



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:23 PM UTC

PDB ID : 4BC7 / pdb_00004bc7
Title : MAMMALIAN ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE: Arg419His mutant
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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)
Xtrriage (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

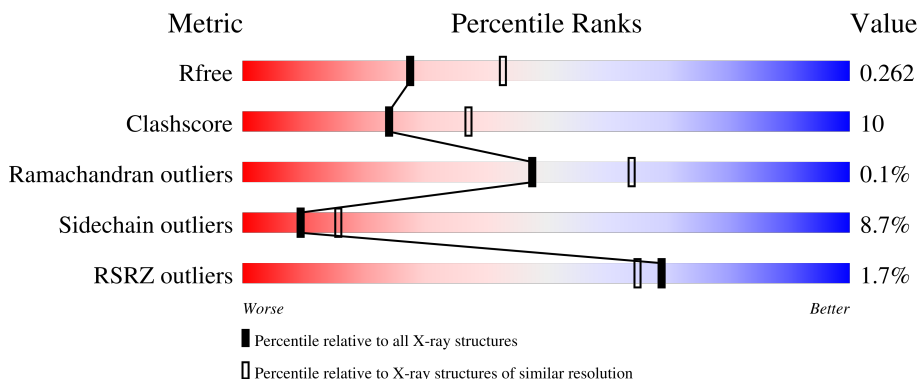
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	 2% 62% 19% 16%
1	B	658	 2% 61% 18% 17%
1	C	658	 % 63% 19% 15%
1	D	658	 2% 63% 18% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17858 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	Total 4396	C 2791	N 761	O 820	S 24	0	1	0
1	B	543	Total 4300	C 2732	N 746	O 798	S 24	0	0	0
1	C	557	Total 4404	C 2793	N 765	O 822	S 24	0	0	0
1	D	550	Total 4349	C 2757	N 756	O 812	S 24	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

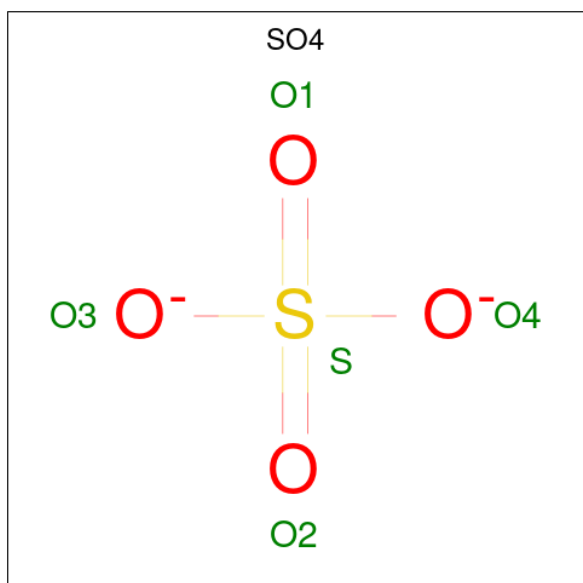
Chain	Residue	Modelled	Actual	Comment	Reference
A	419	HIS	ARG	engineered mutation	UNP P97275
B	419	HIS	ARG	engineered mutation	UNP P97275
C	419	HIS	ARG	engineered mutation	UNP P97275
D	419	HIS	ARG	engineered mutation	UNP P97275

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



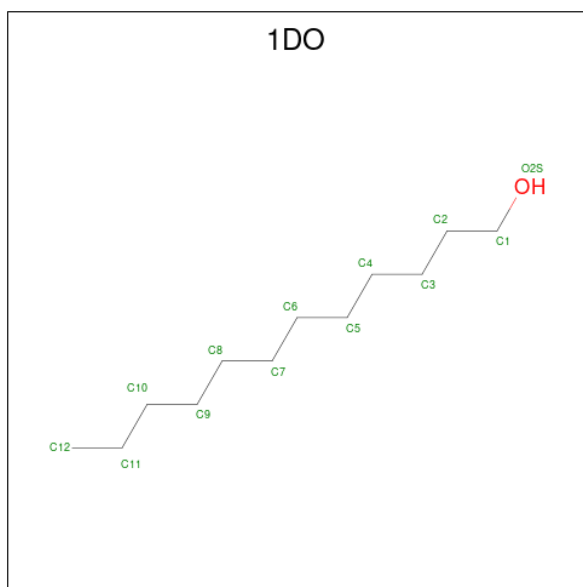
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
2	A	1	Total	53	27	9	15	2	0	0
2	B	1	Total	53	27	9	15	2	0	0
2	C	1	Total	53	27	9	15	2	0	0
2	D	1	Total	53	27	9	15	2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is 1-DODECANOL (CCD ID: 1DO) (formula: C₁₂H₂₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 13 12 1	0	0
4	C	1	Total C O 13 12 1	0	0

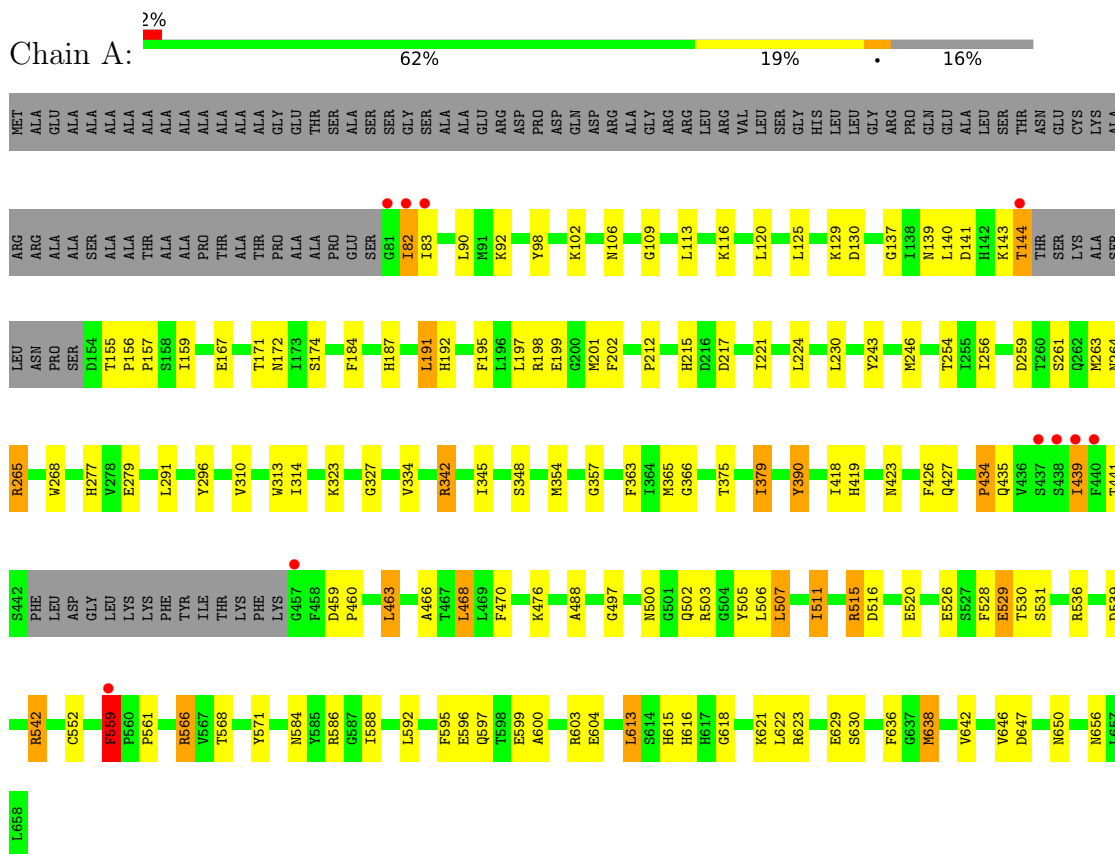
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	46	Total O 46 46	0	0
5	B	36	Total O 36 36	0	0
5	C	49	Total O 49 49	0	0
5	D	30	Total O 30 30	0	0

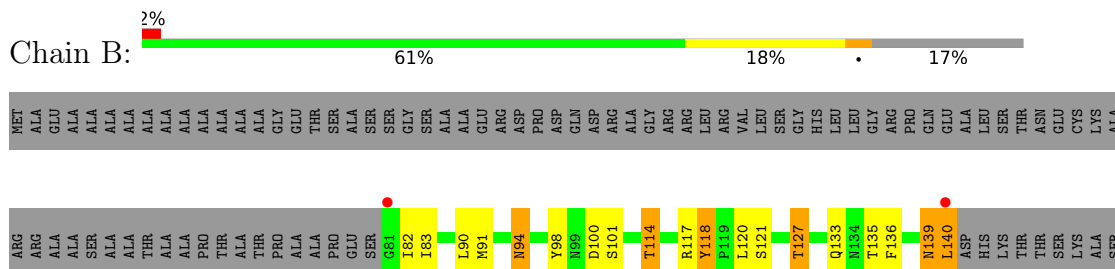
3 Residue-property plots [i](#)

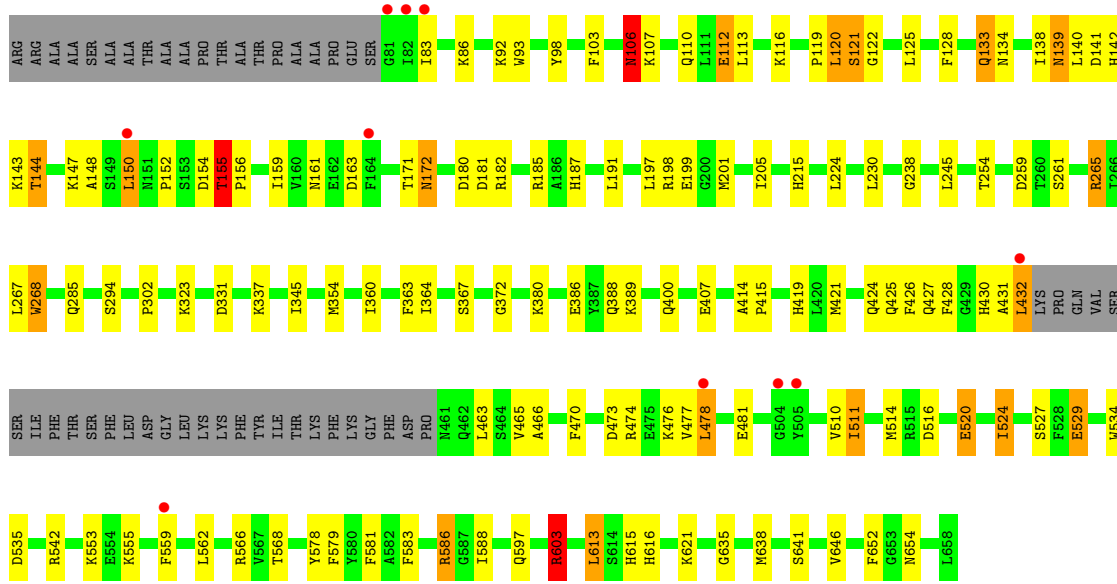
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL



- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.41Å 99.19Å 107.46Å 90.58° 91.88° 95.03°	Depositor
Resolution (Å)	54.17 – 2.40 54.17 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (54.17-2.40) 95.4 (54.17-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.270 0.210 , 0.262	Depositor DCC
R_{free} test set	1077 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17858	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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: SO4, FAD, 1DO

