



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:44 PM UTC

PDB ID : 8IL4 / pdb_00008il4
Title : Crystal structure of alcohol oxidase ParAOX(M59V/Q60P/R61N/F101S/N602H)(Polyporus arcularius)
Authors : Wu, B.; Wang, Y.
Deposited on : 2023-03-01
Resolution : 3.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

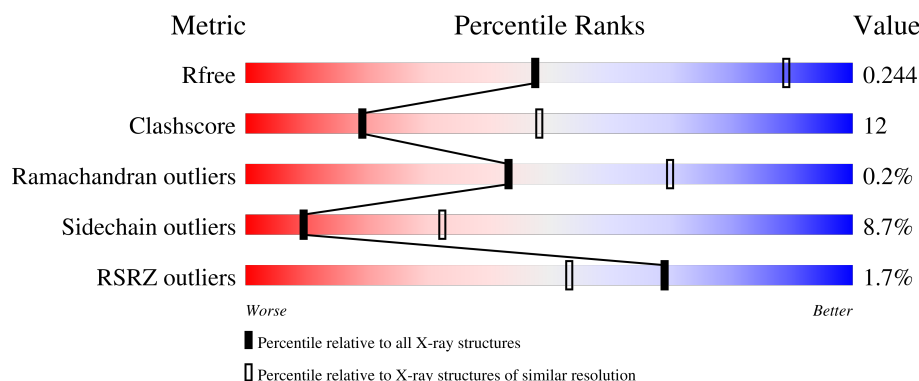
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	649	69% 24% • 5%
1	B	649	68% 23% • 6%
1	C	649	3% 65% 27% • 5%
1	D	649	2% 58% 31% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19024 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.

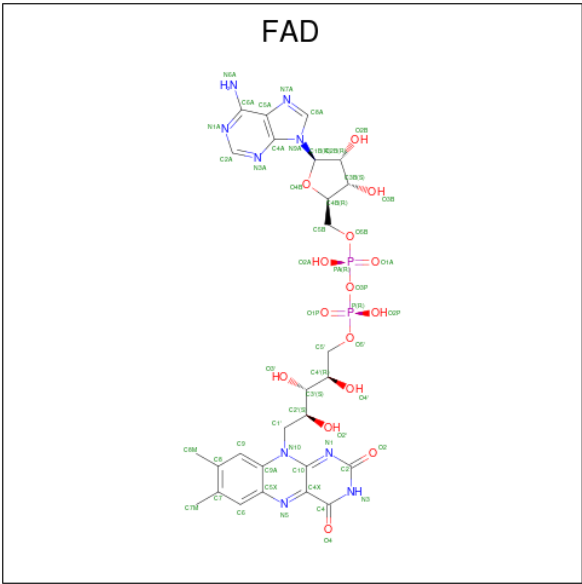
- Molecule 1 is a protein called GMC oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	0	0
			4765	2994	842	909	20			
1	B	607	Total	C	N	O	S	0	0	0
			4648	2916	817	896	19			
1	C	619	Total	C	N	O	S	0	0	0
			4736	2976	830	910	20			
1	D	609	Total	C	N	O	S	0	0	0
			4663	2937	811	895	20			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	VAL	MET	engineered mutation	UNP A0A5C3NW19
A	60	PRO	GLN	engineered mutation	UNP A0A5C3NW19
A	61	ASN	ARG	engineered mutation	UNP A0A5C3NW19
A	101	SER	PHE	engineered mutation	UNP A0A5C3NW19
A	602	HIS	ASN	engineered mutation	UNP A0A5C3NW19
B	59	VAL	MET	engineered mutation	UNP A0A5C3NW19
B	60	PRO	GLN	engineered mutation	UNP A0A5C3NW19
B	61	ASN	ARG	engineered mutation	UNP A0A5C3NW19
B	101	SER	PHE	engineered mutation	UNP A0A5C3NW19
B	602	HIS	ASN	engineered mutation	UNP A0A5C3NW19
C	59	VAL	MET	engineered mutation	UNP A0A5C3NW19
C	60	PRO	GLN	engineered mutation	UNP A0A5C3NW19
C	61	ASN	ARG	engineered mutation	UNP A0A5C3NW19
C	101	SER	PHE	engineered mutation	UNP A0A5C3NW19
C	602	HIS	ASN	engineered mutation	UNP A0A5C3NW19
D	59	VAL	MET	engineered mutation	UNP A0A5C3NW19
D	60	PRO	GLN	engineered mutation	UNP A0A5C3NW19
D	61	ASN	ARG	engineered mutation	UNP A0A5C3NW19
D	101	SER	PHE	engineered mutation	UNP A0A5C3NW19
D	602	HIS	ASN	engineered mutation	UNP A0A5C3NW19

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).

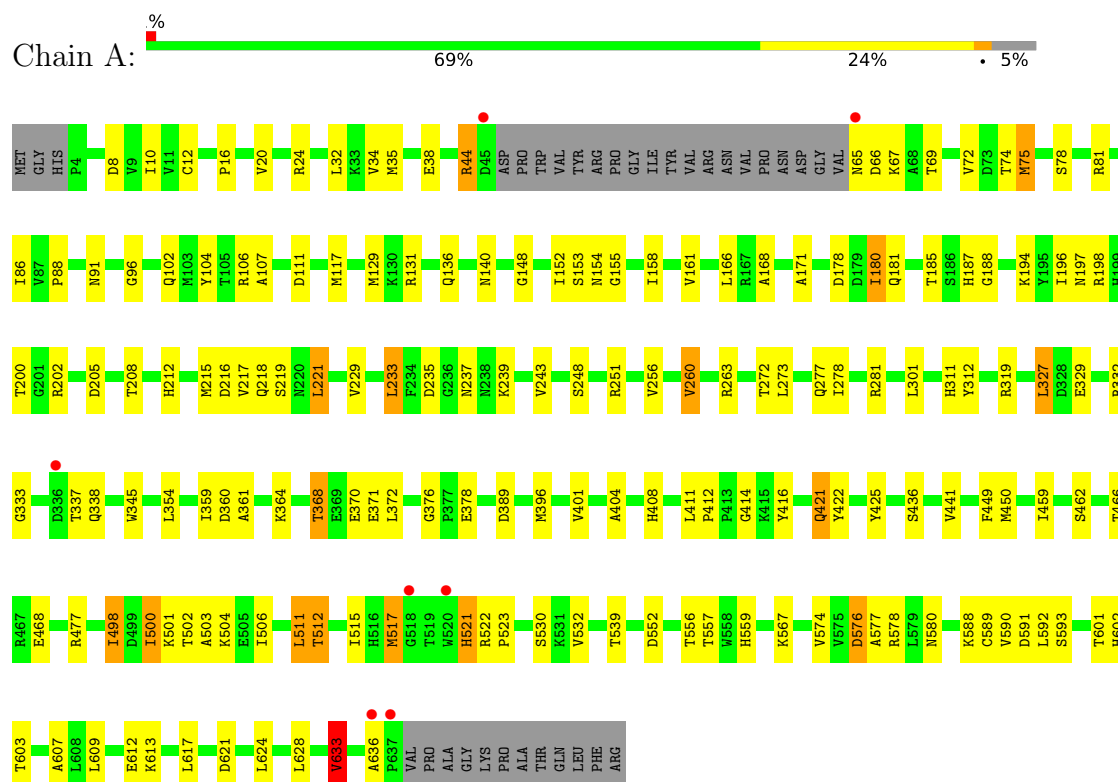


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

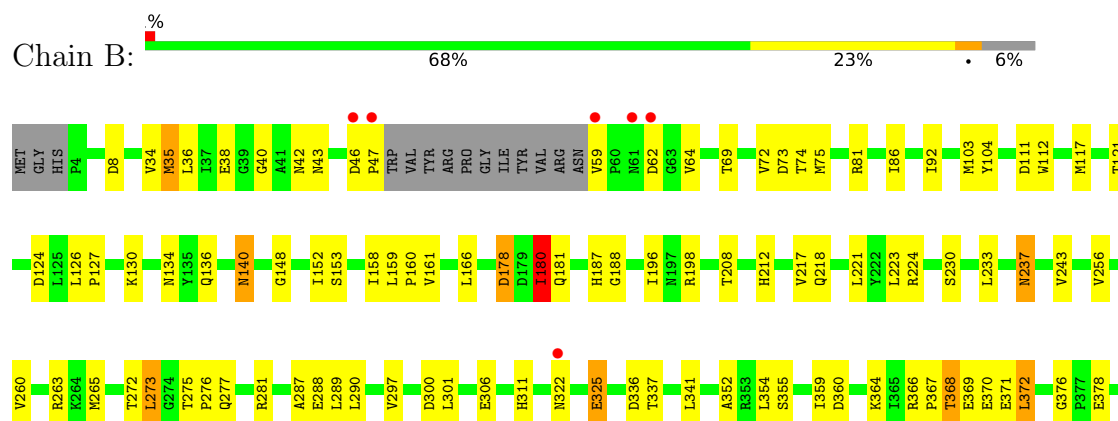
3 Residue-property plots

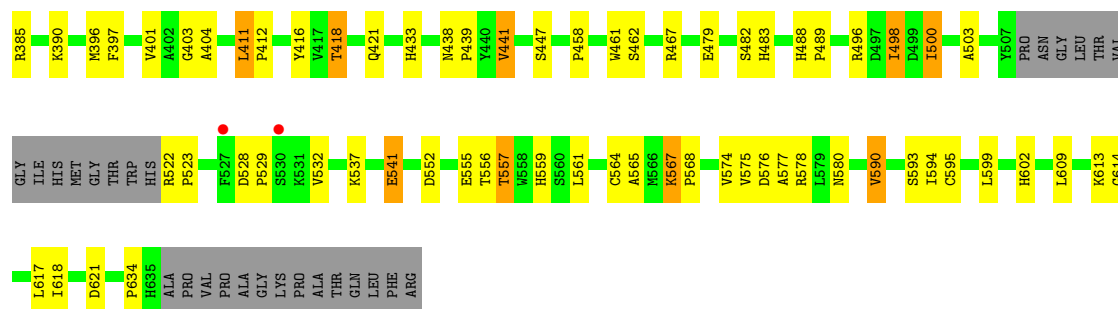
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: GMC oxidoreductase

