	A	354	MET
1	A	379	ILE
1	A	428	PHE
1	A	439	ILE
1	A	462	GLN
1	A	463	LEU
1	A	476	LYS
1	A	498	GLU
1	A	499	ASP
1	A	503	ARG
1	A	508	THR
1	A	510	VAL
1	A	511	ILE
1	A	520	GLU
1	A	526	GLU
1	A	559	PHE
1	A	568	THR
1	A	586	ARG
1	A	588	ILE
1	A	592	LEU
1	A	596	GLU

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Mol	Chain	Res	Type
1	A	613	LEU
1	A	625	GLN
1	A	646	VAL
1	B	86	LYS
1	B	90	LEU
1	B	102	LYS
1	B	116	LYS
1	B	117	ARG
1	B	120	LEU
1	B	170	LYS
1	B	174	SER
1	B	180	ASP
1	B	195	PHE
1	B	199	GLU
1	B	298	THR
1	B	354	MET
1	B	384	THR
1	B	421	MET
1	B	432	LEU
1	B	476	LYS
1	B	478	LEU
1	B	484	VAL
1	B	498	GLU
1	B	500	ASN
1	B	507	LEU
1	B	510	VAL
1	B	515	ARG
1	B	516	ASP
1	B	520	GLU
1	B	526	GLU
1	B	568	THR
1	B	586	ARG
1	B	588	ILE
1	B	603	ARG
1	B	613	LEU
1	C	90	LEU
1	C	105	LEU
1	C	116	LYS
1	C	117	ARG
1	C	120	LEU
1	C	140	LEU
1	C	141	ASP

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Mol	Chain	Res	Type
1	C	150	LEU
1	C	153	SER
1	C	161	ASN
1	C	162	GLU
1	C	224	LEU
1	C	337	LYS
1	C	342	ARG
1	C	498	GLU
1	C	506	LEU
1	C	507	LEU
1	C	508	THR
1	C	526	GLU
1	C	555	LYS
1	C	568	THR
1	C	586	ARG
1	C	588	ILE
1	C	596	GLU
1	C	613	LEU
1	D	90	LEU
1	D	102	LYS
1	D	105	LEU
1	D	107	LYS
1	D	110	GLN
1	D	116	LYS
1	D	117	ARG
1	D	120	LEU
1	D	144	THR
1	D	150	LEU
1	D	161	ASN
1	D	162	GLU
1	D	174	SER
1	D	180	ASP
1	D	199	GLU
1	D	224	LEU
1	D	231	CYS
1	D	384	THR
1	D	393	VAL
1	D	424	GLN
1	D	432	LEU
1	D	474	ARG
1	D	476	LYS
1	D	482	LYS

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Mol	Chain	Res	Type
1	D	498	GLU
1	D	507	LEU
1	D	526	GLU
1	D	536	ARG
1	D	555	LYS
1	D	568	THR
1	D	586	ARG
1	D	588	ILE
1	D	603	ARG
1	D	646	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	142	HIS
1	A	187	HIS
1	A	189	HIS
1	A	192	HIS
1	A	215	HIS
1	A	262	GLN
1	A	277	HIS
1	A	290	GLN
1	A	328	ASN
1	A	362	HIS
1	A	388	GLN
1	A	400	GLN
1	A	423	ASN
1	A	479	GLN
1	A	597	GLN
1	A	615	HIS
1	A	616	HIS
1	A	650	ASN
1	B	110	GLN
1	B	177	GLN
1	B	277	HIS
1	B	290	GLN
1	B	400	GLN
1	B	423	ASN
1	B	427	GLN
1	B	597	GLN
1	B	650	ASN

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Mol	Chain	Res	Type
1	B	656	ASN
1	C	110	GLN
1	C	192	HIS
1	C	290	GLN
1	C	388	GLN
1	C	400	GLN
1	C	423	ASN
1	C	424	GLN
1	C	462	GLN
1	C	597	GLN
1	C	650	ASN
1	C	656	ASN
1	D	142	HIS
1	D	151	ASN
1	D	192	HIS
1	D	277	HIS
1	D	290	GLN
1	D	424	GLN
1	D	427	GLN
1	D	461	ASN
1	D	462	GLN
1	D	597	GLN
1	D	650	ASN
1	D	656	ASN