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	1.21	47/4500 (1.0%)	1.17	21/6084 (0.3%)
1	B	1.06	8/4398 (0.2%)	1.13	15/5945 (0.3%)
1	C	1.04	5/4505 (0.1%)	1.10	8/6092 (0.1%)
1	D	0.95	4/4447 (0.1%)	1.08	10/6013 (0.2%)
All	All	1.07	64/17850 (0.4%)	1.12	54/24134 (0.2%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	265	ARG	CG-CD	-8.28	1.27	1.52
1	A	542	ARG	CZ-NH1	-8.08	1.21	1.32
1	C	265	ARG	NE-CZ	-7.56	1.24	1.33
1	A	184	PHE	CE2-CZ	-7.47	1.16	1.38
1	B	623	ARG	CZ-NH1	-7.46	1.22	1.32
1	A	638	MET	SD-CE	-7.43	1.60	1.79
1	A	595	PHE	CE1-CZ	-7.41	1.16	1.38
1	A	515	ARG	CZ-NH2	-7.10	1.24	1.33
1	D	265	ARG	CD-NE	-7.08	1.36	1.46
1	A	536	ARG	CZ-NH1	-7.02	1.23	1.32
1	A	568	THR	CB-CG2	-7.00	1.29	1.52
1	A	528	PHE	CG-CD2	-6.89	1.24	1.38
1	A	195	PHE	CG-CD2	-6.70	1.24	1.38
1	A	595	PHE	CG-CD2	-6.69	1.24	1.38
1	A	603	ARG	CZ-NH1	-6.65	1.23	1.32
1	D	265	ARG	NE-CZ	-6.63	1.25	1.33
1	A	559	PHE	CG-CD2	-6.62	1.25	1.38
1	A	195	PHE	CE1-CZ	-6.46	1.19	1.38
1	A	528	PHE	CE1-CZ	-6.45	1.19	1.38
1	A	195	PHE	CG-CD1	-6.31	1.25	1.38
1	A	636	PHE	CE2-CZ	-6.19	1.20	1.38
1	A	636	PHE	CG-CD1	-6.04	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	597	GLN	CD-NE2	-6.01	1.20	1.33
1	A	224	LEU	CG-CD1	-6.00	1.32	1.52
1	A	224	LEU	CG-CD2	-5.87	1.33	1.52
1	A	184	PHE	CG-CD1	-5.87	1.26	1.38
1	B	559	PHE	CA-C	-5.86	1.44	1.52
1	A	191	LEU	CG-CD2	-5.77	1.33	1.52
1	A	470	PHE	CE2-CZ	-5.77	1.21	1.38
1	A	191	LEU	CG-CD1	-5.76	1.33	1.52
1	C	265	ARG	CD-NE	-5.72	1.38	1.46
1	B	334	VAL	CB-CG2	-5.71	1.33	1.52
1	A	195	PHE	CE2-CZ	-5.70	1.21	1.38
1	A	390	TYR	CG-CD1	-5.69	1.27	1.39
1	B	629	GLU	CB-CG	-5.69	1.35	1.52
1	A	470	PHE	CE1-CZ	-5.63	1.21	1.38
1	A	656	ASN	CG-ND2	-5.62	1.21	1.33
1	A	265	ARG	NE-CZ	-5.58	1.26	1.33
1	D	180	ASP	CB-CG	-5.57	1.38	1.52
1	A	291	LEU	CG-CD1	-5.56	1.34	1.52
1	A	342	ARG	CG-CD	-5.55	1.35	1.52
1	A	470	PHE	CG-CD1	-5.51	1.27	1.38
1	A	559	PHE	CE1-CZ	-5.50	1.22	1.38
1	A	363	PHE	CG-CD2	-5.44	1.27	1.38
1	C	265	ARG	CG-CD	-5.42	1.36	1.52
1	A	265	ARG	CZ-NH2	-5.37	1.26	1.33
1	A	488	ALA	CA-C	5.36	1.59	1.52
1	B	568	THR	C-O	-5.35	1.17	1.23
1	A	636	PHE	CE1-CZ	-5.33	1.22	1.38
1	A	613	LEU	CG-CD2	-5.32	1.34	1.52
1	A	265	ARG	CD-NE	-5.32	1.38	1.46
1	B	265	ARG	NE-CZ	-5.31	1.27	1.33
1	C	266	ILE	CA-C	-5.23	1.47	1.53
1	A	515	ARG	CZ-NH1	-5.22	1.25	1.32
1	B	559	PHE	CB-CG	-5.17	1.38	1.50
1	A	184	PHE	CE1-CZ	-5.15	1.23	1.38
1	A	390	TYR	CG-CD2	-5.14	1.28	1.39
1	A	167	GLU	CD-OE1	-5.14	1.15	1.25
1	A	470	PHE	CG-CD2	-5.13	1.28	1.38
1	A	595	PHE	CE2-CZ	-5.13	1.23	1.38
1	B	406	ARG	CG-CD	-5.09	1.37	1.52
1	C	177	GLN	CD-OE1	-5.07	1.14	1.23
1	A	650	ASN	CG-ND2	-5.06	1.22	1.33
1	A	566	ARG	CZ-NH1	-5.04	1.25	1.32

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ARG	NE-CZ-NH2	9.85	128.06	119.20
1	B	623	ARG	NE-CZ-NH2	8.87	127.18	119.20
1	A	191	LEU	CD1-CG-CD2	-8.86	91.30	110.80
1	A	542	ARG	NE-CZ-NH2	8.76	127.08	119.20
1	B	155	THR	CA-C-N	8.28	125.70	119.66
1	B	155	THR	C-N-CA	8.28	125.70	119.66
1	B	265	ARG	CG-CD-NE	-8.04	94.31	112.00
1	A	603	ARG	NE-CZ-NH2	7.72	126.14	119.20
1	A	224	LEU	CD1-CG-CD2	-7.66	93.94	110.80
1	A	265	ARG	CB-CG-CD	-7.42	94.23	111.30
1	A	566	ARG	NE-CZ-NH2	7.16	125.65	119.20
1	C	354	MET	N-CA-C	7.05	120.44	109.52
1	B	298	THR	N-CA-C	-6.81	105.51	113.88
1	D	180	ASP	CB-CA-C	-6.73	100.60	110.96
1	B	118	TYR	CA-C-N	6.57	126.81	119.32
1	B	118	TYR	C-N-CA	6.57	126.81	119.32
1	A	515	ARG	CG-CD-NE	-6.55	97.59	112.00
1	B	474	ARG	N-CA-C	6.53	118.05	111.07
1	D	566	ARG	CB-CG-CD	-6.50	96.35	111.30
1	D	265	ARG	CD-NE-CZ	-6.29	115.59	124.40
1	A	647	ASP	CA-C-N	6.16	126.34	119.32
1	A	647	ASP	C-N-CA	6.16	126.34	119.32
1	A	291	LEU	CD1-CG-CD2	-6.07	97.44	110.80
1	A	536	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	C	354	MET	CA-CB-CG	5.99	126.08	114.10
1	D	603	ARG	CD-NE-CZ	5.94	132.72	124.40
1	A	342	ARG	CA-CB-CG	-5.93	102.24	114.10
1	B	559	PHE	CB-CA-C	-5.92	100.65	108.76
1	B	265	ARG	CD-NE-CZ	-5.92	116.11	124.40
1	A	125	LEU	CA-C-N	5.79	125.92	119.32
1	A	125	LEU	C-N-CA	5.79	125.92	119.32
1	C	361	HIS	N-CA-C	-5.79	104.97	111.28
1	A	613	LEU	CD1-CG-CD2	-5.74	98.18	110.80
1	D	265	ARG	CA-CB-CG	-5.53	103.03	114.10
1	D	566	ARG	CD-NE-CZ	-5.49	116.72	124.40
1	A	515	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	C	503	ARG	N-CA-C	5.48	116.94	111.07
1	D	268	TRP	N-CA-C	5.28	116.55	108.52
1	A	334	VAL	N-CA-C	-5.27	107.26	113.42
1	A	379	ILE	CB-CA-C	-5.22	102.84	110.62
1	C	603	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	C	461	ASN	N-CA-C	5.19	120.38	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	GLY	N-CA-C	-5.15	106.52	112.29
1	D	302	PRO	N-CA-C	-5.14	103.70	111.41
1	B	139	ASN	N-CA-C	5.13	119.29	112.72
1	A	296	TYR	N-CA-C	5.09	117.59	109.81
1	D	155	THR	CA-C-N	5.08	125.62	120.38
1	D	155	THR	C-N-CA	5.08	125.62	120.38
1	B	334	VAL	CG1-CB-CG2	-5.08	99.62	110.80
1	C	564	THR	OG1-CB-CG2	-5.08	99.14	109.30
1	C	537	VAL	N-CA-C	5.06	115.28	110.42
1	B	559	PHE	CB-CG-CD2	5.02	129.23	120.70
1	B	332	LEU	N-CA-C	5.01	116.82	111.36
1	B	261	SER	N-CA-C	5.01	118.16	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4396	0	4325	83	0
1	B	4300	0	4236	107	2
1	C	4404	0	4336	90	2
1	D	4349	0	4285	89	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	B	13	0	26	2	0
4	C	13	0	26	2	0
5	A	46	0	0	1	0
5	B	36	0	0	1	0
5	C	49	0	0	3	0
5	D	30	0	0	0	0
All	All	17858	0	17358	352	2