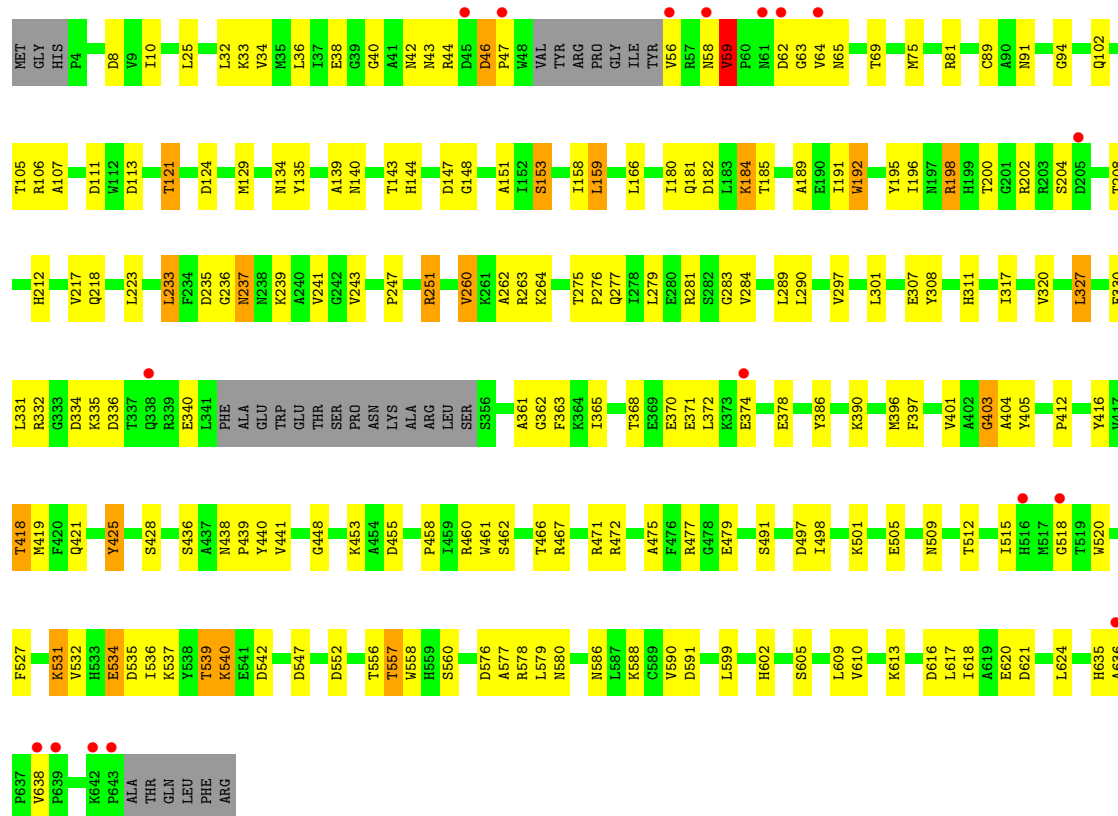


• Molecule 1: GMC oxidoreductase

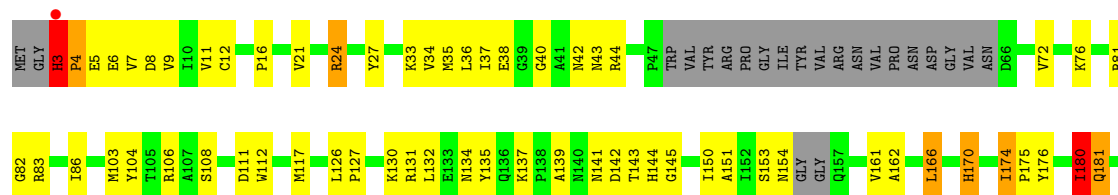


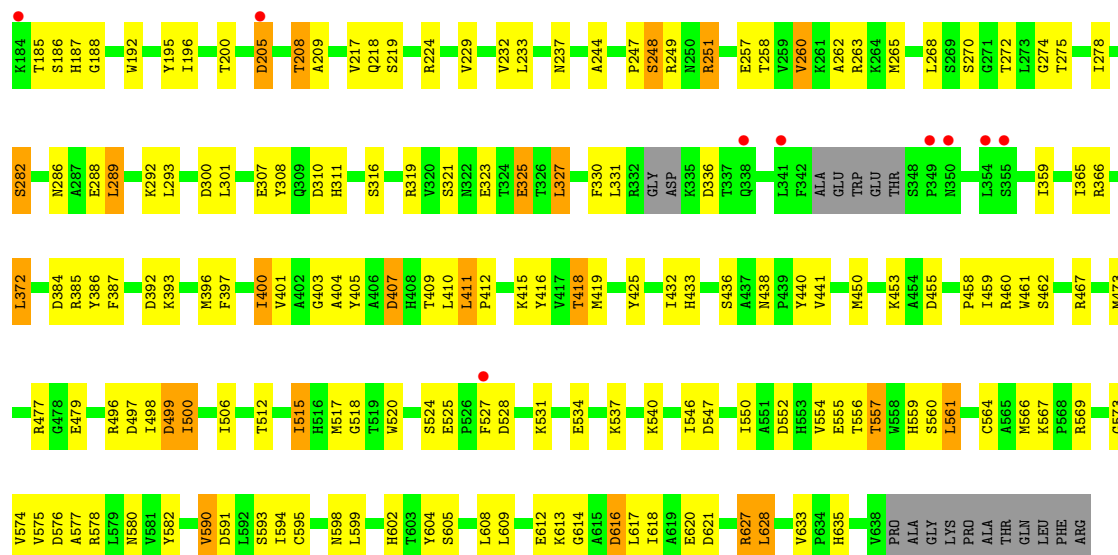


• Molecule 1: GMC oxidoreductase



• Molecule 1: GMC oxidoreductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.71Å 187.43Å 118.53Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	45.57 – 3.36 45.57 – 3.36	Depositor EDS
% Data completeness (in resolution range)	94.1 (45.57-3.36) 94.0 (45.57-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.9_1692+SVN	Depositor
R, R_{free}	0.194 , 0.243 0.198 , 0.244	Depositor DCC
R_{free} test set	1998 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19024	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	0/4880	1.02	13/6630 (0.2%)
1	B	0.93	0/4754	1.00	10/6464 (0.2%)
1	C	0.86	0/4849	1.02	15/6596 (0.2%)
1	D	0.73	0/4775	0.99	9/6499 (0.1%)
All	All	0.88	0/19258	1.01	47/26189 (0.2%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	VAL	CA-C-N	-9.79	107.03	120.25
1	C	59	VAL	C-N-CA	-9.79	107.03	120.25
1	C	46	ASP	CA-C-N	-8.63	109.06	119.84
1	C	46	ASP	C-N-CA	-8.63	109.06	119.84
1	A	376	GLY	CA-C-N	8.16	127.45	118.97
1	A	376	GLY	C-N-CA	8.16	127.45	118.97
1	A	511	LEU	N-CA-C	-7.26	101.17	110.53
1	D	174	ILE	CA-C-N	7.25	127.25	119.78
1	D	174	ILE	C-N-CA	7.25	127.25	119.78
1	A	256	VAL	N-CA-C	7.20	118.25	108.17
1	C	527	PHE	N-CA-C	7.02	119.25	109.15
1	C	390	LYS	CA-C-N	7.00	127.16	119.87
1	C	390	LYS	C-N-CA	7.00	127.16	119.87
1	C	94	GLY	N-CA-C	-6.10	106.99	114.92
1	C	403	GLY	N-CA-C	-5.82	102.26	110.88
1	C	180	ILE	N-CA-C	-5.81	107.09	113.43
1	A	589	CYS	CA-C-N	-5.74	117.51	122.96
1	A	589	CYS	C-N-CA	-5.74	117.51	122.96
1	A	603	THR	N-CA-C	5.66	119.88	112.92
1	C	425	TYR	CA-C-N	5.62	125.57	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	425	TYR	C-N-CA	5.62	125.57	119.78
1	A	633	VAL	CA-C-N	5.54	125.47	119.76
1	A	633	VAL	C-N-CA	5.54	125.47	119.76
1	D	3	HIS	CA-C-N	5.53	126.75	119.84
1	D	3	HIS	C-N-CA	5.53	126.75	119.84
1	D	400	ILE	N-CA-C	5.53	115.91	108.17
1	B	528	ASP	CA-C-N	5.48	125.00	119.19
1	B	528	ASP	C-N-CA	5.48	125.00	119.19
1	B	529	PRO	N-CA-C	-5.44	106.44	113.57
1	B	376	GLY	CA-C-N	5.41	124.59	118.97
1	B	376	GLY	C-N-CA	5.41	124.59	118.97
1	A	577	ALA	N-CA-C	-5.40	106.64	113.18
1	B	575	VAL	N-CA-C	5.40	116.68	108.80
1	B	180	ILE	N-CA-C	-5.39	107.50	112.83
1	B	411	LEU	CA-C-N	5.24	123.49	119.66
1	B	411	LEU	C-N-CA	5.24	123.49	119.66
1	A	180	ILE	N-CA-C	-5.23	107.88	112.90
1	A	148	GLY	CA-C-N	5.20	124.70	119.19
1	A	148	GLY	C-N-CA	5.20	124.70	119.19
1	C	63	GLY	N-CA-C	-5.19	108.83	115.42
1	D	411	LEU	CA-C-N	5.15	125.69	120.38
1	D	411	LEU	C-N-CA	5.15	125.69	120.38
1	D	575	VAL	N-CA-C	5.14	116.31	108.80
1	C	334	ASP	N-CA-C	5.11	117.12	110.43
1	B	256	VAL	N-CA-C	5.07	115.15	107.80
1	C	335	LYS	N-CA-C	5.01	118.65	112.24
1	D	180	ILE	N-CA-C	-5.00	107.98	113.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4765	0	4608	95	0
1	B	4648	0	4454	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4736	0	4540	110	0
1	D	4663	0	4436	139	0
2	A	53	0	30	3	0
2	B	53	0	30	2	0
2	C	53	0	30	1	0
2	D	53	0	30	4	0
All	All	19024	0	18158	436	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (436) 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:D:137:LYS:HE3	1:D:154:ASN:HB3	1.55	0.86
1:D:72:VAL:HG12	1:D:86:ILE:HG12	1.58	0.86
1:B:136:GLN:O	1:B:198:ARG:NH1	2.08	0.86
1:D:528:ASP:HB3	1:D:531:LYS:HG3	1.56	0.85
1:D:217:VAL:HG23	1:D:218:GLN:HG3	1.60	0.83
1:A:436:SER:HB3	1:A:441:VAL:HG21	1.60	0.82
1:C:460:ARG:NH1	1:C:547:ASP:OD1	2.14	0.79
1:D:35:MET:HE1	1:D:260:VAL:HG11	1.64	0.79
1:D:83:ARG:NH2	1:D:554:VAL:O	2.18	0.77
1:C:182:ASP:CG	1:C:184:LYS:HZ1	1.94	0.75
1:C:81:ARG:NH1	1:C:552:ASP:OD2	2.20	0.74
1:A:576:ASP:HB3	1:A:578:ARG:H	1.53	0.74
1:C:412:PRO:O	1:C:416:TYR:OH	2.05	0.73
1:D:141:ASN:OD1	1:D:142:ASP:N	2.21	0.73
1:C:580:ASN:OD1	1:C:588:LYS:NZ	2.20	0.73
1:C:69:THR:HG23	1:C:91:ASN:HB2	1.71	0.73
1:D:278:ILE:O	1:D:282:SER:OG	2.07	0.73
1:D:401:VAL:HB	1:D:418:THR:HG23	1.69	0.72
1:B:576:ASP:HB3	1:B:578:ARG:H	1.54	0.72
1:D:24:ARG:NH1	1:D:612:GLU:OE2	2.22	0.72
1:D:613:LYS:HE3	1:D:617:LEU:HD21	1.71	0.72
1:C:251:ARG:HB2	1:C:251:ARG:HH21	1.55	0.72
1:B:35:MET:HE2	1:B:260:VAL:HG11	1.71	0.71
1:C:158:ILE:HG12	1:C:191:ILE:HD12	1.72	0.71
1:A:35:MET:HE1	1:A:260:VAL:HG11	1.72	0.71
1:D:407:ASP:OD1	1:D:407:ASP:N	2.17	0.69
1:C:578:ARG:NH1	1:C:621:ASP:OD1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ALA:HB2	1:B:416:TYR:HB2	1.72	0.69
1:C:471:ARG:NH1	1:C:479:GLU:OE2	2.26	0.69