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](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	1660	-	4,4,4	0.38	0	6,6,6	0.79	0
2	FAD	B	999	-	58,58,58	1.38	8 (13%)	85,89,89	1.94	25 (29%)
2	FAD	C	999	-	58,58,58	1.13	5 (8%)	85,89,89	1.99	25 (29%)
2	FAD	A	999	-	58,58,58	1.30	6 (10%)	85,89,89	1.66	16 (18%)
4	SO4	B	1661	-	4,4,4	0.31	0	6,6,6	0.72	0
4	SO4	D	1661	-	4,4,4	0.42	0	6,6,6	0.91	0
4	SO4	A	1660	-	4,4,4	0.23	0	6,6,6	1.01	0
4	SO4	C	1660	-	4,4,4	0.36	0	6,6,6	0.46	0
2	FAD	D	999	-	58,58,58	1.30	8 (13%)	85,89,89	1.76	24 (28%)
4	SO4	D	1660	-	4,4,4	0.17	0	6,6,6	0.49	0
4	SO4	A	1661	-	4,4,4	0.47	0	6,6,6	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	999	-	-	4/34/50/50	0/6/6/6
2	FAD	C	999	-	-	2/34/50/50	0/6/6/6
2	FAD	D	999	-	-	3/34/50/50	0/6/6/6
2	FAD	A	999	-	-	4/34/50/50	0/6/6/6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	FAD	C4X-N5	6.13	1.44	1.30
2	D	999	FAD	C4X-N5	4.29	1.40	1.30
2	A	999	FAD	C4X-N5	4.03	1.39	1.30
2	D	999	FAD	PA-O3P	3.82	1.63	1.59
2	C	999	FAD	C4X-N5	3.67	1.38	1.30
2	A	999	FAD	PA-O3P	3.36	1.63	1.59
2	B	999	FAD	P-O3P	2.92	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	FAD	C10-N1	2.75	1.38	1.33
2	B	999	FAD	O4'-C4'	-2.66	1.37	1.43
2	C	999	FAD	C10-N1	2.64	1.38	1.33
2	B	999	FAD	C2A-N1A	2.62	1.38	1.33
2	C	999	FAD	C8A-N7A	2.50	1.36	1.31
2	D	999	FAD	P-O3P	2.48	1.62	1.59
2	C	999	FAD	C2A-N3A	2.43	1.38	1.33
2	D	999	FAD	C10-N1	2.35	1.38	1.33
2	A	999	FAD	C2A-N1A	2.35	1.38	1.33
2	C	999	FAD	C1'-C2'	2.27	1.55	1.52
2	A	999	FAD	C8A-N7A	2.27	1.36	1.31
2	B	999	FAD	C1'-C2'	2.24	1.55	1.52
2	D	999	FAD	C4X-C10	-2.22	1.37	1.44
2	D	999	FAD	C8A-N7A	2.22	1.35	1.31
2	D	999	FAD	C5A-N7A	-2.21	1.35	1.39
2	B	999	FAD	C2A-N3A	2.18	1.37	1.33
2	B	999	FAD	C10-N1	2.13	1.37	1.33
2	B	999	FAD	C10-N10	2.13	1.41	1.37
2	A	999	FAD	O4-C4	2.09	1.27	1.23
2	D	999	FAD	C2A-N1A	2.06	1.37	1.33