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 (352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:LEU:O	1:B:511:ILE:CD1	1.65	1.44
1:B:511:ILE:HD13	1:B:511:ILE:N	1.47	1.24
1:B:511:ILE:CD1	1:B:511:ILE:H	1.57	1.13
1:B:621:LYS:NZ	1:B:654:ASN:O	1.80	1.13
1:B:507:LEU:O	1:B:511:ILE:HD12	1.49	1.11
1:B:507:LEU:O	1:B:511:ILE:HD11	1.33	1.07
1:C:586:ARG:HG3	1:C:586:ARG:HH11	1.03	1.07
1:B:507:LEU:C	1:B:511:ILE:HD11	1.79	1.06
1:B:265:ARG:NH1	1:B:265:ARG:HA	1.71	1.05
1:C:139:ASN:HB3	1:C:141:ASP:OD1	1.53	1.05
1:B:265:ARG:HA	1:B:265:ARG:HH11	1.24	0.99
1:B:265:ARG:HH11	1:B:265:ARG:CA	1.77	0.98
1:A:615:HIS:HD2	1:A:616:HIS:HD2	1.10	0.98
1:C:100:ASP:O	1:C:114:THR:HG22	1.63	0.98
1:B:511:ILE:HD13	1:B:511:ILE:H	0.81	0.97
1:B:139:ASN:O	1:B:140:LEU:HB2	1.65	0.97
1:D:586:ARG:HH11	1:D:586:ARG:HG3	1.29	0.96
1:B:511:ILE:CD1	1:B:511:ILE:N	2.26	0.90
1:C:586:ARG:HG3	1:C:586:ARG:NH1	1.82	0.89
1:C:419:HIS:HD2	1:C:566:ARG:HH21	1.20	0.89
1:A:82:ILE:HG13	1:A:264:ASN:ND2	1.87	0.89
1:A:615:HIS:HD2	1:A:616:HIS:CD2	1.93	0.86
1:A:265:ARG:HH11	1:A:265:ARG:HG2	1.40	0.85
1:B:406:ARG:HG3	1:B:406:ARG:HH11	1.39	0.85
1:A:615:HIS:CD2	1:A:616:HIS:HD2	1.95	0.84
1:B:192:HIS:ND1	1:B:592:LEU:HD11	1.93	0.83
1:B:100:ASP:O	1:B:114:THR:HG22	1.80	0.82
1:D:586:ARG:HG3	1:D:586:ARG:NH1	1.90	0.81
1:C:139:ASN:CB	1:C:141:ASP:OD1	2.28	0.80
1:D:133:GLN:HG3	1:D:138:ILE:O	1.81	0.80
1:D:389:LYS:HE3	1:D:481:GLU:OE2	1.82	0.80
1:D:106:ASN:HD21	1:D:110:GLN:H	1.29	0.78
1:D:86:LYS:NZ	1:D:181:ASP:OD2	2.16	0.76
1:D:106:ASN:ND2	1:D:110:GLN:H	1.83	0.75
1:A:439:ILE:HG13	1:D:535:ASP:HB2	1.67	0.75
1:A:265:ARG:HG2	1:A:265:ARG:NH1	2.02	0.75
1:D:430:HIS:C	1:D:432:LEU:H	1.95	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:LYS:NZ	1:C:654:ASN:O	2.20	0.74
1:C:100:ASP:O	1:C:114:THR:CG2	2.35	0.74
1:D:473:ASP:O	1:D:477:VAL:HG23	1.88	0.73
1:D:529:GLU:OE2	1:D:615:HIS:N	2.18	0.73
1:A:507:LEU:O	1:A:511:ILE:HG12	1.87	0.72
1:D:154:ASP:O	1:D:201:MET:HG2	1.89	0.72
1:D:139:ASN:H	1:D:139:ASN:ND2	1.88	0.71
1:D:603:ARG:HG2	1:D:603:ARG:HH11	1.56	0.71
1:D:555:LYS:NZ	1:D:597:GLN:HE21	1.89	0.71
1:C:139:ASN:O	1:C:140:LEU:HB2	1.91	0.70
1:A:571:TYR:OH	1:A:615:HIS:HE1	1.72	0.70
1:B:192:HIS:CB	1:B:243:TYR:OH	2.39	0.70
1:C:342:ARG:NE	1:C:645:TYR:O	2.21	0.70
1:D:92:LYS:HE3	1:D:98:TYR:O	1.93	0.69
1:C:144:THR:HG21	1:C:519:LEU:O	1.93	0.69
1:C:526:GLU:HG3	1:C:527:SER:N	2.08	0.68
1:C:638:MET:HE1	1:D:345:ILE:HD13	1.75	0.68
1:A:463:LEU:HD12	1:A:463:LEU:O	1.92	0.68
1:B:527:SER:OG	4:B:888:1DO:H1C2	1.93	0.68
1:C:106:ASN:HD21	1:C:110:GLN:HE21	1.41	0.68
1:B:192:HIS:HB3	1:B:243:TYR:OH	1.94	0.68
1:B:421:MET:HE3	1:B:426:PHE:HA	1.75	0.67
1:C:421:MET:HE3	1:C:426:PHE:HA	1.74	0.67
1:C:345:ILE:HD13	1:D:638:MET:HE1	1.76	0.66
1:D:93:TRP:NE1	1:D:148:ALA:O	2.26	0.66
1:C:434:PRO:O	1:C:435:GLN:HB2	1.95	0.66
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.77	0.66
1:C:586:ARG:HH11	1:C:586:ARG:CG	1.94	0.66
1:D:511:ILE:HA	1:D:514:MET:HE3	1.78	0.66
1:A:265:ARG:HH11	1:A:265:ARG:CG	2.01	0.65
1:B:481:GLU:HG3	1:B:485:TYR:CE2	2.31	0.65
1:C:144:THR:HG22	1:C:520:GLU:HA	1.76	0.65
1:C:419:HIS:CD2	1:C:566:ARG:HH21	2.08	0.65
1:D:139:ASN:H	1:D:139:ASN:HD22	1.43	0.65
1:D:635:GLY:HA2	1:D:638:MET:HE3	1.78	0.65
1:A:82:ILE:HG13	1:A:264:ASN:HD21	1.61	0.64
1:B:592:LEU:O	1:B:595:PHE:HB3	1.96	0.64
1:B:225:ALA:HA	1:B:230:LEU:HD12	1.79	0.64
1:B:265:ARG:NH1	1:B:265:ARG:HG3	2.03	0.64
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.79	0.64
1:C:421:MET:CE	1:C:426:PHE:HA	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:586:ARG:HH11	1:D:586:ARG:CG	2.06	0.64
1:D:139:ASN:ND2	1:D:139:ASN:N	2.45	0.64
1:C:510:VAL:HG23	1:C:514:MET:HE3	1.79	0.63
1:A:187:HIS:CE1	1:A:197:LEU:HD11	2.34	0.63
1:D:86:LYS:NZ	1:D:181:ASP:CG	2.57	0.63
1:B:133:GLN:OE1	1:B:139:ASN:O	2.17	0.62
1:B:507:LEU:O	1:B:511:ILE:CG1	2.45	0.62
1:A:215:HIS:HD2	1:A:375:THR:OG1	1.83	0.62
1:C:192:HIS:HB3	1:C:243:TYR:OH	1.99	0.62
1:D:144:THR:HG22	1:D:520:GLU:HA	1.81	0.62
1:B:650:ASN:HD21	1:B:653:GLY:HA2	1.65	0.61
1:B:481:GLU:HG3	1:B:485:TYR:HE2	1.65	0.61
1:D:142:HIS:CE1	1:D:586:ARG:HH22	2.18	0.61
1:B:340:THR:HB	1:B:646:VAL:HG13	1.82	0.61
1:D:474:ARG:O	1:D:478:LEU:HG	2.01	0.60
1:B:246:MET:HE2	1:B:621:LYS:HD2	1.81	0.60
1:C:98:TYR:CD2	1:C:117:ARG:HD3	2.36	0.60
1:B:265:ARG:NH1	1:B:265:ARG:CG	2.53	0.60
1:C:419:HIS:HD2	1:C:566:ARG:NH2	1.96	0.60
1:A:439:ILE:HG13	1:D:535:ASP:CB	2.31	0.60
1:B:243:TYR:HD2	1:B:622:LEU:HB2	1.67	0.59
1:D:555:LYS:HZ1	1:D:597:GLN:HE21	1.48	0.59
1:B:182:ARG:HB3	1:B:205:ILE:HD12	1.85	0.59
1:A:419:HIS:O	1:A:466:ALA:HA	2.03	0.59
1:D:428:PHE:HZ	1:D:514:MET:SD	2.25	0.58
1:B:507:LEU:C	1:B:511:ILE:CD1	2.54	0.58
1:D:142:HIS:CG	1:D:586:ARG:HH12	2.21	0.58
1:A:642:VAL:HG13	1:B:638:MET:HG2	1.84	0.58
1:B:190:CYS:SG	1:B:241:VAL:O	2.61	0.58
1:B:83:ILE:HG23	1:B:91:MET:HE1	1.85	0.58
1:A:212:PRO:HG2	1:A:263:MET:HE2	1.85	0.57
1:C:421:MET:HE1	5:C:2039:HOH:O	2.04	0.57
1:C:243:TYR:HE2	1:C:622:LEU:HD13	1.70	0.57
1:C:555:LYS:NZ	1:C:597:GLN:HE21	2.03	0.57
1:D:182:ARG:HB3	1:D:205:ILE:HD12	1.86	0.57
1:B:185:ARG:HG2	1:B:235:ILE:HD13	1.87	0.57
1:D:524:ILE:HD11	1:D:583:PHE:CZ	2.39	0.57
1:C:142:HIS:CD2	1:C:586:ARG:NH2	2.73	0.57
1:C:467:THR:HG21	1:C:504:GLY:HA3	1.87	0.56
1:C:526:GLU:HB3	1:C:595:PHE:HZ	1.69	0.56
1:A:171:THR:O	1:A:172:ASN:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:HIS:CD2	1:A:616:HIS:CD2	2.81	0.56
1:B:526:GLU:HG3	1:B:527:SER:H	1.70	0.56
1:A:265:ARG:NH1	1:A:265:ARG:CG	2.58	0.56
1:B:298:THR:CG2	1:B:300:HIS:H	2.18	0.56
1:B:265:ARG:NH1	1:B:265:ARG:CA	2.47	0.56
1:A:129:LYS:HG3	1:A:140:LEU:HD23	1.88	0.56
1:B:481:GLU:CG	1:B:485:TYR:HE2	2.19	0.56
1:C:342:ARG:HD3	1:C:645:TYR:CZ	2.41	0.56
1:B:419:HIS:HD2	1:B:566:ARG:HH21	1.54	0.55
1:C:133:GLN:HG2	1:C:138:ILE:O	2.06	0.55
1:C:524:ILE:O	1:C:582:ALA:HA	2.06	0.55
1:B:470:PHE:HB3	1:B:477:VAL:HG13	1.88	0.55
1:C:192:HIS:CB	1:C:243:TYR:OH	2.55	0.55
1:D:430:HIS:O	1:D:432:LEU:N	2.38	0.55
1:A:426:PHE:CD2	1:A:463:LEU:HD11	2.42	0.54
1:A:497:GLY:HA2	5:A:2038:HOH:O	2.06	0.54
1:B:288:GLU:OE1	1:B:298:THR:HB	2.07	0.54
1:C:481:GLU:HG2	1:C:485:TYR:CE2	2.43	0.54
1:D:120:LEU:HD13	1:D:120:LEU:N	2.22	0.54
1:A:92:LYS:HE3	1:A:98:TYR:O	2.07	0.54
1:B:243:TYR:HE2	1:B:622:LEU:HD13	1.72	0.54
1:C:185:ARG:HG2	1:C:235:ILE:HD13	1.89	0.54
1:C:511:ILE:HD13	4:C:888:1DO:H5C2	1.89	0.54
1:D:150:LEU:O	1:D:152:PRO:HD3	2.07	0.54
1:A:613:LEU:HD11	1:A:623:ARG:HB3	1.90	0.54
1:C:139:ASN:O	1:C:140:LEU:CB	2.56	0.53
1:C:638:MET:CE	1:D:345:ILE:HD13	2.37	0.53
1:D:185:ARG:NE	1:D:259:ASP:OD2	2.31	0.53
1:A:345:ILE:HD13	1:B:638:MET:HE1	1.91	0.53
1:A:531:SER:HB3	1:A:615:HIS:HB2	1.89	0.53
1:C:528:PHE:HZ	1:C:548:ILE:HD11	1.72	0.53
1:B:303:ASP:OD2	1:B:508:THR:HB	2.09	0.53
1:D:407:GLU:OE1	1:D:407:GLU:HA	2.08	0.53
1:D:112:GLU:OE2	1:D:122:GLY:HA2	2.08	0.53
1:C:635:GLY:HA2	1:C:638:MET:HE3	1.91	0.52
1:B:555:LYS:NZ	1:B:597:GLN:HE21	2.07	0.52
1:D:86:LYS:NZ	1:D:181:ASP:OD1	2.42	0.52
1:B:335:HIS:HD2	5:B:2023:HOH:O	1.92	0.52
1:A:243:TYR:CE2	1:A:622:LEU:HD13	2.44	0.51
1:B:525:GLY:HA3	4:B:888:1DO:H8C2	1.92	0.51
1:A:459:ASP:OD1	1:A:460:PRO:HD2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASP:O	1:B:380:LYS:HE3	2.11	0.51
1:C:526:GLU:HG3	1:C:527:SER:H	1.73	0.51
1:A:129:LYS:HG3	1:A:140:LEU:CD2	2.40	0.51
1:C:230:LEU:HD13	1:C:256:ILE:HD11	1.93	0.51
1:B:506:LEU:O	1:B:510:VAL:HG22	2.10	0.51
1:A:426:PHE:CE2	1:A:463:LEU:HD11	2.46	0.50
1:B:98:TYR:CD2	1:B:117:ARG:HD3	2.46	0.50
1:B:155:THR:HG21	1:B:179:ALA:HB1	1.93	0.50
1:B:528:PHE:HZ	1:B:548:ILE:HD11	1.76	0.50
1:A:82:ILE:CG1	1:A:264:ASN:ND2	2.70	0.50
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.46	0.50
1:A:137:GLY:HA3	1:A:559:PHE:CE2	2.46	0.50
1:A:434:PRO:HD2	1:A:435:GLN:OE1	2.12	0.49
1:A:515:ARG:O	1:A:515:ARG:HG2	2.04	0.49