1:D:205:ASP:OD2	1:D:208:THR:OG1	2.10	0.68
1:C:184:LYS:NZ	1:C:185:THR:HG23	2.07	0.68
1:D:436:SER:HB3	1:D:441:VAL:HG21	1.74	0.68
1:A:311:HIS:O	1:A:557:THR:OG1	2.10	0.68
1:A:153:SER:OG	1:A:196:ILE:O	2.10	0.68
1:A:412:PRO:O	1:A:416:TYR:OH	2.11	0.67
1:B:482:SER:HG	1:B:483:HIS:HD1	1.42	0.67
1:D:308:TYR:OH	1:D:310:ASP:OD2	2.09	0.67
1:B:217:VAL:HG23	1:B:218:GLN:HG3	1.75	0.67
1:C:217:VAL:HG13	1:C:218:GLN:HG3	1.75	0.66
1:D:321:SER:OG	1:D:323:GLU:OE2	2.14	0.66
1:B:412:PRO:O	1:B:416:TYR:OH	2.11	0.65
1:D:265:MET:HE3	1:D:618:ILE:HG23	1.77	0.65
1:C:401:VAL:HB	1:C:418:THR:HG23	1.78	0.65
1:D:400:ILE:HD12	1:D:473:MET:HE1	1.79	0.65
1:D:117:MET:HG3	1:D:566:MET:HG2	1.78	0.65
1:D:576:ASP:OD1	1:D:577:ALA:N	2.30	0.64
1:B:341:LEU:HD12	1:B:354:LEU:HG	1.79	0.64
1:D:403:GLY:O	1:D:418:THR:HG22	1.98	0.64
1:A:217:VAL:HG23	1:A:218:GLN:HG3	1.80	0.63
1:D:407:ASP:HB2	1:D:409:THR:HG22	1.81	0.63
1:A:219:SER:OG	1:C:124:ASP:OD2	2.16	0.63
1:A:301:LEU:HD13	1:A:574:VAL:HG13	1.81	0.62
1:C:184:LYS:HZ2	1:C:185:THR:HG23	1.64	0.62
1:B:496:ARG:HD2	1:B:522:ARG:HH21	1.63	0.62
1:C:235:ASP:OD1	1:C:237:ASN:N	2.30	0.62
1:B:153:SER:OG	1:B:196:ILE:O	2.17	0.62
2:D:1000:FAD:O1A	2:D:1000:FAD:O4'	2.15	0.62
1:C:311:HIS:O	1:C:557:THR:OG1	2.17	0.61
1:C:38:GLU:HG3	1:C:40:GLY:H	1.66	0.61
1:B:237:ASN:OD1	1:B:237:ASN:N	2.33	0.61
1:B:311:HIS:O	1:B:557:THR:OG1	2.12	0.61
1:B:488:HIS:ND1	1:B:489:PRO:HD2	2.15	0.61
1:D:289:LEU:HD11	1:D:433:HIS:HB3	1.83	0.61
1:B:81:ARG:NH1	1:B:552:ASP:OD2	2.34	0.61
1:D:153:SER:OG	1:D:196:ILE:O	2.18	0.60
1:D:412:PRO:O	1:D:416:TYR:OH	2.13	0.60
1:C:371:GLU:O	1:C:374:GLU:HG2	2.02	0.60
1:C:613:LYS:HE3	1:C:617:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:602:HIS:HB3	2:D:1000:FAD:C2	2.32	0.60
1:A:180:ILE:HD11	1:A:188:GLY:HA3	1.83	0.60
1:C:531:LYS:HD3	1:C:532:VAL:N	2.17	0.60
1:D:135:TYR:HE2	1:D:139:ALA:HB2	1.67	0.59
1:D:192:TRP:CZ2	1:D:397:PHE:HE2	2.19	0.59
1:D:405:TYR:H	1:D:418:THR:HG21	1.67	0.59
1:D:497:ASP:OD1	1:D:498:ILE:N	2.35	0.59
1:B:72:VAL:HG22	1:B:86:ILE:HG12	1.85	0.59
1:B:117:MET:HE3	1:B:577:ALA:HB2	1.83	0.59
1:A:69:THR:HG23	1:A:91:ASN:HB2	1.85	0.58
1:B:401:VAL:HB	1:B:418:THR:HG23	1.85	0.58
1:C:200:THR:OG1	1:C:202:ARG:HG2	2.04	0.58
1:C:290:LEU:HD12	1:C:297:VAL:HG22	1.85	0.58
1:C:386:TYR:HH	1:C:425:TYR:HD2	1.51	0.58
1:B:613:LYS:HE3	1:B:617:LEU:HD21	1.85	0.58
1:D:112:TRP:CZ2	1:D:609:LEU:HD23	2.40	0.57
1:A:396:MET:HE2	1:A:462:SER:HB2	1.85	0.57
1:C:404:ALA:HB2	1:C:416:TYR:HB2	1.85	0.57
1:B:366:ARG:NH2	1:B:390:LYS:O	2.38	0.57
1:D:232:VAL:H	1:D:282:SER:HB3	1.70	0.57
1:D:311:HIS:O	1:D:557:THR:OG1	2.20	0.57
1:B:158:ILE:HD12	1:B:360:ASP:HB3	1.86	0.57
1:A:450:MET:HE1	1:A:459:ILE:HD12	1.87	0.56
1:B:482:SER:OG	1:B:483:HIS:ND1	2.38	0.56
1:D:247:PRO:O	1:D:440:TYR:OH	2.11	0.56
1:D:12:CYS:HB3	1:D:229:VAL:HG21	1.87	0.56
1:D:438:ASN:HB3	1:D:441:VAL:HG13	1.87	0.56
1:C:405:TYR:H	1:C:418:THR:HG21	1.70	0.56
1:C:531:LYS:HD3	1:C:532:VAL:H	1.71	0.56
1:A:408:HIS:HA	1:A:411:LEU:HB2	1.87	0.56
1:A:65:ASN:HD21	1:A:67:LYS:HE2	1.71	0.55
1:A:131:ARG:NH2	1:A:612:GLU:OE1	2.31	0.55
1:B:467:ARG:NH2	1:B:479:GLU:OE1	2.36	0.55
1:D:170:HIS:CE1	1:D:176:TYR:HB2	2.41	0.55
1:C:534:GLU:N	1:C:534:GLU:OE1	2.40	0.55
1:D:162:ALA:O	1:D:166:LEU:HD22	2.07	0.55
1:C:471:ARG:HD2	1:C:536:ILE:HD11	1.88	0.55
1:C:602:HIS:HB3	2:C:1000:FAD:C2	2.37	0.54
1:A:556:THR:OG1	1:A:557:THR:N	2.39	0.54
1:B:38:GLU:HG3	1:B:40:GLY:H	1.72	0.54
1:C:111:ASP:HB3	1:C:599:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ILE:HG13	1:D:608:LEU:HD13	1.89	0.54
1:A:601:THR:OG1	1:A:602:HIS:O	2.23	0.54
1:A:396:MET:HE2	1:A:462:SER:CB	2.38	0.54
1:A:613:LYS:HE3	1:A:617:LEU:HD21	1.89	0.54
1:C:403:GLY:O	1:C:418:THR:HG22	2.07	0.54
1:D:8:ASP:OD1	1:D:263:ARG:NE	2.40	0.54
1:D:602:HIS:HB3	2:D:1000:FAD:O2	2.06	0.54
1:C:239:LYS:HD2	1:C:586:ASN:ND2	2.23	0.54
1:B:180:ILE:HD11	1:B:188:GLY:HA3	1.89	0.53
1:A:65:ASN:ND2	1:A:67:LYS:HE2	2.22	0.53
1:C:134:ASN:HB3	1:C:151:ALA:HA	1.90	0.53
1:C:284:VAL:HG13	1:C:301:LEU:HD12	1.89	0.53
1:A:332:ARG:NH2	1:A:414:GLY:O	2.41	0.53
1:B:62:ASP:HB3	1:B:64:VAL:HG12	1.89	0.53
1:A:602:HIS:HB3	2:A:1000:FAD:C2	2.38	0.53
1:C:113:ASP:OD1	1:C:121:THR:HG22	2.09	0.53
1:D:244:ALA:HB1	1:D:257:GLU:HG2	1.90	0.53
1:D:311:HIS:HE1	1:D:598:ASN:OD1	1.92	0.53
1:D:321:SER:HB2	1:D:527:PHE:CE2	2.43	0.53
1:D:576:ASP:HB3	1:D:580:ASN:H	1.74	0.53
1:B:8:ASP:OD1	1:B:263:ARG:NH1	2.42	0.53
1:C:308:TYR:HE1	1:C:560:SER:HB3	1.73	0.53
1:D:21:VAL:HG21	1:D:590:VAL:HG21	1.90	0.53
1:A:272:THR:HA	1:A:593:SER:HB3	1.91	0.53