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	999	FAD	C5A-C4A-N3A	-6.34	117.99	126.72
2	A	999	FAD	N3A-C2A-N1A	-5.91	119.63	128.58
2	C	999	FAD	N3A-C2A-N1A	-5.42	120.37	128.58
2	B	999	FAD	N9A-C8A-N7A	-5.21	106.55	113.94
2	B	999	FAD	C5A-N7A-C8A	4.57	110.64	103.45
2	B	999	FAD	O4'-C4'-C5'	-4.45	100.18	109.99
2	C	999	FAD	C2A-N3A-C4A	4.37	122.52	111.83
2	B	999	FAD	C4-C4X-N5	4.37	124.24	118.21
2	B	999	FAD	N3A-C2A-N1A	-4.35	122.00	128.58
2	D	999	FAD	N3A-C2A-N1A	-4.30	122.07	128.58
2	C	999	FAD	C9A-C5X-N5	-4.09	118.11	122.45
2	B	999	FAD	C4A-C5A-N7A	-4.07	105.93	110.58
2	D	999	FAD	N9A-C8A-N7A	-3.96	108.32	113.94
2	A	999	FAD	C9A-C5X-N5	-3.94	118.28	122.45
2	A	999	FAD	C4-N3-C2	-3.87	118.76	125.64
2	C	999	FAD	O4'-C4'-C5'	-3.71	101.81	109.99
2	C	999	FAD	C5A-N7A-C8A	3.68	109.23	103.45
2	B	999	FAD	C10-C4X-N5	-3.65	117.35	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	FAD	C5A-C4A-N3A	-3.56	121.82	126.72
2	B	999	FAD	C4X-C10-N10	3.50	121.49	116.48
2	B	999	FAD	C4A-N9A-C8A	3.49	109.41	105.74
2	D	999	FAD	C4X-C10-N10	3.49	121.48	116.48
2	D	999	FAD	C9A-C5X-N5	-3.46	118.79	122.45
2	C	999	FAD	N3A-C4A-N9A	3.45	133.03	127.17
2	C	999	FAD	C4-N3-C2	-3.45	119.52	125.64
2	D	999	FAD	C10-C4X-N5	-3.42	117.82	124.81
2	C	999	FAD	O2-C2-N1	-3.42	116.13	121.80
2	C	999	FAD	C4B-O4B-C1B	3.40	116.98	109.47
2	C	999	FAD	C4A-C5A-N7A	-3.40	106.70	110.58
2	C	999	FAD	C5'-C4'-C3'	3.34	118.53	112.22
2	C	999	FAD	N9A-C8A-N7A	-3.32	109.22	113.94
2	A	999	FAD	C2A-N3A-C4A	3.29	119.87	111.83
2	B	999	FAD	C10-N1-C2	3.29	123.96	116.85
2	A	999	FAD	C10-C4X-N5	-3.22	118.24	124.81
2	D	999	FAD	C5A-N7A-C8A	3.21	108.50	103.45
2	D	999	FAD	C6A-C5A-C4A	3.19	121.54	117.18
2	C	999	FAD	C4X-C10-N10	3.19	121.05	116.48
2	D	999	FAD	C5A-C4A-N3A	-3.19	122.33	126.72
2	D	999	FAD	O4'-C4'-C5'	-3.13	103.08	109.99
2	A	999	FAD	C5X-N5-C4X	3.11	123.12	118.09
2	A	999	FAD	C5A-C4A-N3A	-3.01	122.57	126.72
2	B	999	FAD	C4X-C4-N3	2.94	120.75	113.25
2	A	999	FAD	O4B-C1B-N9A	-2.93	102.47	108.09
2	B	999	FAD	C2A-N3A-C4A	2.88	118.88	111.83
2	D	999	FAD	O3'-C3'-C4'	2.86	115.42	108.93
2	D	999	FAD	C10-N1-C2	2.85	123.03	116.85
2	C	999	FAD	C5A-C4A-N9A	2.84	108.91	105.81
2	B	999	FAD	C5X-C9A-N10	2.83	120.53	117.97
2	C	999	FAD	O5'-C5'-C4'	-2.83	101.81	109.36
2	D	999	FAD	C5X-N5-C4X	2.82	122.65	118.09
2	C	999	FAD	O4B-C1B-C2B	-2.81	100.60	106.62
2	B	999	FAD	O4-C4-N3	-2.74	114.97	120.11
2	B	999	FAD	C4-N3-C2	-2.73	120.80	125.64
2	C	999	FAD	C10-C4X-N5	-2.71	119.28	124.81
2	D	999	FAD	O4'-C4'-C3'	2.70	115.56	109.25
2	D	999	FAD	C6-C5X-C9A	2.68	122.73	119.05
2	D	999	FAD	C2A-N1A-C6A	2.67	123.11	118.73
2	D	999	FAD	C4-C4X-N5	2.66	121.88	118.21
2	A	999	FAD	N9A-C8A-N7A	-2.65	110.18	113.94
2	D	999	FAD	C4X-C10-N1	-2.57	118.29	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	C4X-C10-N10	2.55	120.13	116.48
2	B	999	FAD	C4X-C10-N1	-2.53	118.40	124.59
2	B	999	FAD	C9A-C5X-N5	-2.49	119.82	122.45
2	D	999	FAD	O2-C2-N3	2.48	123.34	118.58
2	B	999	FAD	O2P-P-O3P	2.48	113.97	107.27
2	D	999	FAD	C4A-C5A-N7A	-2.47	107.76	110.58
2	A	999	FAD	C5X-C9A-N10	2.41	120.15	117.97
2	A	999	FAD	C4-C4X-N5	2.37	121.48	118.21
2	A	999	FAD	O2A-PA-O3P	2.35	113.63	107.27
2	A	999	FAD	O3'-C3'-C2'	-2.35	103.59	108.93
2	C	999	FAD	O3P-PA-O1A	2.32	117.67	110.70
2	A	999	FAD	C4X-C4-N3	2.29	119.09	113.25
2	B	999	FAD	C5'-C4'-C3'	2.29	116.54	112.22
2	D	999	FAD	O2A-PA-O3P	2.29	113.45	107.27
2	C	999	FAD	O4-C4-C4X	-2.27	120.53	126.53
2	D	999	FAD	C4X-C4-N3	2.27	119.04	113.25
2	C	999	FAD	C5X-N5-C4X	2.26	121.74	118.09
2	C	999	FAD	C4-C4X-C10	2.22	120.74	116.93
2	B	999	FAD	C9-C9A-N10	-2.22	118.87	121.85
2	B	999	FAD	C6A-C5A-C4A	2.19	120.17	117.18
2	B	999	FAD	O2-C2-N3	2.19	122.79	118.58
2	C	999	FAD	C5X-C9A-N10	2.13	119.89	117.97
2	B	999	FAD	O2A-PA-O3P	2.13	113.03	107.27
2	C	999	FAD	C4X-C4-N3	2.13	118.67	113.25
2	B	999	FAD	N3A-C4A-N9A	2.11	130.75	127.17
2	C	999	FAD	C4X-C10-N1	-2.09	119.47	124.59
2	A	999	FAD	O4'-C4'-C5'	-2.05	105.46	109.99
2	D	999	FAD	O4B-C1B-N9A	-2.05	104.16	108.09
2	D	999	FAD	O5'-C5'-C4'	-2.04	103.91	109.36
2	D	999	FAD	C4-N3-C2	-2.03	122.03	125.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	FAD	N10-C1'-C2'-O2'
2	A	999	FAD	N10-C1'-C2'-C3'
2	B	999	FAD	N10-C1'-C2'-O2'
2	B	999	FAD	N10-C1'-C2'-C3'
2	C	999	FAD	N10-C1'-C2'-O2'
2	C	999	FAD	N10-C1'-C2'-C3'
2	D	999	FAD	N10-C1'-C2'-O2'