1:B:435:GLN:HA	1:B:435:GLN:OE1	2.11	0.49
1:C:481:GLU:HG2	1:C:485:TYR:HE2	1.77	0.49
1:B:569:GLN:HB2	1:B:576:CYS:HB3	1.94	0.49
1:D:147:LYS:HG3	1:D:198:ARG:O	2.12	0.49
1:A:129:LYS:HD2	1:A:140:LEU:HD23	1.95	0.49
1:B:470:PHE:CB	1:B:477:VAL:HG13	2.42	0.49
1:A:323:LYS:HD2	1:A:323:LYS:C	2.38	0.49
1:A:348:SER:HB3	1:B:629:GLU:O	2.12	0.49
1:C:526:GLU:CB	1:C:595:PHE:HZ	2.26	0.49
1:D:421:MET:HG2	1:D:465:VAL:O	2.13	0.49
1:D:529:GLU:O	1:D:603:ARG:NH2	2.46	0.49
1:A:463:LEU:C	1:A:463:LEU:CD1	2.86	0.49
1:C:525:GLY:HA2	1:C:581:PHE:O	2.12	0.49
1:D:171:THR:O	1:D:172:ASN:HB2	2.12	0.49
1:D:555:LYS:NZ	1:D:597:GLN:NE2	2.60	0.49
1:B:212:PRO:HG2	1:B:263:MET:HE2	1.95	0.48
1:B:192:HIS:ND1	1:B:592:LEU:CD1	2.72	0.48
1:A:357:GLY:HA2	1:B:366:GLY:O	2.13	0.48
1:B:187:HIS:NE2	1:B:197:LEU:HD11	2.28	0.48
1:B:406:ARG:HG3	1:B:406:ARG:NH1	2.11	0.48
1:D:421:MET:HE3	1:D:426:PHE:HA	1.95	0.48
1:D:119:PRO:HB2	1:D:120:LEU:HD13	1.94	0.48
1:B:406:ARG:HG3	1:B:406:ARG:O	2.11	0.48
1:A:82:ILE:CG1	1:A:264:ASN:HD21	2.25	0.48
1:A:539:ASP:OD1	1:A:542:ARG:NH2	2.47	0.48
1:A:439:ILE:CG1	1:D:535:ASP:HB2	2.40	0.48
1:A:463:LEU:HD12	1:A:463:LEU:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:MET:HG2	1:B:642:VAL:HG13	1.96	0.48
1:C:243:TYR:CE2	1:C:622:LEU:HD13	2.49	0.48
1:D:419:HIS:O	1:D:466:ALA:HA	2.13	0.48
1:B:277:HIS:HD2	1:B:378:THR:OG1	1.97	0.48
1:C:345:ILE:HD13	1:D:638:MET:CE	2.43	0.47
1:D:230:LEU:HD22	1:D:254:THR:HB	1.96	0.47
1:D:516:ASP:O	1:D:520:GLU:HG2	2.14	0.47
1:D:586:ARG:HD2	1:D:586:ARG:C	2.39	0.47
1:B:394:ALA:O	1:B:493:GLY:HA2	2.14	0.47
1:C:569:GLN:HB2	1:C:576:CYS:HB3	1.97	0.47
1:C:586:ARG:NH1	1:C:586:ARG:CG	2.63	0.47
1:B:372:GLY:HA2	1:B:652:PHE:CZ	2.50	0.47
1:A:314:ILE:HG23	1:A:365:MET:HG2	1.95	0.47
1:B:564:THR:HG23	1:B:580:TYR:HB2	1.97	0.47
1:B:82:ILE:HG12	1:B:264:ASN:ND2	2.30	0.47
1:C:400:GLN:HA	1:C:400:GLN:NE2	2.28	0.47
1:A:629:GLU:O	1:B:348:SER:HB3	2.15	0.47
1:D:527:SER:HA	1:D:579:PHE:O	2.15	0.47
1:A:155:THR:HG22	1:A:201:MET:HE3	1.97	0.47
1:C:463:LEU:HD23	1:C:463:LEU:O	2.15	0.46
1:D:238:GLY:HA2	1:D:245:LEU:HD11	1.96	0.46
1:A:192:HIS:HB3	1:A:243:TYR:OH	2.15	0.46
1:C:267:LEU:O	1:C:268:TRP:HB3	2.15	0.46
1:C:511:ILE:HG23	4:C:888:IDO:H4C1	1.97	0.46
1:A:366:GLY:O	1:B:357:GLY:HA2	2.15	0.46
1:C:355:SER:HB2	1:D:616:HIS:HA	1.98	0.46
1:D:155:THR:HA	1:D:156:PRO:HD2	1.76	0.46
1:A:230:LEU:HD22	1:A:254:THR:HB	1.96	0.46
1:B:94:ASN:HD22	1:B:94:ASN:C	2.22	0.46
1:B:298:THR:HG22	1:B:300:HIS:H	1.79	0.46
1:C:424:GLN:HB2	1:C:564:THR:HG22	1.98	0.46
1:C:511:ILE:HD12	1:C:580:TYR:CE1	2.51	0.46
1:A:516:ASP:O	1:A:520:GLU:HG3	2.16	0.46
1:C:144:THR:HG22	1:C:520:GLU:CA	2.43	0.46
1:C:251:GLU:OE2	1:C:253:ARG:HB2	2.16	0.45
1:C:522:TYR:CG	1:C:586:ARG:HG2	2.51	0.45
1:D:103:PHE:HA	1:D:112:GLU:O	2.16	0.45
1:C:524:ILE:HD11	1:C:583:PHE:CZ	2.51	0.45
1:B:127:THR:HG22	1:B:431:ALA:HB1	1.98	0.45
1:B:590:ASP:O	1:B:594:VAL:HG23	2.16	0.45
1:A:230:LEU:HD13	1:A:256:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PRO:HD2	1:A:259:ASP:O	2.16	0.45
1:B:298:THR:HG23	1:B:300:HIS:H	1.82	0.45
1:A:102:LYS:C	1:A:113:LEU:HD12	2.41	0.45
1:A:143:LYS:O	1:A:144:THR:HB	2.16	0.45
1:C:144:THR:CG2	1:C:520:GLU:HA	2.43	0.45
1:B:516:ASP:O	1:B:520:GLU:HG2	2.17	0.45
1:C:340:THR:HB	1:C:646:VAL:HG13	1.99	0.45
1:D:331:ASP:O	1:D:380:LYS:HE3	2.16	0.45
1:B:520:GLU:HG2	1:B:520:GLU:H	1.57	0.44
1:B:557:VAL:HA	1:B:588:ILE:HD11	1.99	0.44
1:A:439:ILE:HD13	1:A:439:ILE:HA	1.81	0.44
1:A:423:ASN:HD21	1:A:427:GLN:NE2	2.15	0.44
1:A:618:GLY:O	1:A:623:ARG:NH1	2.46	0.44
1:B:643:LYS:NZ	1:B:647:ASP:OD2	2.50	0.44
1:C:273:ASN:OD1	1:D:534:TRP:HB2	2.17	0.44
1:D:323:LYS:HD2	1:D:323:LYS:C	2.42	0.44
1:D:400:GLN:NE2	1:D:400:GLN:HA	2.33	0.44
1:B:171:THR:O	1:B:172:ASN:HB2	2.16	0.44
1:B:301:GLU:CD	1:B:322:LYS:HE2	2.42	0.44
1:D:83:ILE:HB	1:D:261:SER:HB2	1.98	0.44
1:A:265:ARG:HD2	1:A:279:GLU:OE1	2.17	0.44
1:A:500:ASN:ND2	1:A:503:ARG:HH12	2.15	0.44
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.84	0.44
1:B:243:TYR:O	1:B:621:LYS:HE2	2.17	0.44
1:C:507:LEU:O	1:C:511:ILE:HB	2.17	0.44
1:C:83:ILE:HG23	1:C:91:MET:HE1	1.99	0.44
1:D:529:GLU:HG3	1:D:616:HIS:CE1	2.53	0.44
1:B:284:GLY:O	1:B:288:GLU:HG2	2.18	0.43
1:C:584:ASN:OD1	1:C:584:ASN:C	2.60	0.43
1:D:142:HIS:CD2	1:D:586:ARG:HH12	2.35	0.43
1:D:364:ILE:O	1:D:367:SER:OG	2.29	0.43
1:C:643:LYS:NZ	1:C:650:ASN:HD22	2.16	0.43
1:D:265:ARG:HH11	1:D:265:ARG:HD2	1.38	0.43
1:B:118:TYR:O	1:B:121:SER:HB2	2.19	0.43
1:C:555:LYS:HZ1	1:C:597:GLN:HE21	1.65	0.43
1:A:143:LYS:HB3	1:A:144:THR:H	1.53	0.43
1:A:268:TRP:CZ2	1:A:277:HIS:HB2	2.54	0.43
1:B:526:GLU:HB3	1:B:595:PHE:HZ	1.83	0.43
1:C:498:GLU:HG2	5:C:2038:HOH:O	2.18	0.43
1:A:529:GLU:HG2	1:A:530:THR:N	2.32	0.43
1:C:82:ILE:HG12	1:C:264:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASP:O	1:C:201:MET:HG2	2.18	0.43
1:D:616:HIS:HD2	2:D:999:FAD:C2	2.32	0.43
1:A:600:ALA:O	1:A:604:GLU:HG2	2.18	0.43
1:D:150:LEU:HD21	1:D:201:MET:HE1	2.01	0.43
1:D:171:THR:O	1:D:172:ASN:CB	2.67	0.43
1:D:562:LEU:O	1:D:581:PHE:HA	2.19	0.43
1:C:422:ASP:OD1	1:C:422:ASP:C	2.62	0.42
1:D:113:LEU:HB3	1:D:121:SER:HA	2.01	0.42
1:B:397:ASN:HA	1:B:462:GLN:O	2.19	0.42
1:B:510:VAL:O	1:B:513:TYR:N	2.45	0.42
1:D:426:PHE:CD1	1:D:465:VAL:HG21	2.53	0.42
1:D:621:LYS:NZ	1:D:654:ASN:O	2.52	0.42
1:B:243:TYR:CD2	1:B:622:LEU:HB2	2.50	0.42
1:C:529:GLU:OE2	1:C:617:HIS:HB2	2.19	0.42
1:B:265:ARG:HH11	1:B:265:ARG:CG	2.20	0.42
1:C:118:TYR:O	1:C:121:SER:HB2	2.19	0.42
1:A:507:LEU:O	1:A:511:ILE:CG1	2.63	0.42
1:B:187:HIS:CD2	1:B:197:LEU:HD11	2.55	0.42
1:B:526:GLU:HG3	1:B:527:SER:N	2.34	0.42
1:B:527:SER:HA	1:B:579:PHE:O	2.20	0.42
1:A:268:TRP:CE2	1:A:277:HIS:HB2	2.55	0.42
1:B:425:GLN:OE1	1:B:566:ARG:HB3	2.20	0.42
1:C:171:THR:O	1:C:172:ASN:HB2	2.20	0.42
1:D:161:ASN:OD1	1:D:163:ASP:N	2.51	0.42
1:D:187:HIS:CE1	1:D:197:LEU:HD11	2.55	0.42
1:A:390:TYR:HE2	1:A:505:TYR:HB2	1.85	0.42
1:A:418:ILE:HG13	1:A:468:LEU:HD23	2.02	0.42
1:C:619:VAL:HB	1:C:657:LEU:HD23	2.02	0.42
1:D:215:HIS:CE1	1:D:337:LYS:HD3	2.54	0.42
2:A:999:FAD:H9	2:A:999:FAD:H1'2	1.87	0.41
1:A:198:ARG:C	1:A:199:GLU:HG2	2.45	0.41
1:A:217:ASP:O	1:A:221:ILE:HG13	2.20	0.41
1:A:310:VAL:HA	1:A:313:TRP:CE3	2.55	0.41
1:C:510:VAL:CG2	1:C:514:MET:HE3	2.50	0.41
1:C:616:HIS:HD2	2:C:999:FAD:C2	2.33	0.41
1:A:83:ILE:HB	1:A:261:SER:HB2	2.01	0.41
1:B:127:THR:HG22	1:B:431:ALA:CB	2.51	0.41
1:B:265:ARG:HB2	1:B:279:GLU:OE1	2.20	0.41
1:D:187:HIS:NE2	1:D:197:LEU:HD11	2.36	0.41
1:D:267:LEU:O	1:D:268:TRP:HB3	2.21	0.41
1:B:127:THR:CG2	1:B:431:ALA:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ARG:HB3	1:C:118:TYR:CD2	2.56	0.41
1:C:305:LEU:C	1:C:305:LEU:HD12	2.45	0.41
1:D:421:MET:HB2	1:D:425:GLN:HB2	2.02	0.41
1:D:613:LEU:HD23	1:D:613:LEU:HA	1.89	0.41
1:A:552:CYS:SG	1:A:561:PRO:HG3	2.61	0.41
1:C:190:CYS:HB2	1:C:193:GLU:OE1	2.21	0.41
1:D:470:PHE:HB3	1:D:477:VAL:HG13	2.03	0.41
1:A:156:PRO:HA	1:A:157:PRO:HD3	1.94	0.40
1:B:135:THR:HG22	1:B:136:PHE:CD1	2.57	0.40
1:B:481:GLU:CG	1:B:485:TYR:CE2	2.99	0.40
1:B:487:ILE:HA	1:B:490:LYS:HE2	2.03	0.40
1:C:191:LEU:HD13	1:C:191:LEU:C	2.46	0.40
1:C:293:GLU:HG3	5:C:2020:HOH:O	2.21	0.40
1:D:372:GLY:HA2	1:D:652:PHE:CZ	2.57	0.40
1:A:439:ILE:CD1	1:D:535:ASP:HB2	2.50	0.40
1:D:414:ALA:HA	1:D:415:PRO:HD3	1.85	0.40
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.80	0.40
1:D:363:PHE:CD1	1:D:363:PHE:N	2.89	0.40
1:A:197:LEU:HG	1:A:202:PHE:CZ	2.56	0.40
1:B:277:HIS:CD2	1:B:378:THR:OG1	2.74	0.40
1:B:481:GLU:O	1:B:485:TYR:CD2	2.74	0.40
1:A:106:ASN:OD1	1:A:106:ASN:C	2.65	0.40
1:A:246:MET:HE2	1:A:621:LYS:HE3	2.03	0.40
1:A:379:ILE:HG21	1:A:379:ILE:HD13	1.78	0.40
1:B:192:HIS:HB2	1:B:243:TYR:OH	2.19	0.40
1:C:187:HIS:CE1	1:C:197:LEU:HD11	2.57	0.40
1:C:288:GLU:O	1:C:292:LYS:HB2	2.21	0.40
1:D:128:PHE:HD1	1:D:128:PHE:O	2.05	0.40