1:B:403:GLY:O	1:B:418:THR:HG22	2.08	0.53
1:D:27:TYR:CE2	1:D:627:ARG:HG2	2.44	0.52
1:D:76:LYS:HD3	1:D:82:GLY:O	2.09	0.52
1:D:131:ARG:NH2	1:D:612:GLU:OE1	2.39	0.52
1:D:106:ARG:HH21	1:D:144:HIS:CE1	2.28	0.52
1:A:512:THR:O	1:A:515:ILE:HG23	2.09	0.52
1:A:251:ARG:NH2	1:B:300:ASP:OD2	2.43	0.52
1:B:359:ILE:HG12	1:B:401:VAL:HG22	1.91	0.52
1:C:534:GLU:CD	1:C:534:GLU:H	2.18	0.52
1:A:404:ALA:HB2	1:A:416:TYR:HB2	1.91	0.52
1:C:135:TYR:CE2	1:C:139:ALA:HB2	2.45	0.52
1:D:366:ARG:NH2	1:D:387:PHE:O	2.41	0.52
1:D:126:LEU:HG	1:D:130:LYS:HE3	1.92	0.52
1:B:576:ASP:HB2	1:B:580:ASN:H	1.75	0.51
1:D:132:LEU:HD23	1:D:612:GLU:HG3	1.92	0.51
1:C:105:THR:O	1:C:605:SER:OG	2.19	0.51
1:C:202:ARG:HH22	1:C:636:ALA:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:ARG:NH1	1:D:621:ASP:OD1	2.42	0.51
1:A:208:THR:HG22	1:A:212:HIS:HD2	1.74	0.51
1:C:121:THR:OG1	1:C:124:ASP:OD2	2.28	0.51
1:C:198:ARG:HH11	1:C:198:ARG:HB2	1.75	0.51
1:C:436:SER:HB3	1:C:441:VAL:HG21	1.92	0.51
1:C:134:ASN:HB2	1:C:148:GLY:O	2.11	0.51
1:B:230:SER:O	1:B:281:ARG:HD2	2.11	0.50
1:D:499:ASP:OD1	1:D:500:ILE:N	2.44	0.50
1:C:277:GLN:O	1:C:281:ARG:HG3	2.11	0.50
1:C:327:LEU:O	1:C:330:PHE:HB3	2.11	0.50
1:D:559:HIS:CE1	1:D:602:HIS:HA	2.46	0.50
1:B:36:LEU:HD23	1:B:223:LEU:HD13	1.94	0.50
1:C:59:VAL:HG21	1:C:558:TRP:CZ2	2.46	0.50
1:D:170:HIS:NE2	1:D:176:TYR:HB2	2.27	0.50
1:A:498:ILE:HD13	1:A:503:ALA:HB2	1.94	0.50
1:D:518:GLY:HA3	1:D:520:TRP:NE1	2.27	0.50
1:A:578:ARG:HB2	1:A:580:ASN:ND2	2.26	0.50
1:D:288:GLU:O	1:D:292:LYS:HG3	2.10	0.50
1:B:272:THR:HA	1:B:593:SER:HB3	1.94	0.50
1:A:187:HIS:HA	1:A:364:LYS:O	2.11	0.49
1:D:111:ASP:OD1	1:D:425:TYR:OH	2.24	0.49
1:C:192:TRP:HZ3	1:C:362:GLY:C	2.19	0.49
1:C:419:MET:HG3	1:C:466:THR:HB	1.94	0.49
1:D:117:MET:HE2	1:D:567:LYS:HA	1.95	0.49
1:A:10:ILE:HD11	1:A:260:VAL:HG22	1.94	0.49
1:B:369:GLU:H	1:B:369:GLU:CD	2.21	0.49
1:C:235:ASP:OD2	1:C:239:LYS:HB3	2.12	0.49
1:C:105:THR:HG23	1:C:181:GLN:NE2	2.28	0.49
1:B:565:ALA:HB1	1:B:567:LYS:HE3	1.94	0.49
1:A:44:ARG:NH2	1:A:216:ASP:OD2	2.42	0.49
1:D:556:THR:OG1	1:D:557:THR:N	2.46	0.49
1:C:576:ASP:OD1	1:C:577:ALA:N	2.46	0.49
1:B:111:ASP:HB3	1:B:599:LEU:HD23	1.95	0.49
1:C:363:PHE:CD1	1:C:365:ILE:HG23	2.48	0.49
1:C:518:GLY:HA3	1:C:520:TRP:CZ3	2.48	0.49
1:B:73:ASP:OD1	1:B:447:SER:HB2	2.14	0.48
1:C:198:ARG:HB2	1:C:198:ARG:NH1	2.27	0.48
1:C:467:ARG:NH2	1:C:479:GLU:OE1	2.44	0.48
1:D:567:LYS:O	1:D:573:GLY:HA3	2.12	0.48
1:D:35:MET:HE3	1:D:37:ILE:HD11	1.96	0.48
1:A:155:GLY:O	1:A:198:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:MET:HE3	1:B:618:ILE:HG23	1.95	0.48
1:B:482:SER:HG	1:B:483:HIS:CE1	2.31	0.48
1:D:321:SER:HB2	1:D:527:PHE:CZ	2.49	0.48
1:C:102:GLN:HB2	1:C:195:TYR:HB2	1.96	0.48
1:C:8:ASP:O	1:C:264:LYS:HB2	2.13	0.48
1:A:333:GLY:HA2	1:A:338:GLN:NE2	2.28	0.48
1:A:166:LEU:HD21	1:A:361:ALA:HB1	1.95	0.48
1:D:270:SER:O	1:D:274:GLY:HA3	2.14	0.48
1:A:106:ARG:H	1:A:181:GLN:HG3	1.78	0.48
1:C:539:THR:HG22	1:C:540:LYS:H	1.79	0.48
1:D:200:THR:HG21	1:D:635:HIS:O	2.13	0.48
1:D:404:ALA:HB2	1:D:416:TYR:HB2	1.96	0.48
1:A:277:GLN:O	1:A:281:ARG:HG2	2.14	0.47
1:A:578:ARG:NH1	1:A:621:ASP:OD1	2.47	0.47
1:B:578:ARG:NH1	1:B:621:ASP:OD1	2.47	0.47
1:C:56:VAL:C	1:C:58:ASN:H	2.22	0.47
1:D:131:ARG:NH2	1:D:616:ASP:OD1	2.46	0.47
1:C:540:LYS:HD2	1:C:540:LYS:N	2.27	0.47
1:A:117:MET:HE2	1:A:567:LYS:HA	1.95	0.47
1:B:325:GLU:CD	1:B:325:GLU:H	2.23	0.47
1:D:268:LEU:HB3	1:D:275:THR:HG23	1.96	0.47
1:A:359:ILE:HG12	1:A:401:VAL:HG22	1.97	0.47
1:A:421:GLN:HG2	1:A:466:THR:HG21	1.95	0.47
1:C:153:SER:OG	1:C:196:ILE:O	2.31	0.47
1:D:16:PRO:HB3	1:D:604:TYR:HE1	1.80	0.47
1:D:308:TYR:HE1	1:D:560:SER:HB3	1.78	0.47
1:D:327:LEU:O	1:D:330:PHE:HB3	2.15	0.47
1:D:534:GLU:CD	1:D:537:LYS:HZ1	2.21	0.47
1:D:4:PRO:O	1:D:6:GLU:N	2.48	0.47
1:D:248:SER:HA	1:D:249:ARG:HA	1.71	0.47
1:B:578:ARG:HA	1:B:617:LEU:HD13	1.96	0.47
1:D:564:CYS:HA	1:D:574:VAL:HG21	1.97	0.47
1:D:316:SER:HB2	1:D:419:MET:HB2	1.96	0.46
1:B:112:TRP:CZ2	1:B:609:LEU:HD23	2.49	0.46
1:B:368:THR:OG1	1:B:371:GLU:OE1	2.31	0.46
1:C:166:LEU:HD21	1:C:361:ALA:HB1	1.97	0.46
1:D:42:ASN:OD1	1:D:43:ASN:N	2.49	0.46
1:D:564:CYS:O	1:D:594:ILE:HA	2.15	0.46
1:A:65:ASN:OD1	1:A:66:ASP:N	2.34	0.46
1:A:81:ARG:NH1	1:A:552:ASP:OD2	2.48	0.46
1:C:308:TYR:CE1	1:C:560:SER:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:TYR:OH	1:D:106:ARG:NE	2.49	0.46
1:D:458:PRO:O	1:D:461:TRP:HB3	2.15	0.46
1:B:496:ARG:HD2	1:B:522:ARG:NH2	2.31	0.46
1:D:9:VAL:HG22	1:D:265:MET:HB3	1.97	0.46
1:D:477:ARG:HA	1:D:527:PHE:HE1	1.80	0.46
1:A:38:GLU:OE2	2:A:1000:FAD:O3B	2.33	0.46