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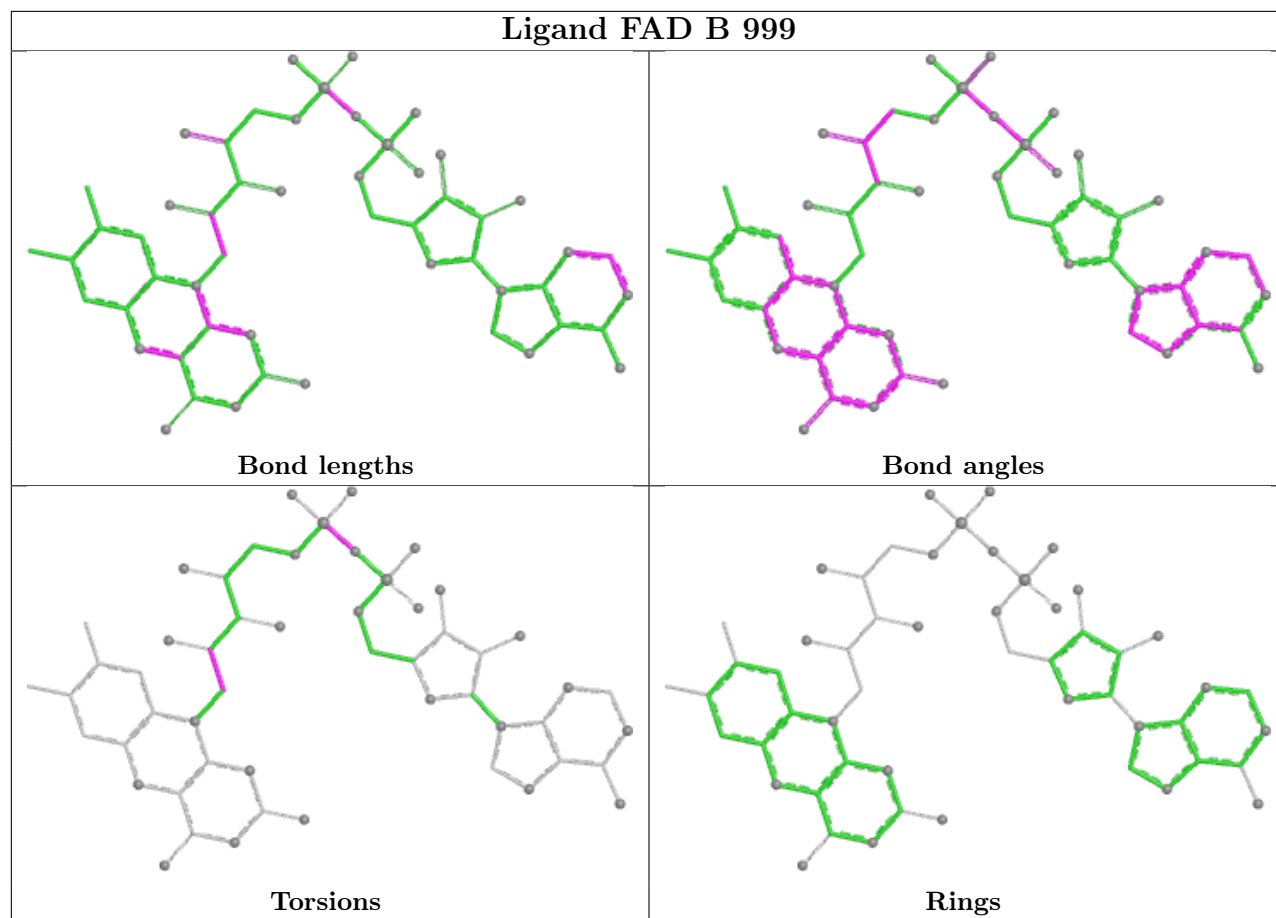
Mol	Chain	Res	Type	Atoms
2	D	999	FAD	N10-C1'-C2'-C3'
2	B	999	FAD	PA-O3P-P-O2P
2	A	999	FAD	PA-O3P-P-O1P
2	A	999	FAD	PA-O3P-P-O2P
2	B	999	FAD	PA-O3P-P-O1P
2	D	999	FAD	PA-O3P-P-O2P

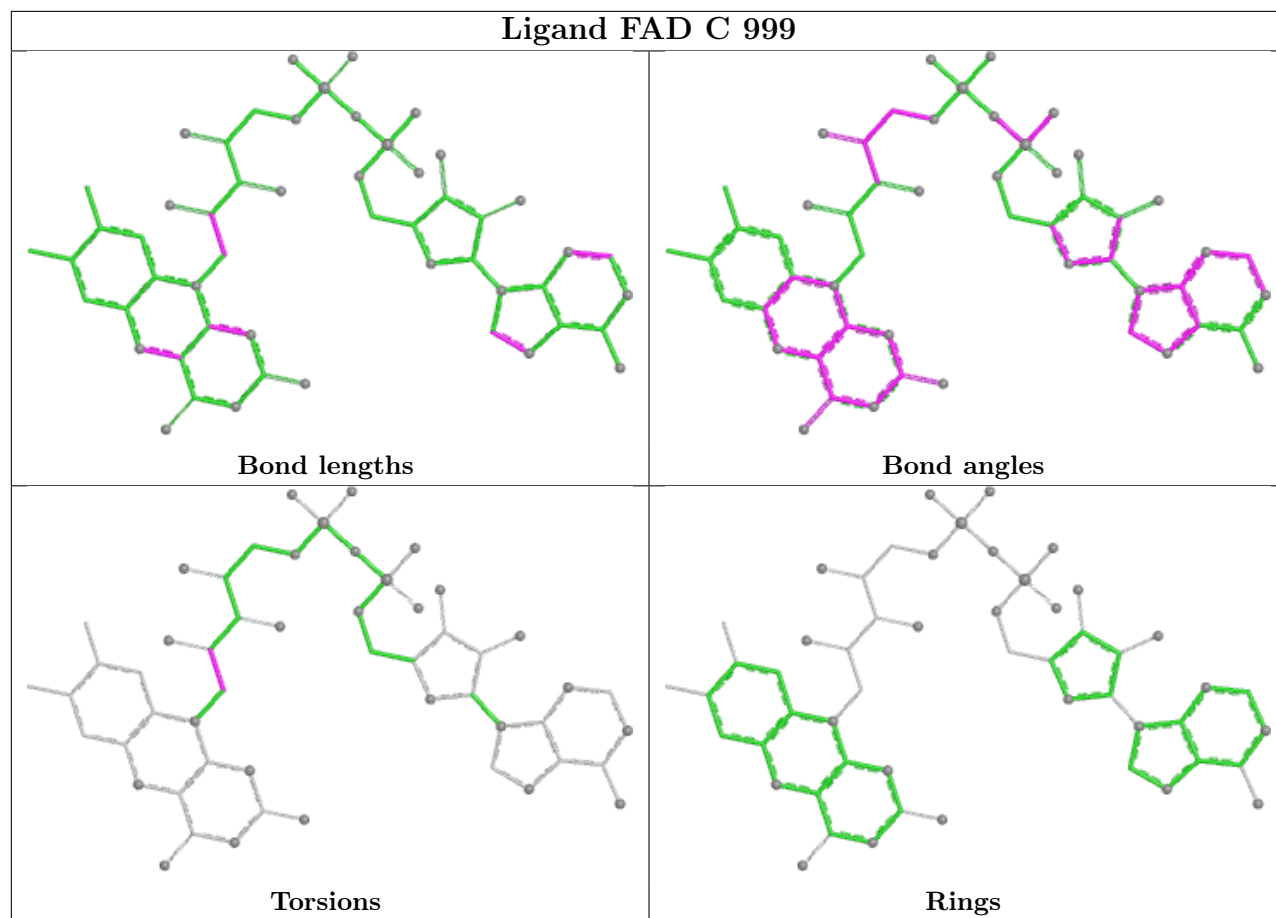
There are no ring outliers.