All (2) 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]	2.04	0.16
1:B:265:ARG:CD	1:C:151:ASN:OD1[1_556]	2.13	0.07

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	550/658 (84%)	539 (98%)	11 (2%)	0	100	100
1	B	537/658 (82%)	521 (97%)	16 (3%)	0	100	100
1	C	553/658 (84%)	536 (97%)	16 (3%)	1 (0%)	43	58
1	D	546/658 (83%)	524 (96%)	20 (4%)	2 (0%)	30	43
All	All	2186/2632 (83%)	2120 (97%)	63 (3%)	3 (0%)	48	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	431	ALA
1	C	140	LEU
1	D	106	ASN

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	477/545 (88%)	443 (93%)	34 (7%)	13	23
1	B	464/545 (85%)	427 (92%)	37 (8%)	11	19
1	C	477/545 (88%)	433 (91%)	44 (9%)	8	14
1	D	471/545 (86%)	422 (90%)	49 (10%)	7	10
All	All	1889/2180 (87%)	1725 (91%)	164 (9%)	9	16

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ILE
1	A	90	LEU
1	A	116	LYS
1	A	120	LEU
1	A	130	ASP
1	A	139	ASN
1	A	141	ASP
1	A	144	THR
1	A	159	ILE
1	A	174	SER
1	A	191	LEU
1	A	342	ARG
1	A	354	MET
1	A	434	PRO
1	A	439	ILE
1	A	441	THR
1	A	463	LEU
1	A	468	LEU
1	A	476	LYS
1	A	502	GLN
1	A	507	LEU
1	A	511	ILE
1	A	526	GLU
1	A	529	GLU
1	A	559	PHE
1	A	566	ARG
1	A	584	ASN
1	A	586	ARG
1	A	588	ILE
1	A	592	LEU
1	A	596	GLU
1	A	599	GLU
1	A	630	SER
1	A	646	VAL
1	B	90	LEU
1	B	94	ASN
1	B	101	SER
1	B	114	THR
1	B	120	LEU
1	B	127	THR
1	B	140	LEU
1	B	170	LYS
1	B	199	GLU

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Mol	Chain	Res	Type
1	B	265	ARG
1	B	298	THR
1	B	360	ILE
1	B	379	ILE
1	B	406	ARG
1	B	421	MET
1	B	433	LYS
1	B	435	GLN
1	B	463	LEU
1	B	475	GLU
1	B	476	LYS
1	B	487	ILE
1	B	494	LEU
1	B	502	GLN
1	B	503	ARG
1	B	510	VAL
1	B	511	ILE
1	B	520	GLU
1	B	524	ILE
1	B	526	GLU
1	B	529	GLU
1	B	578	TYR
1	B	592	LEU
1	B	599	GLU
1	B	613	LEU
1	B	614	SER
1	B	633	ASP
1	B	646	VAL
1	C	82	ILE
1	C	83	ILE
1	C	90	LEU
1	C	105	LEU
1	C	108	LYS
1	C	114	THR
1	C	125	LEU
1	C	129	LYS
1	C	140	LEU
1	C	141	ASP
1	C	150	LEU
1	C	159	ILE
1	C	174	SER
1	C	199	GLU

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Mol	Chain	Res	Type
1	C	224	LEU
1	C	265	ARG
1	C	271	GLU
1	C	342	ARG
1	C	354	MET
1	C	360	ILE
1	C	425	GLN
1	C	432	LEU
1	C	462	GLN
1	C	463	LEU
1	C	490	LYS
1	C	499	ASP
1	C	508	THR
1	C	511	ILE
1	C	520	GLU
1	C	526	GLU
1	C	542	ARG
1	C	559	PHE
1	C	566	ARG
1	C	568	THR
1	C	578	TYR
1	C	584	ASN
1	C	586	ARG
1	C	588	ILE
1	C	596	GLU
1	C	613	LEU
1	C	633	ASP
1	C	640	LYS
1	C	641	SER
1	C	646	VAL
1	D	106	ASN
1	D	107	LYS
1	D	112	GLU
1	D	116	LYS
1	D	120	LEU
1	D	121	SER
1	D	125	LEU
1	D	133	GLN
1	D	134	ASN
1	D	139	ASN
1	D	140	LEU
1	D	141	ASP

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Mol	Chain	Res	Type
1	D	143	LYS
1	D	144	THR
1	D	150	LEU
1	D	155	THR
1	D	159	ILE
1	D	172	ASN
1	D	191	LEU
1	D	199	GLU
1	D	224	LEU
1	D	285	GLN
1	D	294	SER
1	D	354	MET
1	D	360	ILE
1	D	386	GLU
1	D	388	GLN
1	D	424	GLN
1	D	427	GLN
1	D	432	LEU
1	D	463	LEU
1	D	476	LYS
1	D	478	LEU
1	D	510	VAL
1	D	511	ILE
1	D	520	GLU
1	D	524	ILE
1	D	529	GLU
1	D	542	ARG
1	D	553	LYS
1	D	559	PHE
1	D	568	THR
1	D	578	TYR
1	D	586	ARG
1	D	588	ILE
1	D	603	ARG
1	D	613	LEU
1	D	641	SER
1	D	646	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS

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Mol	Chain	Res	Type
1	A	189	HIS
1	A	215	HIS
1	A	262	GLN
1	A	290	GLN
1	A	328	ASN
1	A	388	GLN
1	A	423	ASN
1	A	461	ASN
1	A	500	ASN
1	A	615	HIS
1	A	616	HIS
1	B	94	ASN
1	B	110	GLN
1	B	133	GLN
1	B	177	GLN
1	B	277	HIS
1	B	419	HIS
1	B	427	GLN
1	B	479	GLN
1	B	558	GLN
1	B	597	GLN
1	B	650	ASN
1	B	656	ASN
1	C	110	GLN
1	C	142	HIS
1	C	388	GLN
1	C	400	GLN
1	C	419	HIS
1	C	597	GLN
1	C	650	ASN
1	C	656	ASN
1	D	106	ASN
1	D	110	GLN
1	D	139	ASN
1	D	142	HIS
1	D	151	ASN
1	D	277	HIS
1	D	400	GLN
1	D	424	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](#)

8 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
4	1DO	B	888	-	12,12,12	0.80	0	11,11,11	0.41	0
2	FAD	D	999	-	58,58,58	1.33	8 (13%)	85,89,89	1.72	19 (22%)
2	FAD	A	999	-	58,58,58	1.23	5 (8%)	85,89,89	1.88	19 (22%)
2	FAD	B	999	-	58,58,58	1.38	9 (15%)	85,89,89	1.78	24 (28%)
3	SO4	D	1659	-	4,4,4	0.49	0	6,6,6	0.68	0
4	1DO	C	888	-	12,12,12	0.78	0	11,11,11	0.51	0
2	FAD	C	999	-	58,58,58	1.49	6 (10%)	85,89,89	1.61	15 (17%)
3	SO4	A	1659	-	4,4,4	0.32	0	6,6,6	0.37	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
4	1DO	B	888	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	999	-	-	4/34/50/50	0/6/6/6
2	FAD	A	999	-	-	3/34/50/50	0/6/6/6
2	FAD	B	999	-	-	4/34/50/50	0/6/6/6
4	1DO	C	888	-	-	7/10/10/10	-
2	FAD	C	999	-	-	4/34/50/50	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	FAD	P-O3P	5.49	1.65	1.59
2	A	999	FAD	C4X-N5	5.40	1.42	1.30
2	C	999	FAD	PA-O3P	4.76	1.64	1.59
2	B	999	FAD	C4X-N5	4.37	1.40	1.30
2	D	999	FAD	C4X-N5	4.09	1.39	1.30
2	B	999	FAD	C10-N1	3.74	1.40	1.33
2	B	999	FAD	C2A-N3A	3.36	1.39	1.33
2	B	999	FAD	C2A-N1A	3.15	1.39	1.33
2	C	999	FAD	C4X-N5	3.00	1.37	1.30
2	C	999	FAD	C8A-N7A	2.95	1.37	1.31
2	D	999	FAD	P-O3P	2.89	1.62	1.59
2	B	999	FAD	P-O3P	2.79	1.62	1.59
2	A	999	FAD	C8A-N7A	2.71	1.36	1.31
2	D	999	FAD	PA-O3P	2.67	1.62	1.59
2	D	999	FAD	C2A-N1A	2.65	1.38	1.33
2	D	999	FAD	C8A-N7A	2.57	1.36	1.31
2	B	999	FAD	O4'-C4'	-2.55	1.38	1.43
2	C	999	FAD	C10-N1	2.53	1.38	1.33
2	D	999	FAD	C1'-N10	2.28	1.53	1.47
2	B	999	FAD	C1'-N10	2.27	1.53	1.47
2	A	999	FAD	C2A-N1A	2.27	1.38	1.33
2	B	999	FAD	PA-O3P	2.24	1.61	1.59
2	D	999	FAD	C8A-N9A	2.21	1.41	1.37
2	C	999	FAD	C4X-C10	-2.18	1.37	1.44
2	A	999	FAD	C2A-N3A	2.18	1.37	1.33
2	D	999	FAD	C4'-C3'	2.10	1.57	1.53
2	A	999	FAD	C10-N1	2.06	1.37	1.33
2	B	999	FAD	O4B-C4B	-2.02	1.40	1.45