1:C:106:ARG:HH21	1:C:144:HIS:CE1	2.33	0.46
1:C:202:ARG:NH2	1:C:635:HIS:O	2.43	0.46
1:C:247:PRO:O	1:C:440:TYR:OH	2.25	0.46
1:D:518:GLY:HA3	1:D:520:TRP:CD1	2.50	0.46
1:A:129:MET:HG2	1:A:609:LEU:HD22	1.97	0.46
1:D:108:SER:N	1:D:111:ASP:OD2	2.48	0.46
1:D:272:THR:HA	1:D:593:SER:HB3	1.97	0.46
1:D:249:ARG:O	1:D:251:ARG:HG3	2.15	0.46
1:D:546:ILE:O	1:D:550:ILE:HG12	2.15	0.46
1:A:559:HIS:CE1	1:A:602:HIS:HA	2.50	0.46
1:C:105:THR:HG23	1:C:181:GLN:HE22	1.80	0.46
1:C:235:ASP:OD1	1:C:236:GLY:N	2.49	0.46
1:C:241:VAL:O	1:C:262:ALA:N	2.38	0.46
1:A:500:ILE:H	1:A:500:ILE:HG13	1.46	0.46
1:C:106:ARG:NH2	1:C:144:HIS:CE1	2.84	0.46
1:D:27:TYR:HE2	1:D:627:ARG:HG2	1.80	0.46
1:D:195:TYR:CE2	1:D:604:TYR:HD2	2.34	0.46
1:D:590:VAL:HG11	1:D:614:GLY:HA3	1.98	0.46
1:A:592:LEU:HD23	1:A:592:LEU:HA	1.78	0.45
1:B:160:PRO:HG2	1:B:325:GLU:OE2	2.17	0.45
1:C:556:THR:OG1	1:C:557:THR:N	2.49	0.45
1:D:301:LEU:HD21	1:D:582:TYR:HB2	1.98	0.45
1:D:450:MET:HE1	1:D:459:ILE:HD12	1.97	0.45
1:D:598:ASN:OD1	1:D:599:LEU:N	2.47	0.45
1:D:591:ASP:OD1	1:D:593:SER:OG	2.25	0.45
1:A:576:ASP:HB2	1:A:580:ASN:H	1.82	0.45
1:A:591:ASP:OD1	1:A:593:SER:OG	2.23	0.45
1:A:578:ARG:O	1:A:588:LYS:NZ	2.47	0.45
1:B:306:GLU:OE2	1:B:433:HIS:NE2	2.37	0.45
1:C:472:ARG:NH2	1:C:535:ASP:OD1	2.50	0.45
1:D:3:HIS:NE2	1:D:224:ARG:HD3	2.31	0.45
1:D:38:GLU:HG3	1:D:40:GLY:H	1.80	0.45
1:D:300:ASP:O	1:D:569:ARG:NH2	2.45	0.45
1:A:107:ALA:HB1	1:A:111:ASP:OD2	2.17	0.45
1:A:81:ARG:HH11	1:A:552:ASP:CG	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:MET:HE2	1:B:462:SER:CB	2.47	0.45
1:D:540:LYS:HB3	1:D:540:LYS:HE2	1.75	0.45
1:D:561:LEU:HD23	1:D:595:CYS:HB2	1.99	0.45
1:A:327:LEU:HD22	1:A:327:LEU:HA	1.71	0.45
1:A:16:PRO:O	1:A:20:VAL:HG23	2.18	0.44
1:D:286:ASN:HB3	1:D:289:LEU:HB2	1.99	0.44
1:A:215:MET:HE3	1:A:221:LEU:O	2.18	0.44
1:B:556:THR:OG1	1:B:557:THR:N	2.50	0.44
1:B:38:GLU:OE1	1:B:40:GLY:N	2.50	0.44
1:A:368:THR:O	1:A:371:GLU:N	2.50	0.44
1:B:46:ASP:HA	1:B:47:PRO:HD3	1.80	0.44
1:C:182:ASP:OD2	1:C:184:LYS:NZ	2.49	0.44
1:C:368:THR:OG1	1:C:370:GLU:HG2	2.17	0.44
1:A:24:ARG:NH2	1:A:612:GLU:OE2	2.33	0.44
1:C:33:LYS:HD3	1:C:263:ARG:HH12	1.81	0.44
1:A:477:ARG:HA	1:A:477:ARG:HD3	1.73	0.44
1:C:10:ILE:HD11	1:C:260:VAL:HG22	1.99	0.44
1:A:168:ALA:O	1:A:171:ALA:HB3	2.18	0.44
1:B:590:VAL:HG21	1:B:614:GLY:HA3	2.00	0.44
1:D:180:ILE:HG22	1:D:181:GLN:CD	2.43	0.44
1:B:561:LEU:HD13	1:B:595:CYS:HB2	1.99	0.44
1:C:438:ASN:HA	1:C:439:PRO:HD3	1.89	0.44
1:D:453:LYS:C	1:D:455:ASP:H	2.26	0.44
1:C:106:ARG:NH2	1:C:143:THR:O	2.51	0.43
1:D:419:MET:HE1	1:D:473:MET:CE	2.48	0.43
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.84	0.43
1:A:624:LEU:HD12	1:A:624:LEU:HA	1.82	0.43
1:B:438:ASN:HB3	1:B:441:VAL:HG13	1.98	0.43
1:C:396:MET:HE2	1:C:462:SER:CB	2.47	0.43
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.68	0.43
1:C:75:MET:HE2	1:C:75:MET:HB2	1.86	0.43
1:C:107:ALA:HB1	1:C:111:ASP:OD2	2.18	0.43
1:A:517:MET:HE3	1:A:517:MET:HB2	1.95	0.43
1:B:541:GLU:H	1:B:541:GLU:HG2	1.41	0.43
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.84	0.43
1:C:428:SER:HB3	1:C:448:GLY:O	2.19	0.43
1:D:396:MET:HE2	1:D:462:SER:CB	2.48	0.43
1:A:111:ASP:OD1	1:A:425:TYR:OH	2.33	0.43
1:B:287:ALA:HB2	1:B:300:ASP:CG	2.43	0.43
1:B:522:ARG:HA	1:B:523:PRO:HD3	1.84	0.43
1:C:62:ASP:C	1:C:64:VAL:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:PRO:O	1:C:461:TRP:HB3	2.19	0.43
1:A:154:ASN:O	1:A:194:LYS:NZ	2.52	0.43
1:B:488:HIS:HD1	1:B:489:PRO:HD2	1.84	0.43
1:C:159:LEU:HD12	1:C:159:LEU:HA	1.83	0.43
1:C:208:THR:HG22	1:C:212:HIS:HD2	1.84	0.43
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.84	0.43
1:D:180:ILE:HD11	1:D:188:GLY:HA3	2.01	0.43
1:D:359:ILE:HG12	1:D:401:VAL:HG22	2.01	0.43
1:B:438:ASN:HA	1:B:439:PRO:HD3	1.92	0.43
1:B:458:PRO:O	1:B:461:TRP:HB3	2.19	0.43
1:D:174:ILE:HA	1:D:175:PRO:HD2	1.87	0.43
1:A:32:LEU:HD22	1:A:624:LEU:HD21	2.01	0.42
1:A:158:ILE:HD12	1:A:360:ASP:HB3	2.01	0.42
1:A:235:ASP:HB3	1:A:239:LYS:H	1.84	0.42
1:A:396:MET:HE3	1:A:396:MET:HB3	1.85	0.42
1:C:491:SER:OG	1:C:542:ASP:OD2	2.35	0.42
1:D:11:VAL:O	1:D:36:LEU:HD12	2.19	0.42
1:D:460:ARG:HD3	1:D:547:ASP:OD1	2.19	0.42
1:A:633:VAL:O	1:A:636:ALA:HB3	2.19	0.42
1:B:103:MET:HE1	1:B:397:PHE:HZ	1.84	0.42
1:B:275:THR:N	1:B:276:PRO:HD2	2.35	0.42
1:A:8:ASP:OD1	1:A:263:ARG:NH1	2.44	0.42
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.74	0.42
1:A:521:HIS:O	1:A:522:ARG:HD3	2.19	0.42
1:C:129:MET:HG2	1:C:609:LEU:HD22	2.01	0.42
1:D:131:ARG:HG3	1:D:628:LEU:HD21	2.01	0.42
1:A:88:PRO:HD2	1:A:556:THR:HG21	2.01	0.42