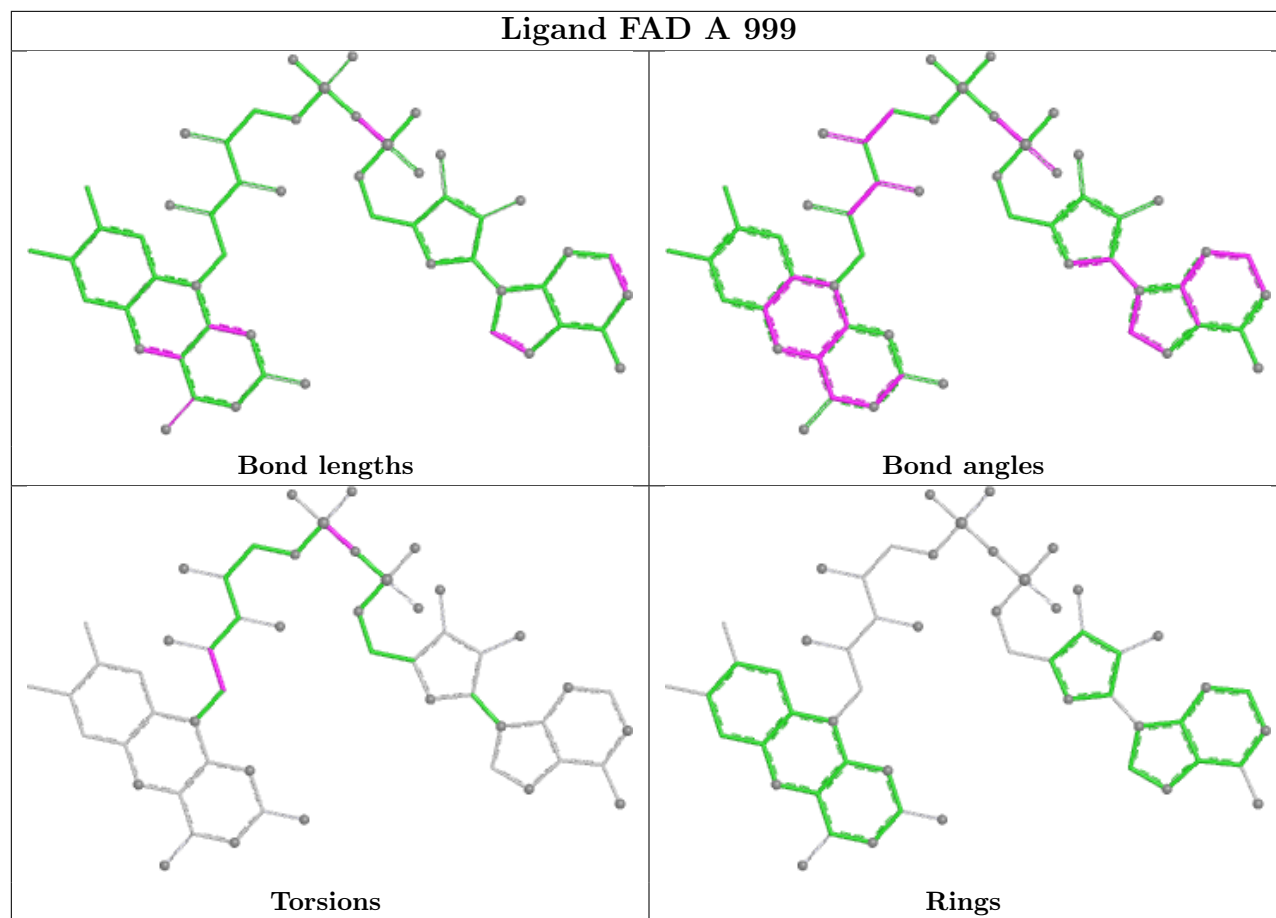
9 monomers are involved in 13 short contacts:

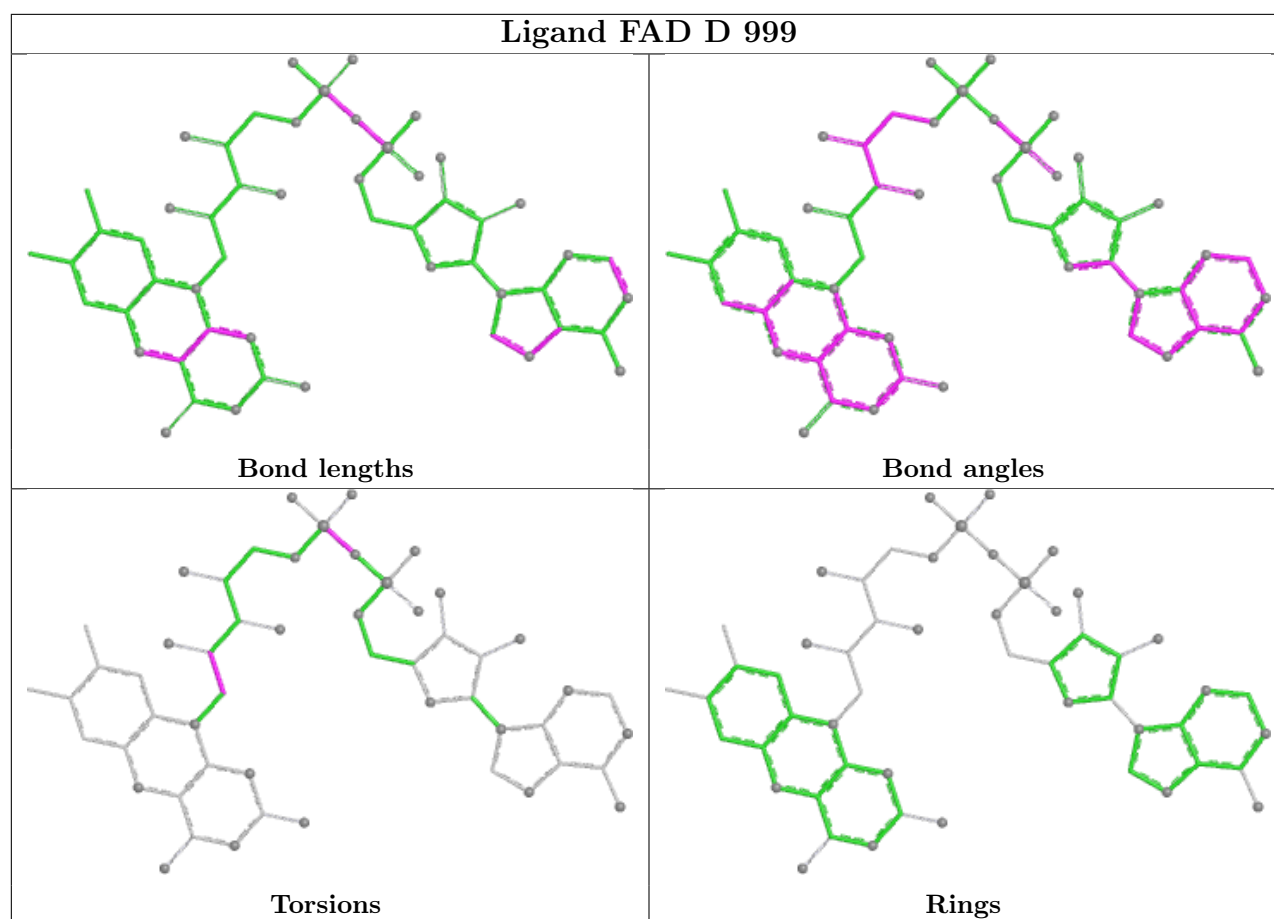
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1660	SO4	2	0
2	B	999	FAD	2	0
2	C	999	FAD	1	0
2	A	999	FAD	3	0
4	D	1661	SO4	1	0
4	C	1660	SO4	1	0
2	D	999	FAD	1	0
4	D	1660	SO4	1	0
4	A	1661	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	555/658 (84%)	-0.40	8 (1%) 73 69	10, 24, 49, 73	0
1	B	543/658 (82%)	-0.21	12 (2%) 62 58	13, 30, 60, 75	0
1	C	557/658 (84%)	-0.41	11 (1%) 65 60	9, 24, 51, 73	2 (0%)
1	D	550/658 (83%)	-0.38	5 (0%) 81 78	9, 25, 53, 67	1 (0%)
All	All	2205/2632 (83%)	-0.35	36 (1%) 70 66	9, 25, 54, 75	3 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	457	GLY	5.6
1	A	82	ILE	4.9
1	B	81	GLY	4.1
1	B	457	GLY	4.1
1	C	82	ILE	4.1
1	A	83	ILE	3.9
1	D	82	ILE	3.8
1	C	509	TYR	3.8
1	B	140	LEU	3.5
1	A	439	ILE	3.5
1	A	457	GLY	3.3
1	B	504	GLY	3.1
1	D	81	GLY	3.0
1	C	432	LEU	2.7
1	C	83	ILE	2.7
1	A	81	GLY	2.7
1	D	504	GLY	2.6
1	D	83	ILE	2.4
1	C	506	LEU	2.4
1	D	559	PHE	2.4
1	C	508	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	142	HIS	2.3
1	A	559	PHE	2.3
1	B	458	PHE	2.3
1	B	586	ARG	2.3
1	C	559	PHE	2.2
1	B	460	PRO	2.2
1	B	475	GLU	2.2
1	B	199	GLU	2.2
1	C	433	LYS	2.2
1	C	435	GLN	2.1
1	C	81	GLY	2.1
1	B	478	LEU	2.1
1	B	509	TYR	2.1
1	A	438	SER	2.1
1	B	435	GLN	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 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.