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	N3A-C2A-N1A	-7.54	117.17	128.58
2	C	999	FAD	N3A-C2A-N1A	-6.13	119.31	128.58
2	D	999	FAD	N3A-C2A-N1A	-5.79	119.82	128.58
2	A	999	FAD	N9A-C8A-N7A	-5.11	106.68	113.94
2	A	999	FAD	O2A-PA-O3P	4.47	119.35	107.27
2	B	999	FAD	N3A-C2A-N1A	-4.42	121.89	128.58
2	C	999	FAD	C5A-C4A-N3A	-4.25	120.87	126.72
2	D	999	FAD	C4-N3-C2	-3.91	118.69	125.64
2	C	999	FAD	C2A-N3A-C4A	3.85	121.23	111.83
2	B	999	FAD	N9A-C8A-N7A	-3.83	108.50	113.94
2	D	999	FAD	O2A-PA-O3P	3.82	117.59	107.27
2	A	999	FAD	C4A-N9A-C8A	3.80	109.72	105.74
2	A	999	FAD	C2A-N3A-C4A	3.77	121.04	111.83
2	B	999	FAD	C5A-C4A-N3A	-3.64	121.71	126.72
2	B	999	FAD	O4B-C1B-N9A	-3.64	101.11	108.09
2	B	999	FAD	O2A-PA-O3P	3.52	116.78	107.27
2	B	999	FAD	C4X-C10-N10	3.50	121.49	116.48
2	C	999	FAD	O4'-C4'-C5'	-3.50	102.27	109.99
2	A	999	FAD	C4-N3-C2	-3.50	119.43	125.64
2	D	999	FAD	C5'-C4'-C3'	3.50	118.81	112.22
2	B	999	FAD	C4A-N9A-C8A	3.44	109.35	105.74
2	B	999	FAD	C4-C4X-N5	3.43	122.95	118.21
2	B	999	FAD	O4'-C4'-C5'	-3.42	102.45	109.99
2	D	999	FAD	C4X-C10-N10	3.33	121.25	116.48
2	B	999	FAD	N3A-C4A-N9A	3.28	132.75	127.17
2	C	999	FAD	N3A-C4A-N9A	3.11	132.45	127.17
2	A	999	FAD	C4X-C10-N10	3.07	120.88	116.48
2	D	999	FAD	O3'-C3'-C2'	-3.06	101.98	108.93
2	A	999	FAD	C5A-N7A-C8A	3.06	108.25	103.45
2	D	999	FAD	C4X-C4-N3	3.05	121.01	113.25
2	C	999	FAD	C4X-C10-N10	3.04	120.84	116.48
2	A	999	FAD	C4X-C4-N3	3.04	120.98	113.25
2	C	999	FAD	O3'-C3'-C2'	-3.00	102.12	108.93
2	D	999	FAD	N9A-C8A-N7A	-2.97	109.72	113.94
2	D	999	FAD	C10-C4X-N5	-2.95	118.79	124.81
2	B	999	FAD	C10-C4X-N5	-2.93	118.83	124.81
2	A	999	FAD	C5A-C4A-N3A	-2.92	122.69	126.72
2	A	999	FAD	C5X-C9A-N10	2.88	120.57	117.97
2	A	999	FAD	C4-C4X-N5	2.85	122.14	118.21
2	C	999	FAD	O2P-P-O3P	2.75	114.70	107.27
2	D	999	FAD	C4-C4X-N5	2.74	122.00	118.21
2	A	999	FAD	C4A-N9A-C1B	-2.73	120.24	126.63
2	B	999	FAD	C4X-C4-N3	2.72	120.17	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	999	FAD	O5'-C5'-C4'	-2.69	102.19	109.36
2	B	999	FAD	O5'-C5'-C4'	-2.63	102.33	109.36
2	A	999	FAD	C5A-C6A-N6A	-2.62	116.80	123.29
2	B	999	FAD	C5'-C4'-C3'	2.61	117.15	112.22
2	B	999	FAD	C2A-N3A-C4A	2.61	118.20	111.83
2	C	999	FAD	C10-C4X-N5	-2.61	119.48	124.81
2	D	999	FAD	C2A-N3A-C4A	2.56	118.08	111.83
2	B	999	FAD	C5A-N7A-C8A	2.50	107.38	103.45
2	C	999	FAD	C4-C4X-C10	2.48	121.19	116.93
2	B	999	FAD	O3P-PA-O1A	-2.44	103.38	110.70
2	C	999	FAD	C4-N3-C2	-2.43	121.32	125.64
2	A	999	FAD	O3B-C3B-C4B	-2.41	104.15	111.08
2	D	999	FAD	O4'-C4'-C3'	2.37	114.80	109.25
2	B	999	FAD	O4-C4-N3	-2.37	115.65	120.11
2	B	999	FAD	C4X-C10-N1	-2.36	118.80	124.59
2	D	999	FAD	C10-N1-C2	2.36	121.95	116.85
2	B	999	FAD	O3B-C3B-C4B	-2.35	104.33	111.08
2	A	999	FAD	N3A-C4A-N9A	2.34	131.15	127.17
2	C	999	FAD	C5A-C6A-N6A	-2.34	117.50	123.29
2	D	999	FAD	O3P-P-O1P	-2.32	103.73	110.70
2	D	999	FAD	C4X-C10-N1	-2.30	118.96	124.59
2	A	999	FAD	C10-C4X-N5	-2.29	120.14	124.81
2	A	999	FAD	O4-C4-N3	-2.28	115.83	120.11
2	C	999	FAD	O3B-C3B-C4B	-2.24	104.64	111.08
2	D	999	FAD	O3'-C3'-C4'	2.22	113.97	108.93
2	B	999	FAD	C10-N1-C2	2.20	121.62	116.85
2	D	999	FAD	O3P-PA-O1A	-2.17	104.18	110.70
2	D	999	FAD	C5A-C4A-N3A	-2.14	123.77	126.72
2	A	999	FAD	C2A-N1A-C6A	2.10	122.17	118.73
2	B	999	FAD	C1'-C2'-C3'	2.08	115.30	109.66
2	C	999	FAD	C9A-C5X-N5	-2.07	120.26	122.45
2	B	999	FAD	C4-N3-C2	-2.03	122.03	125.64
2	C	999	FAD	C4X-C10-N1	-2.03	119.61	124.59
2	B	999	FAD	C5X-C9A-N10	2.02	119.80	117.97

There are no chirality outliers.

All (28) 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'

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Mol	Chain	Res	Type	Atoms
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'
2	D	999	FAD	N10-C1'-C2'-C3'
4	C	888	1DO	C4-C5-C6-C7
4	C	888	1DO	C3-C4-C5-C6
4	B	888	1DO	C3-C4-C5-C6
4	B	888	1DO	C2-C3-C4-C5
4	B	888	1DO	C1-C2-C3-C4
4	B	888	1DO	O2S-C1-C2-C3
4	C	888	1DO	O2S-C1-C2-C3
4	B	888	1DO	C6-C7-C8-C9
4	C	888	1DO	C2-C3-C4-C5
4	B	888	1DO	C7-C8-C9-C10
4	C	888	1DO	C6-C7-C8-C9
2	D	999	FAD	PA-O3P-P-O2P
4	C	888	1DO	C9-C10-C11-C12
2	A	999	FAD	PA-O3P-P-O2P
4	C	888	1DO	C1-C2-C3-C4
2	B	999	FAD	PA-O3P-P-O2P
2	C	999	FAD	C3'-C4'-C5'-O5'
2	D	999	FAD	C3'-C4'-C5'-O5'
2	C	999	FAD	PA-O3P-P-O2P
2	B	999	FAD	PA-O3P-P-O1P

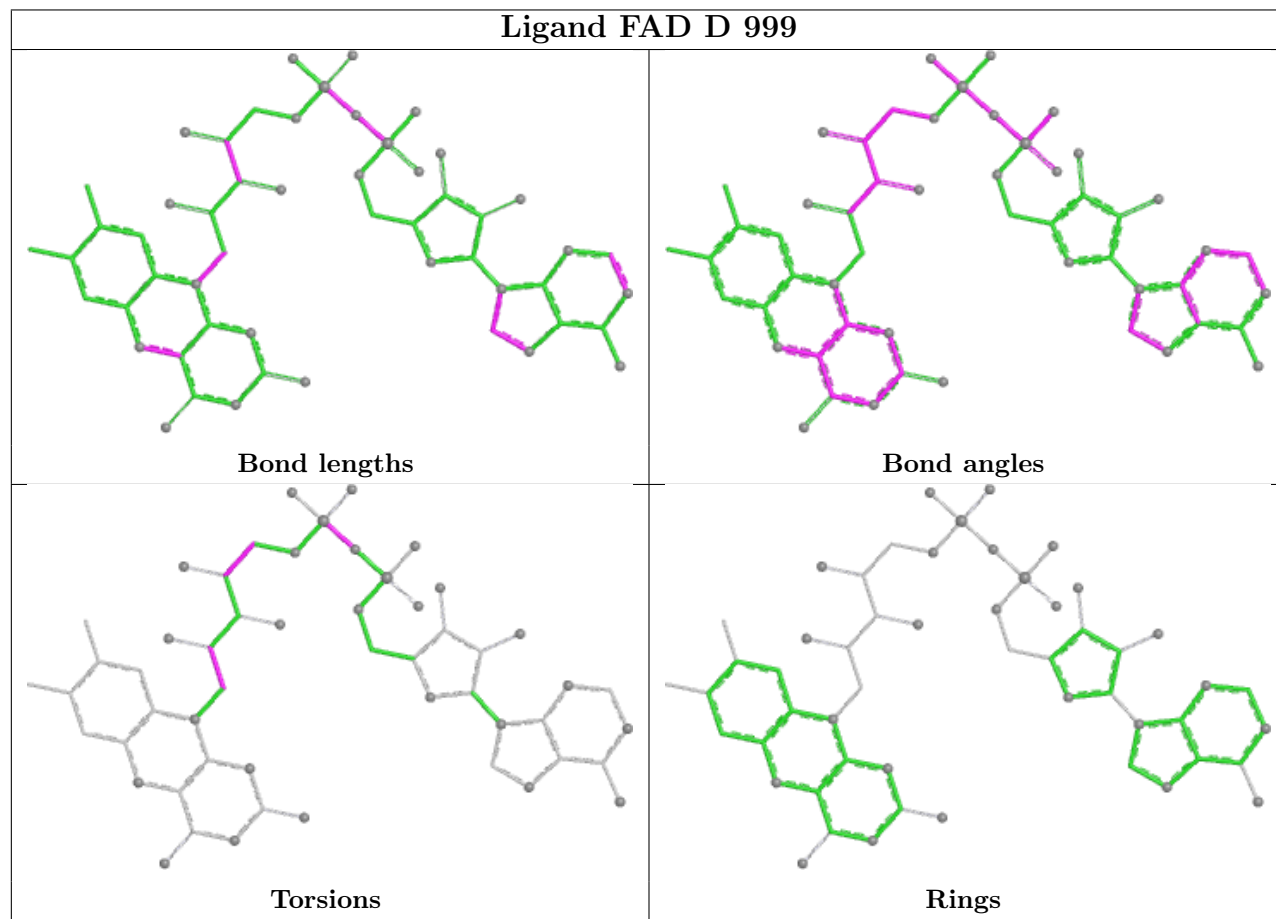
There are no ring outliers.