1:A:200:THR:OG1	1:A:202:ARG:HG2	2.20	0.42
1:A:251:ARG:NH1	1:B:288:GLU:HG2	2.34	0.42
1:B:498:ILE:CG2	1:B:503:ALA:HB2	2.50	0.42
1:C:184:LYS:HZ3	1:C:185:THR:HG23	1.81	0.42
1:C:233:LEU:O	1:C:241:VAL:HG22	2.19	0.42
1:C:591:ASP:O	1:C:610:VAL:HG11	2.18	0.42
1:D:209:ALA:HA	1:D:633:VAL:HG22	2.01	0.42
1:B:140:ASN:ND2	1:B:178:ASP:HB2	2.34	0.42
1:B:187:HIS:HA	1:B:364:LYS:O	2.18	0.42
1:B:301:LEU:HD13	1:B:574:VAL:HG13	2.02	0.42
1:D:130:LYS:O	1:D:145:GLY:HA3	2.18	0.42
1:A:12:CYS:HB3	1:A:229:VAL:HG21	2.01	0.42
1:D:3:HIS:NE2	1:D:224:ARG:HB2	2.34	0.42
1:D:386:TYR:HE1	1:D:393:LYS:HZ2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TYR:CE1	1:B:152:ILE:HD13	2.55	0.42
1:B:126:LEU:HG	1:B:130:LYS:HE3	2.01	0.42
1:C:25:LEU:HD11	1:C:618:ILE:HG21	2.02	0.42
1:C:283:GLY:HA2	1:C:290:LEU:HD13	2.02	0.42
1:D:576:ASP:CB	1:D:580:ASN:H	2.32	0.42
1:B:42:ASN:OD1	1:B:43:ASN:N	2.53	0.42
1:B:121:THR:O	1:B:124:ASP:HB2	2.20	0.42
1:B:500:ILE:H	1:B:500:ILE:HG13	1.56	0.42
1:D:103:MET:HE3	1:D:602:HIS:NE2	2.35	0.42
1:B:180:ILE:HG22	1:B:181:GLN:NE2	2.34	0.42
1:B:277:GLN:O	1:B:281:ARG:HG2	2.20	0.42
1:D:141:ASN:OD1	1:D:143:THR:N	2.53	0.42
1:D:175:PRO:HD2	1:D:187:HIS:CD2	2.55	0.42
1:D:325:GLU:H	1:D:325:GLU:HG2	1.57	0.42
1:A:511:LEU:O	1:A:512:THR:HB	2.20	0.42
1:B:277:GLN:HB3	1:B:281:ARG:NH2	2.35	0.42
1:B:354:LEU:HD23	1:B:354:LEU:HA	1.92	0.42
2:B:1000:FAD:H8A	2:B:1000:FAD:H2B	1.83	0.42
1:C:208:THR:HA	1:C:212:HIS:CD2	2.55	0.42
1:D:3:HIS:HD1	1:D:3:HIS:HA	1.80	0.42
1:A:96:GLY:O	1:A:102:GLN:NE2	2.53	0.41
1:A:312:TYR:O	1:A:422:TYR:HA	2.20	0.41
1:B:290:LEU:HD12	1:B:297:VAL:HG22	2.02	0.41
1:C:275:THR:N	1:C:276:PRO:HD2	2.35	0.41
1:C:453:LYS:C	1:C:455:ASP:H	2.27	0.41
1:D:251:ARG:HG3	1:D:251:ARG:H	1.35	0.41
1:C:579:LEU:HD13	1:C:590:VAL:HG22	2.02	0.41
1:D:372:LEU:HA	1:D:372:LEU:HD13	1.82	0.41
1:D:450:MET:HE2	1:D:554:VAL:HG21	2.02	0.41
1:A:74:THR:HG22	1:A:75:MET:HG2	2.01	0.41
1:B:352:ALA:O	1:B:355:SER:HB2	2.21	0.41
1:D:81:ARG:HD3	1:D:552:ASP:OD1	2.21	0.41
1:D:467:ARG:NH2	1:D:479:GLU:OE1	2.54	0.41
1:D:616:ASP:O	1:D:620:GLU:HG3	2.20	0.41
1:A:312:TYR:CE1	1:A:449:PHE:CD1	3.08	0.41
1:A:502:THR:O	1:A:506:ILE:HG13	2.20	0.41
1:A:522:ARG:HA	1:A:523:PRO:HD3	1.85	0.41
1:B:159:LEU:HA	1:B:160:PRO:HD3	1.91	0.41
1:B:273:LEU:HD12	1:B:273:LEU:HA	1.93	0.41
1:C:189:ALA:HB2	1:C:363:PHE:HB3	2.02	0.41
1:D:131:ARG:HD2	1:D:628:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ARG:NH2	1:D:412:PRO:HB2	2.36	0.41
1:D:432:ILE:O	1:D:433:HIS:ND1	2.51	0.41
1:A:607:ALA:HB2	2:A:1000:FAD:H5'2	2.03	0.41
1:B:35:MET:CE	1:B:260:VAL:HG21	2.51	0.41
1:C:397:PHE:CD1	1:C:397:PHE:C	2.98	0.41
1:D:134:ASN:HB3	1:D:151:ALA:HA	2.01	0.41
1:B:74:THR:HG22	1:B:75:MET:HG3	2.02	0.41
1:B:367:PRO:HB2	1:B:372:LEU:HD22	2.02	0.41
1:A:104:TYR:CE1	1:A:152:ILE:HD13	2.56	0.41
1:C:284:VAL:CG1	1:C:301:LEU:HD12	2.51	0.41
1:C:320:VAL:HG13	1:C:475:ALA:HB1	2.03	0.41
1:D:7:VAL:O	1:D:262:ALA:HA	2.21	0.41
1:D:365:ILE:HG13	1:D:396:MET:HB2	2.03	0.41
1:D:512:THR:O	1:D:515:ILE:HB	2.20	0.41
2:D:1000:FAD:H9	2:D:1000:FAD:H1'1	1.85	0.41
1:A:72:VAL:HG22	1:A:86:ILE:HG12	2.02	0.41
1:A:329:GLU:N	1:A:329:GLU:OE1	2.53	0.41
1:B:557:THR:O	1:B:559:HIS:CD2	2.74	0.41
1:C:32:LEU:HD22	1:C:624:LEU:HD21	2.02	0.41
1:D:506:ILE:HG21	1:D:506:ILE:HD13	1.83	0.41
1:A:136:GLN:NE2	1:A:197:ASN:OD1	2.38	0.40
1:A:205:ASP:OD1	1:A:208:THR:HG23	2.21	0.40
1:A:278:ILE:HD13	1:A:278:ILE:HG21	1.88	0.40
1:C:42:ASN:OD1	1:C:43:ASN:N	2.54	0.40
1:B:208:THR:HA	1:B:212:HIS:HB2	2.03	0.40
1:B:564:CYS:O	1:B:594:ILE:HA	2.21	0.40
1:C:336:ASP:O	1:C:340:GLU:HG3	2.21	0.40
1:C:497:ASP:OD1	1:C:498:ILE:N	2.53	0.40
1:A:81:ARG:HD3	1:A:552:ASP:OD1	2.22	0.40
1:B:153:SER:CB	1:B:198:ARG:HB3	2.51	0.40
1:B:567:LYS:HB2	1:B:568:PRO:HD2	2.02	0.40
1:D:186:SER:HB3	1:D:392:ASP:C	2.45	0.40
1:B:126:LEU:N	1:B:127:PRO:HD2	2.36	0.40
1:B:396:MET:HE3	1:B:396:MET:HB3	1.89	0.40
1:C:36:LEU:HD23	1:C:223:LEU:HD13	2.03	0.40
1:C:135:TYR:HE2	1:C:139:ALA:HB2	1.85	0.40
1:D:409:THR:HG23	1:D:410:LEU:HG	2.03	0.40
1:B:134:ASN:HB2	1:B:148:GLY:O	2.21	0.40
1:B:602:HIS:HB3	2:B:1000:FAD:C2	2.52	0.40
1:D:126:LEU:N	1:D:127:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	611/649 (94%)	591 (97%)	20 (3%)	0	100	100
1	B	601/649 (93%)	573 (95%)	27 (4%)	1 (0%)	43	70
1	C	613/649 (94%)	584 (95%)	26 (4%)	3 (0%)	24	52
1	D	599/649 (92%)	570 (95%)	27 (4%)	2 (0%)	36	63
All	All	2424/2596 (93%)	2318 (96%)	100 (4%)	6 (0%)	43	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	5	GLU
1	C	47	PRO
1	D	4	PRO
1	C	46	ASP
1	C	59	VAL
1	B	634	PRO