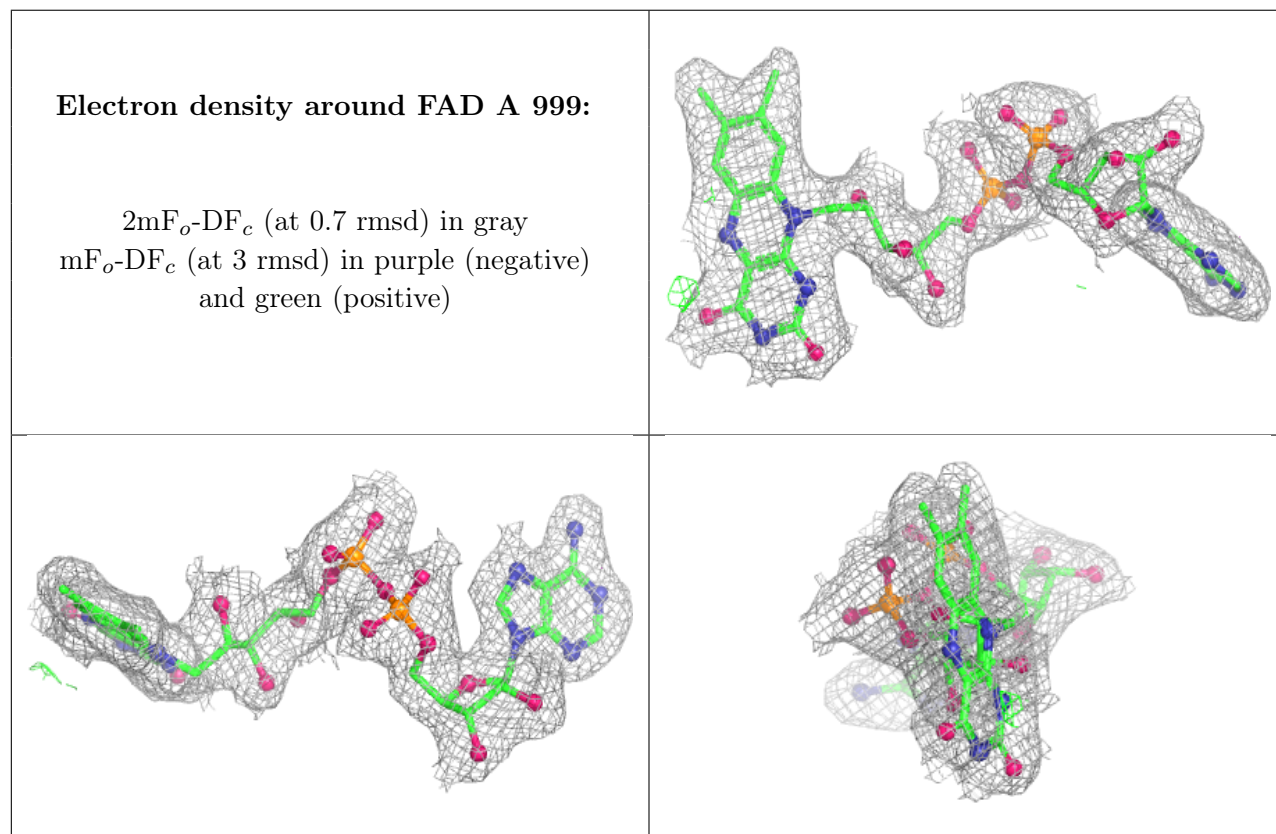
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	D	1661	5/5	0.87	0.13	41,44,53,53	0
4	SO4	B	1661	5/5	0.89	0.16	64,66,66,67	0
4	SO4	B	1660	5/5	0.91	0.14	47,49,51,51	0
3	CL	A	1659	1/1	0.92	0.12	36,36,36,36	0
3	CL	B	1659	1/1	0.93	0.16	56,56,56,56	0
4	SO4	A	1660	5/5	0.94	0.12	42,42,46,49	0
3	CL	C	1659	1/1	0.96	0.09	39,39,39,39	0
3	CL	D	1659	1/1	0.96	0.17	44,44,44,44	0

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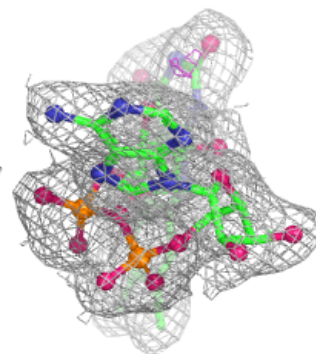
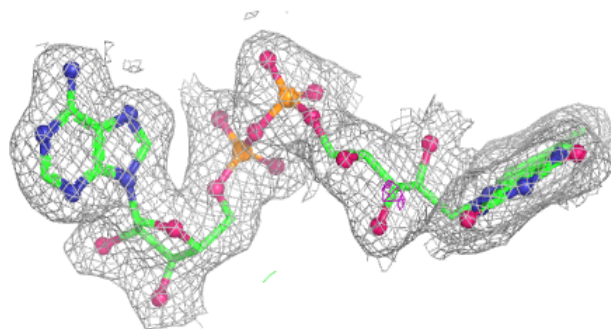
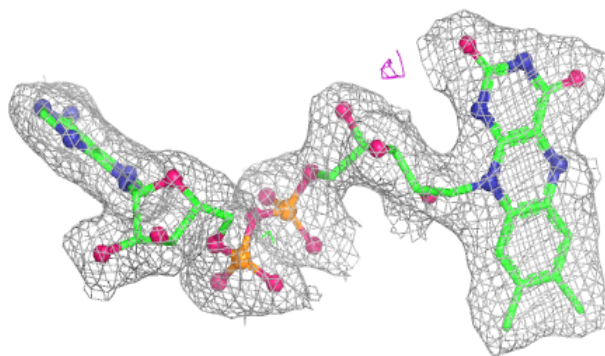
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	C	1660	5/5	0.97	0.09	44,44,47,49	0
2	FAD	A	999	53/53	0.98	0.05	9,11,14,16	0
4	SO4	A	1661	5/5	0.98	0.06	30,30,33,33	0
4	SO4	D	1660	5/5	0.98	0.09	36,38,39,43	0
2	FAD	B	999	53/53	0.98	0.05	12,15,18,21	0
2	FAD	D	999	53/53	0.99	0.04	8,10,13,15	0
2	FAD	C	999	53/53	0.99	0.04	7,9,12,15	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.