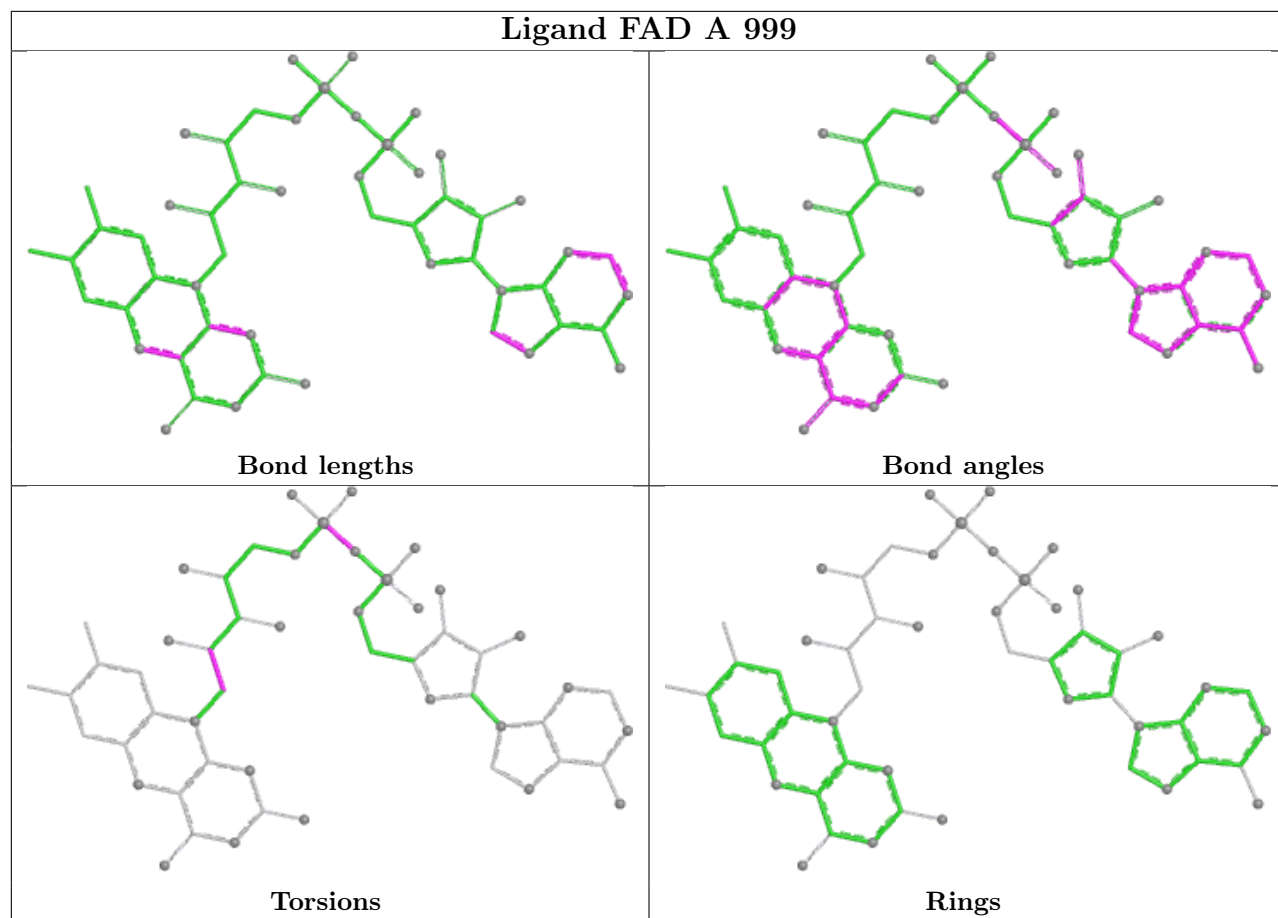
5 monomers are involved in 7 short contacts:

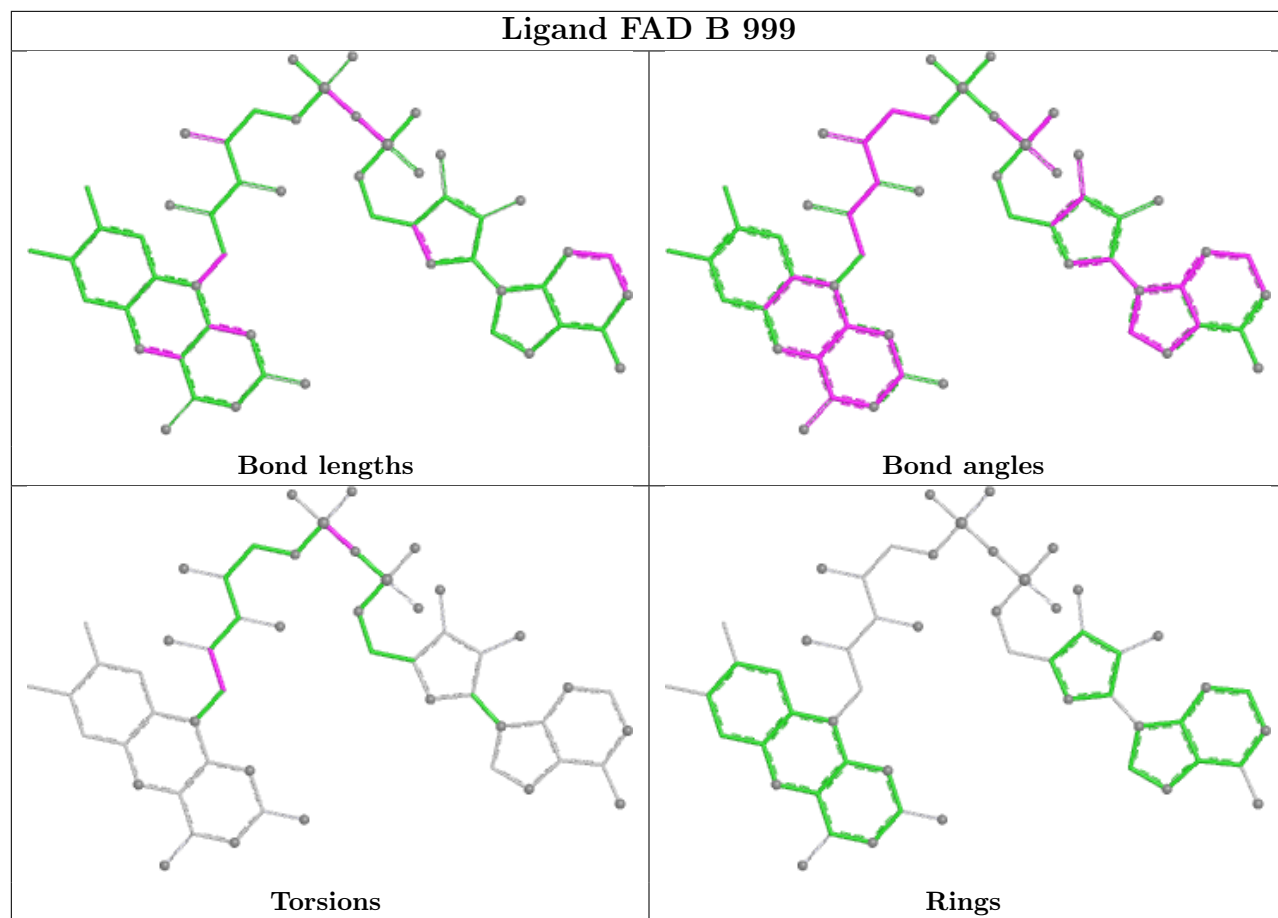
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	888	1DO	2	0
2	D	999	FAD	1	0
2	A	999	FAD	1	0
4	C	888	1DO	2	0
2	C	999	FAD	1	0

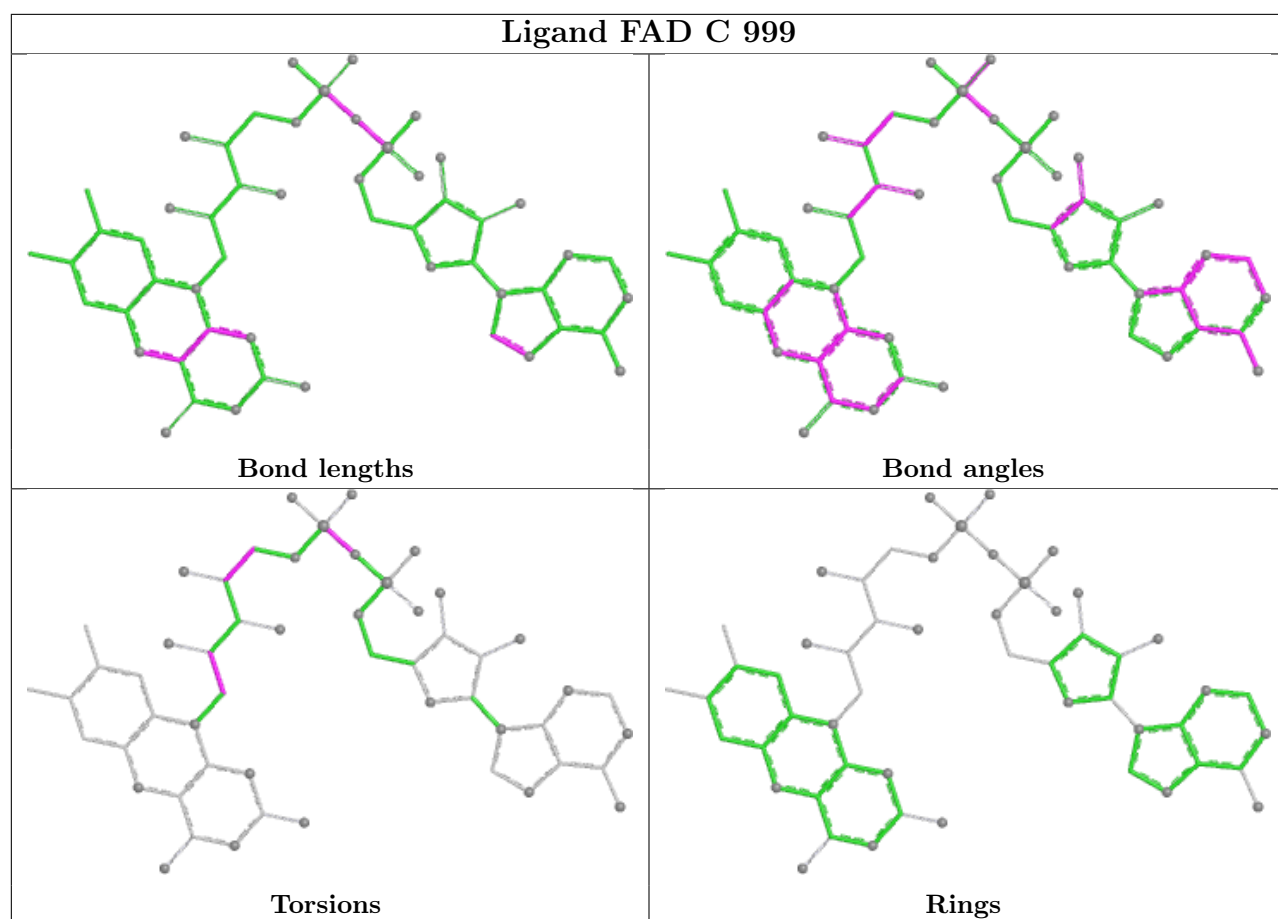
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	555/658 (84%)	-0.13	10 (1%) 67 63	13, 33, 63, 83	1 (0%)
1	B	543/658 (82%)	-0.06	11 (2%) 65 60	14, 35, 65, 85	0
1	C	557/658 (84%)	-0.14	6 (1%) 78 74	14, 33, 59, 72	0
1	D	550/658 (83%)	0.06	10 (1%) 67 63	15, 39, 71, 84	0
All	All	2205/2632 (83%)	-0.07	37 (1%) 69 65	13, 35, 66, 85	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	457	GLY	5.6
1	C	82	ILE	5.3
1	D	83	ILE	4.8
1	D	82	ILE	4.7
1	D	432	LEU	4.4
1	B	81	GLY	4.2
1	C	81	GLY	3.8
1	A	82	ILE	3.7
1	A	83	ILE	3.7
1	A	439	ILE	3.3
1	B	458	PHE	3.1
1	B	559	PHE	3.1
1	B	558	GLN	3.1
1	A	559	PHE	3.0
1	C	83	ILE	3.0
1	A	81	GLY	3.0
1	A	457	GLY	2.6
1	A	438	SER	2.6
1	A	440	PHE	2.5
1	C	432	LEU	2.5
1	A	144	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	162	GLU	2.4
1	B	460	PRO	2.4
1	D	504	GLY	2.4
1	D	81	GLY	2.3
1	D	505	TYR	2.3
1	D	164	PHE	2.3
1	C	457	GLY	2.2
1	B	140	LEU	2.2
1	D	150	LEU	2.1
1	D	478	LEU	2.1
1	B	199	GLU	2.1
1	B	180	ASP	2.1
1	C	159	ILE	2.1
1	A	437	SER	2.1
1	B	166	HIS	2.1
1	D	559	PHE	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.