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	506/544 (93%)	466 (92%)	40 (8%)	11	37
1	B	489/544 (90%)	450 (92%)	39 (8%)	11	36
1	C	498/544 (92%)	455 (91%)	43 (9%)	10	33
1	D	488/544 (90%)	438 (90%)	50 (10%)	7	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1981/2176 (91%)	1809 (91%)	172 (9%)	9 32

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	44	ARG
1	A	75	MET
1	A	78	SER
1	A	140	ASN
1	A	161	VAL
1	A	178	ASP
1	A	185	THR
1	A	221	LEU
1	A	233	LEU
1	A	237	ASN
1	A	243	VAL
1	A	248	SER
1	A	260	VAL
1	A	273	LEU
1	A	319	ARG
1	A	327	LEU
1	A	337	THR
1	A	345	TRP
1	A	368	THR
1	A	370	GLU
1	A	372	LEU
1	A	378	GLU
1	A	389	ASP
1	A	421	GLN
1	A	468	GLU
1	A	498	ILE
1	A	500	ILE
1	A	501	LYS
1	A	504	LYS
1	A	512	THR
1	A	517	MET
1	A	521	HIS
1	A	530	SER
1	A	532	VAL
1	A	539	THR
1	A	576	ASP

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Mol	Chain	Res	Type
1	A	590	VAL
1	A	628	LEU
1	A	633	VAL
1	B	34	VAL
1	B	35	MET
1	B	59	VAL
1	B	69	THR
1	B	92	ILE
1	B	140	ASN
1	B	161	VAL
1	B	166	LEU
1	B	178	ASP
1	B	180	ILE
1	B	221	LEU
1	B	224	ARG
1	B	233	LEU
1	B	237	ASN
1	B	243	VAL
1	B	273	LEU
1	B	289	LEU
1	B	322	ASN
1	B	325	GLU
1	B	336	ASP
1	B	337	THR
1	B	368	THR
1	B	370	GLU
1	B	372	LEU
1	B	378	GLU
1	B	385	ARG
1	B	411	LEU
1	B	418	THR
1	B	421	GLN
1	B	441	VAL
1	B	498	ILE
1	B	500	ILE
1	B	532	VAL
1	B	537	LYS
1	B	541	GLU
1	B	555	GLU
1	B	557	THR
1	B	567	LYS
1	B	590	VAL

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Mol	Chain	Res	Type
1	C	34	VAL
1	C	44	ARG
1	C	65	ASN
1	C	89	CYS
1	C	121	THR
1	C	140	ASN
1	C	147	ASP
1	C	153	SER
1	C	159	LEU
1	C	184	LYS
1	C	192	TRP
1	C	198	ARG
1	C	204	SER
1	C	233	LEU
1	C	237	ASN
1	C	243	VAL
1	C	251	ARG
1	C	260	VAL
1	C	289	LEU
1	C	307	GLU
1	C	317	ILE
1	C	327	LEU
1	C	331	LEU
1	C	332	ARG
1	C	372	LEU
1	C	378	GLU
1	C	418	THR
1	C	421	GLN
1	C	477	ARG
1	C	501	LYS
1	C	505	GLU
1	C	509	ASN
1	C	512	THR
1	C	515	ILE
1	C	531	LYS
1	C	534	GLU
1	C	537	LYS
1	C	539	THR
1	C	540	LYS
1	C	557	THR
1	C	616	ASP
1	C	620	GLU

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Mol	Chain	Res	Type
1	C	638	VAL
1	D	3	HIS
1	D	24	ARG
1	D	33	LYS
1	D	34	VAL
1	D	44	ARG
1	D	161	VAL
1	D	166	LEU
1	D	170	HIS
1	D	180	ILE
1	D	181	GLN
1	D	185	THR
1	D	205	ASP
1	D	208	THR
1	D	219	SER
1	D	233	LEU
1	D	237	ASN
1	D	248	SER
1	D	251	ARG
1	D	258	THR
1	D	260	VAL
1	D	282	SER
1	D	289	LEU
1	D	293	LEU
1	D	307	GLU
1	D	325	GLU
1	D	327	LEU
1	D	331	LEU
1	D	336	ASP
1	D	372	LEU
1	D	384	ASP
1	D	385	ARG
1	D	407	ASP
1	D	411	LEU
1	D	415	LYS
1	D	418	THR
1	D	496	ARG
1	D	499	ASP
1	D	500	ILE
1	D	515	ILE
1	D	517	MET
1	D	524	SER

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Mol	Chain	Res	Type
1	D	525	GLU
1	D	555	GLU
1	D	557	THR
1	D	561	LEU
1	D	590	VAL
1	D	605	SER
1	D	616	ASP
1	D	627	ARG
1	D	628	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	181	GLN
1	A	309	GLN
1	A	322	ASN
1	A	380	ASN
1	A	533	HIS
1	A	553	HIS
1	B	218	GLN
1	B	553	HIS
1	C	212	HIS
1	C	322	ASN
1	C	380	ASN
1	C	421	GLN
1	C	452	ASN
1	C	553	HIS
1	D	309	GLN
1	D	311	HIS
1	D	553	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	C	1000	-	58,58,58	2.69	18 (31%)	85,89,89	1.98	19 (22%)
2	FAD	A	1000	-	58,58,58	2.82	17 (29%)	85,89,89	2.20	26 (30%)
2	FAD	D	1000	-	58,58,58	2.70	19 (32%)	85,89,89	2.07	22 (25%)
2	FAD	B	1000	-	58,58,58	2.73	18 (31%)	85,89,89	2.20	23 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	1000	-	-	12/34/50/50	0/6/6/6
2	FAD	A	1000	-	-	8/34/50/50	0/6/6/6
2	FAD	D	1000	-	-	9/34/50/50	0/6/6/6
2	FAD	B	1000	-	-	8/34/50/50	0/6/6/6

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	FAD	O4B-C1B	8.42	1.61	1.42
2	A	1000	FAD	C2B-C1B	-8.38	1.27	1.53
2	B	1000	FAD	O4B-C1B	8.36	1.61	1.42
2	B	1000	FAD	C2B-C1B	-8.31	1.27	1.53
2	D	1000	FAD	O4B-C1B	8.19	1.60	1.42
2	C	1000	FAD	O4B-C1B	8.02	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1000	FAD	C2B-C1B	-8.00	1.28	1.53
2	C	1000	FAD	C2B-C1B	-7.89	1.28	1.53
2	D	1000	FAD	O4B-C4B	-7.18	1.29	1.45
2	B	1000	FAD	O4B-C4B	-6.90	1.29	1.45
2	A	1000	FAD	O4B-C4B	-6.79	1.29	1.45
2	C	1000	FAD	O4B-C4B	-6.57	1.30	1.45
2	D	1000	FAD	C4X-N5	5.73	1.43	1.30
2	C	1000	FAD	C4X-N5	5.67	1.43	1.30
2	C	1000	FAD	C10-N1	5.59	1.44	1.33
2	A	1000	FAD	C10-N1	5.59	1.44	1.33
2	A	1000	FAD	C4X-N5	5.51	1.42	1.30
2	B	1000	FAD	C4X-N5	5.40	1.42	1.30
2	B	1000	FAD	C10-N1	5.27	1.43	1.33
2	D	1000	FAD	C10-N1	5.09	1.43	1.33
2	A	1000	FAD	C2-N1	4.97	1.47	1.36
2	A	1000	FAD	C9A-N10	4.87	1.49	1.41
2	A	1000	FAD	O3B-C3B	-4.83	1.31	1.43
2	B	1000	FAD	O3B-C3B	-4.77	1.31	1.43
2	D	1000	FAD	O3B-C3B	-4.51	1.31	1.43
2	C	1000	FAD	C2-N1	4.45	1.46	1.36
2	B	1000	FAD	C2-N1	4.25	1.46	1.36
2	C	1000	FAD	O3B-C3B	-4.23	1.32	1.43
2	D	1000	FAD	C2-N1	4.18	1.46	1.36
2	C	1000	FAD	C9A-N10	4.15	1.48	1.41
2	D	1000	FAD	C9A-N10	4.15	1.48	1.41
2	C	1000	FAD	C2-N3	4.12	1.48	1.39
2	B	1000	FAD	C9A-N10	4.07	1.48	1.41
2	B	1000	FAD	C2-N3	4.02	1.47	1.39
2	D	1000	FAD	C2-N3	3.94	1.47	1.39
2	D	1000	FAD	C6A-N6A	3.88	1.44	1.34
2	C	1000	FAD	C6A-N6A	3.83	1.44	1.34
2	A	1000	FAD	C2-N3	3.82	1.47	1.39
2	B	1000	FAD	C6A-N6A	3.81	1.43	1.34
2	D	1000	FAD	C5X-N5	3.66	1.46	1.39
2	B	1000	FAD	C5X-N5	3.50	1.45	1.39
2	A	1000	FAD	C6A-N6A	3.37	1.42	1.34
2	A	1000	FAD	C5A-C4A	-3.31	1.33	1.39
2	C	1000	FAD	C5X-N5	3.30	1.45	1.39
2	B	1000	FAD	C5A-C4A	-3.28	1.33	1.39
2	A	1000	FAD	C5X-N5	3.13	1.45	1.39
2	A	1000	FAD	C4'-C3'	-3.08	1.48	1.53
2	A	1000	FAD	O2'-C2'	-3.07	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	FAD	O2'-C2'	-3.06	1.36	1.43
2	C	1000	FAD	O2B-C2B	3.02	1.50	1.43
2	A	1000	FAD	O2B-C2B	2.93	1.50	1.43
2	A	1000	FAD	C5A-N7A	-2.86	1.33	1.39
2	B	1000	FAD	O2'-C2'	-2.78	1.37	1.43
2	D	1000	FAD	O2B-C2B	2.77	1.49	1.43
2	C	1000	FAD	C5A-C4A	-2.73	1.34	1.39
2	D	1000	FAD	O2'-C2'	-2.69	1.37	1.43
2	C	1000	FAD	C4-N3	2.67	1.43	1.38
2	D	1000	FAD	C5A-C4A	-2.65	1.34	1.39
2	B	1000	FAD	C5A-N7A	-2.50	1.34	1.39
2	D	1000	FAD	C4-N3	2.38	1.43	1.38
2	B	1000	FAD	O2B-C2B	2.38	1.48	1.43
2	C	1000	FAD	C5A-N7A	-2.26	1.35	1.39
2	B	1000	FAD	C4'-C3'	-2.23	1.49	1.53
2	D	1000	FAD	C8A-N9A	-2.23	1.33	1.37
2	C	1000	FAD	C8A-N9A	-2.21	1.33	1.37
2	D	1000	FAD	C2A-N1A	2.20	1.37	1.33
2	B	1000	FAD	C8A-N9A	-2.17	1.33	1.37
2	C	1000	FAD	C8A-N7A	2.13	1.35	1.31
2	B	1000	FAD	C4-N3	2.05	1.42	1.38
2	D	1000	FAD	C5A-N7A	-2.04	1.35	1.39
2	A	1000	FAD	C8A-N7A	2.03	1.35	1.31
2	D	1000	FAD	C8A-N7A	2.02	1.35	1.31