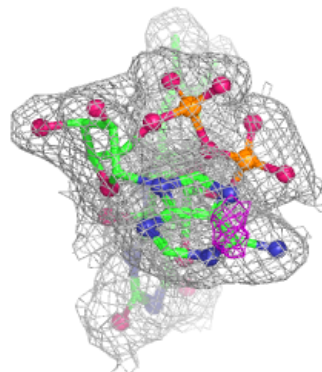
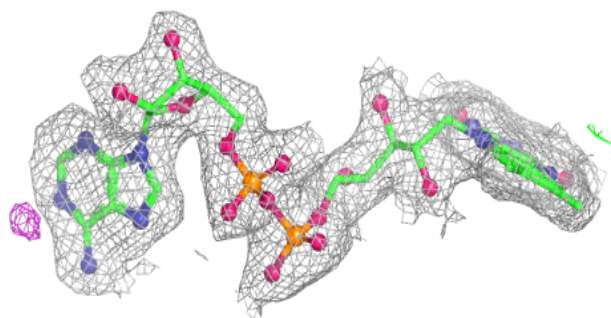
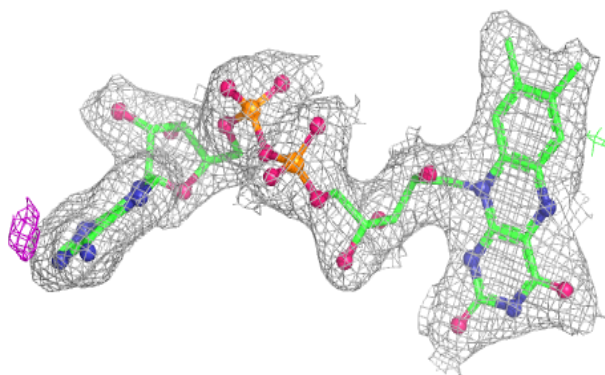


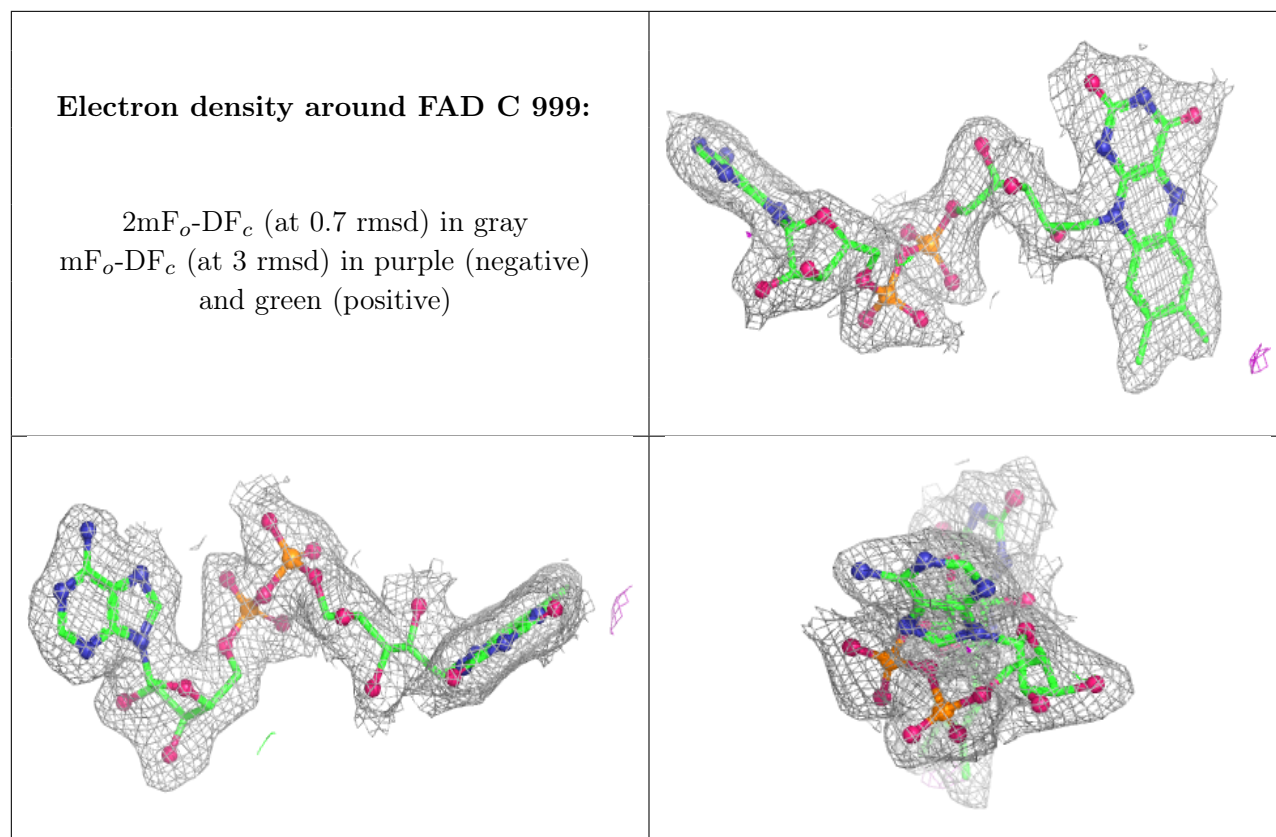
Electron density around FAD B 999:

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

**Electron density around FAD D 999:**

$2mF_o-DF_c$ (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.