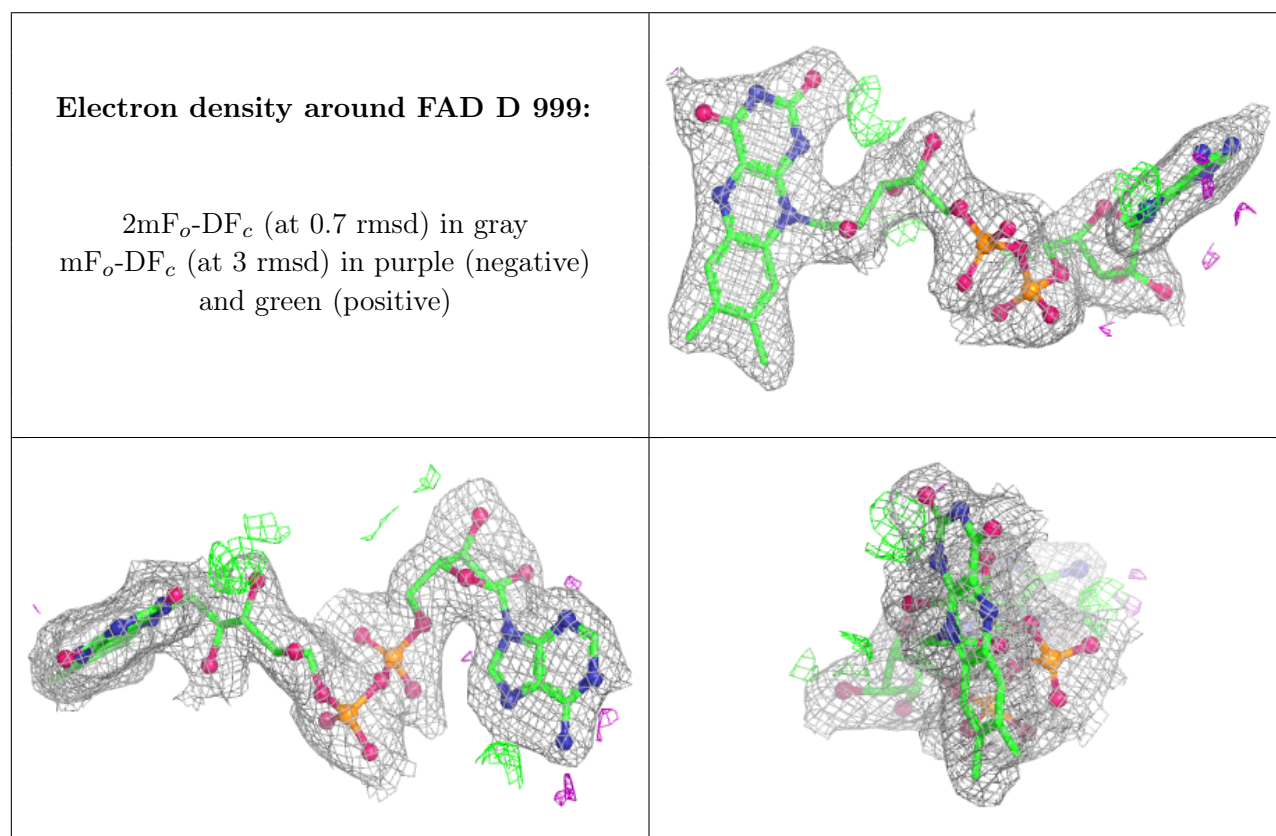
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	1DO	B	888	13/13	0.86	0.12	29,33,36,37	0
4	1DO	C	888	13/13	0.88	0.12	31,34,41,42	0
3	SO4	D	1659	5/5	0.90	0.15	48,49,51,53	0
3	SO4	A	1659	5/5	0.93	0.14	53,53,54,57	0
2	FAD	D	999	53/53	0.97	0.06	15,22,26,27	0
2	FAD	C	999	53/53	0.98	0.04	6,11,16,18	0
2	FAD	A	999	53/53	0.98	0.05	15,19,24,28	0

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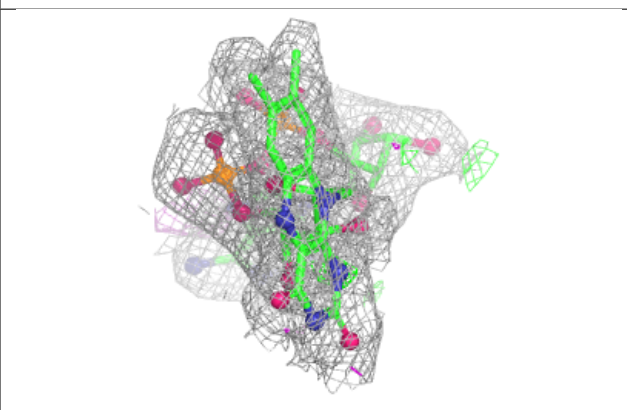
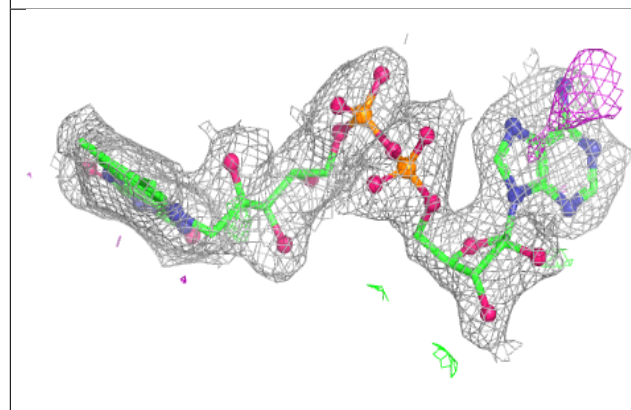
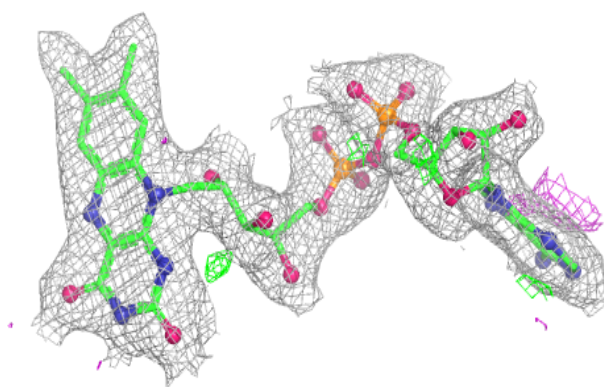
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	B	999	53/53	0.98	0.05	12,17,21,23	0

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.

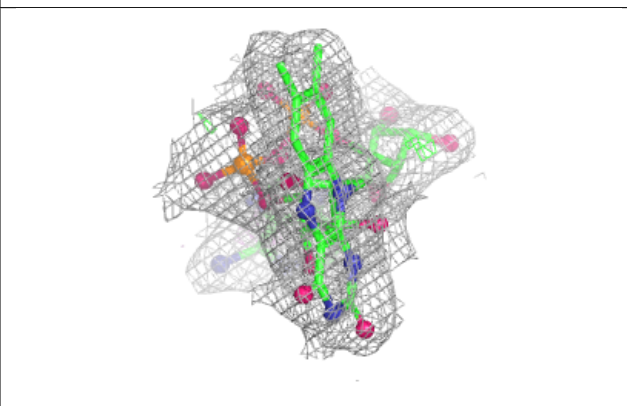
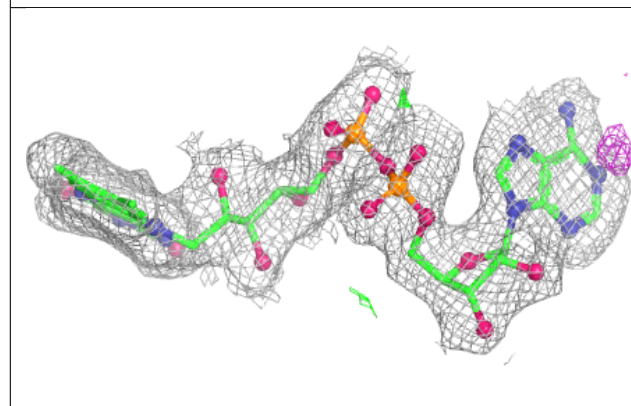
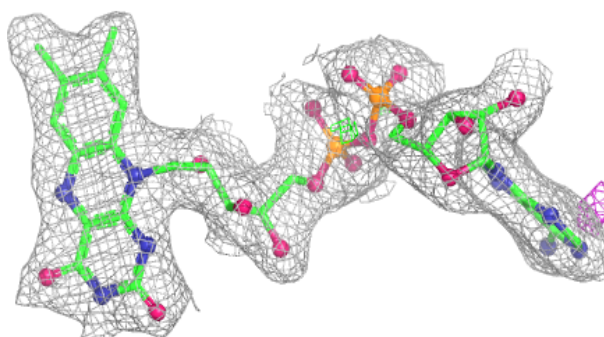


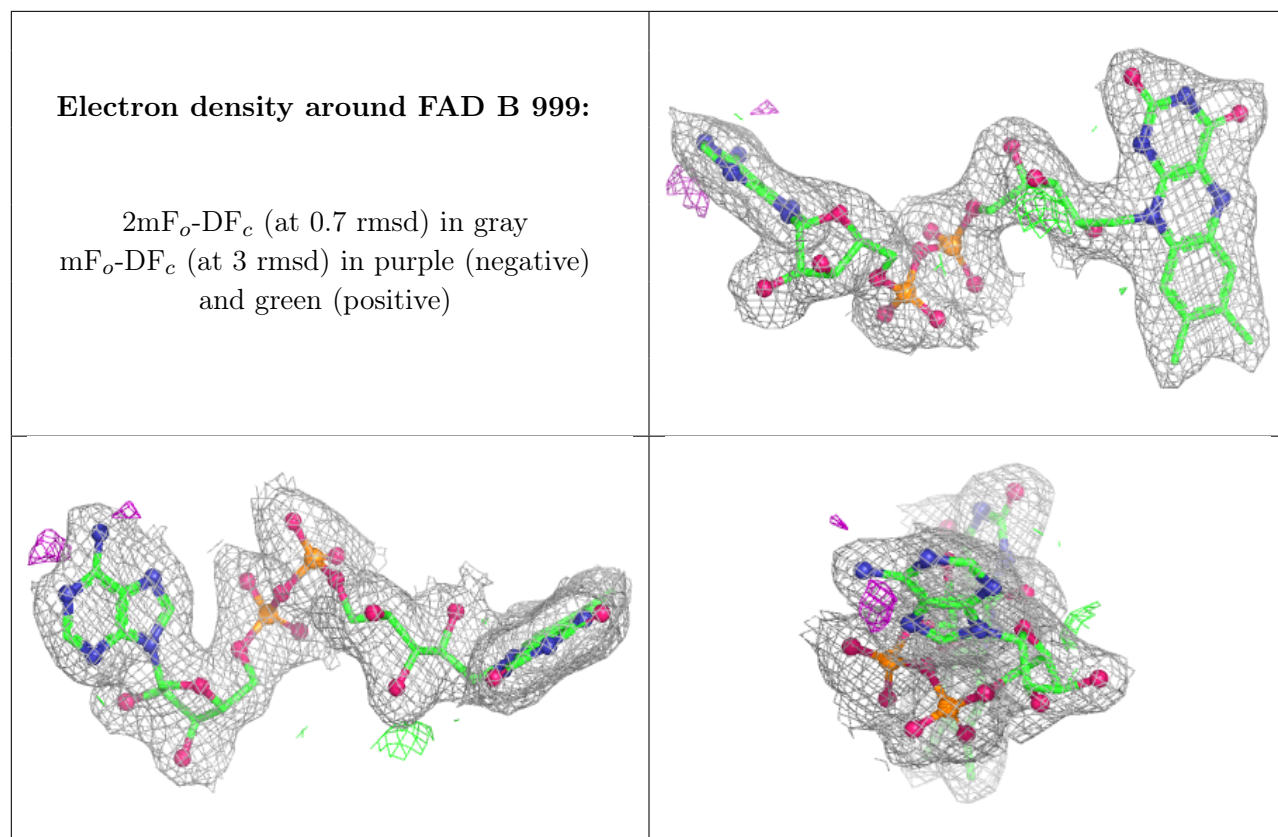
Electron density around FAD C 999:

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

**Electron density around FAD A 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.