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	FAD	C7M-C7-C6	-7.03	107.18	119.57
2	C	1000	FAD	N6A-C6A-N1A	-6.46	103.98	118.38
2	A	1000	FAD	N6A-C6A-N1A	-6.19	104.59	118.38
2	B	1000	FAD	N6A-C6A-N1A	-6.14	104.70	118.38
2	D	1000	FAD	N6A-C6A-N1A	-6.14	104.71	118.38
2	A	1000	FAD	C7M-C7-C6	-6.04	108.94	119.57
2	B	1000	FAD	C7M-C7-C8	5.90	132.81	120.76
2	B	1000	FAD	N3A-C2A-N1A	-5.85	119.73	128.58
2	D	1000	FAD	C7M-C7-C6	-5.84	109.29	119.57
2	A	1000	FAD	N3A-C2A-N1A	-5.82	119.77	128.58
2	D	1000	FAD	N3A-C2A-N1A	-5.62	120.07	128.58
2	C	1000	FAD	N3A-C2A-N1A	-5.35	120.48	128.58
2	A	1000	FAD	C5A-C4A-N3A	-5.33	119.38	126.72
2	C	1000	FAD	C7M-C7-C6	-5.29	110.25	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	FAD	C5A-C4A-N3A	-5.28	119.44	126.72
2	C	1000	FAD	C5A-C4A-N3A	-5.23	119.52	126.72
2	D	1000	FAD	C5A-C6A-N6A	5.19	136.13	123.29
2	C	1000	FAD	C5A-C6A-N6A	5.13	135.98	123.29
2	B	1000	FAD	C5A-C6A-N6A	5.03	135.74	123.29
2	A	1000	FAD	C7M-C7-C8	4.86	130.68	120.76
2	A	1000	FAD	C4'-C3'-C2'	-4.77	105.63	113.57
2	A	1000	FAD	C5A-C6A-N6A	4.77	135.10	123.29
2	D	1000	FAD	C7M-C7-C8	4.56	130.08	120.76
2	D	1000	FAD	N9A-C8A-N7A	-4.56	107.47	113.94
2	B	1000	FAD	N9A-C8A-N7A	-4.51	107.53	113.94
2	D	1000	FAD	C5A-C4A-N3A	-4.50	120.53	126.72
2	C	1000	FAD	C7M-C7-C8	4.14	129.21	120.76
2	C	1000	FAD	N9A-C8A-N7A	-4.02	108.23	113.94
2	A	1000	FAD	C4-N3-C2	-3.84	118.83	125.64
2	A	1000	FAD	N9A-C8A-N7A	-3.79	108.56	113.94
2	B	1000	FAD	C4'-C3'-C2'	-3.77	107.30	113.57
2	D	1000	FAD	C4-N3-C2	-3.62	119.21	125.64
2	B	1000	FAD	C4-N3-C2	-3.55	119.34	125.64
2	A	1000	FAD	C2A-N3A-C4A	3.52	120.42	111.83
2	B	1000	FAD	C2A-N3A-C4A	3.52	120.42	111.83
2	B	1000	FAD	N3A-C4A-N9A	3.43	133.00	127.17
2	C	1000	FAD	C2A-N3A-C4A	3.37	120.07	111.83
2	A	1000	FAD	O4B-C1B-C2B	-3.33	99.48	106.62
2	C	1000	FAD	N3A-C4A-N9A	3.33	132.83	127.17
2	A	1000	FAD	N3A-C4A-N9A	3.20	132.62	127.17
2	C	1000	FAD	C4-N3-C2	-3.15	120.05	125.64
2	D	1000	FAD	C4A-N9A-C8A	3.14	109.04	105.74
2	A	1000	FAD	C4X-C4-N3	3.14	121.25	113.25
2	B	1000	FAD	O4-C4-C4X	-3.11	118.33	126.53
2	D	1000	FAD	C2A-N3A-C4A	3.11	119.42	111.83
2	D	1000	FAD	N3A-C4A-N9A	3.07	132.39	127.17
2	A	1000	FAD	C2B-C1B-N9A	-3.05	105.72	113.30
2	A	1000	FAD	O4-C4-C4X	-2.99	118.64	126.53
2	A	1000	FAD	C5'-C4'-C3'	-2.98	106.59	112.22
2	B	1000	FAD	C5A-N7A-C8A	2.98	108.13	103.45
2	D	1000	FAD	C5A-N7A-C8A	2.86	107.95	103.45
2	A	1000	FAD	C9A-C5X-N5	-2.76	119.52	122.45
2	D	1000	FAD	C10-C4X-N5	-2.70	119.30	124.81
2	D	1000	FAD	C1'-C2'-C3'	-2.68	102.40	109.66
2	D	1000	FAD	C4X-C4-N3	2.67	120.06	113.25
2	B	1000	FAD	C1'-C2'-C3'	-2.66	102.44	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1000	FAD	C4X-C10-N10	2.64	120.26	116.48
2	A	1000	FAD	O4B-C1B-N9A	2.64	113.15	108.09
2	A	1000	FAD	C5X-C9A-N10	2.63	120.34	117.97
2	B	1000	FAD	O4B-C1B-C2B	-2.60	101.05	106.62
2	B	1000	FAD	C5X-C9A-N10	2.60	120.32	117.97
2	B	1000	FAD	C4X-C4-N3	2.57	119.80	113.25
2	B	1000	FAD	C6A-C5A-C4A	2.57	120.69	117.18
2	C	1000	FAD	C4X-C4-N3	2.55	119.74	113.25
2	C	1000	FAD	C5A-N7A-C8A	2.55	107.45	103.45
2	C	1000	FAD	O4-C4-C4X	-2.47	120.02	126.53
2	A	1000	FAD	C6A-C5A-C4A	2.46	120.54	117.18
2	D	1000	FAD	O4'-C4'-C5'	-2.45	104.59	109.99
2	B	1000	FAD	C4-C4X-C10	2.43	121.10	116.93
2	B	1000	FAD	C4A-N9A-C8A	2.42	108.28	105.74
2	B	1000	FAD	C9A-C5X-N5	-2.38	119.93	122.45
2	D	1000	FAD	C5B-C4B-C3B	-2.36	106.72	115.21
2	C	1000	FAD	C5X-C9A-N10	2.34	120.08	117.97
2	C	1000	FAD	C2B-C1B-N9A	-2.33	107.52	113.30
2	D	1000	FAD	C9A-C5X-N5	-2.28	120.04	122.45
2	C	1000	FAD	C6A-C5A-C4A	2.27	120.28	117.18
2	D	1000	FAD	O4-C4-C4X	-2.26	120.57	126.53
2	C	1000	FAD	C4A-N9A-C8A	2.26	108.11	105.74
2	A	1000	FAD	C4X-C10-N1	-2.26	119.06	124.59
2	D	1000	FAD	C6A-C5A-C4A	2.25	120.25	117.18
2	A	1000	FAD	C5A-N7A-C8A	2.24	106.97	103.45
2	C	1000	FAD	C9A-C5X-N5	-2.20	120.12	122.45
2	A	1000	FAD	O3B-C3B-C4B	-2.14	104.93	111.08
2	C	1000	FAD	C10-C4X-N5	-2.14	120.44	124.81
2	A	1000	FAD	C5B-C4B-C3B	-2.11	107.62	115.21
2	A	1000	FAD	C4-C4X-C10	2.11	120.55	116.93
2	D	1000	FAD	O5'-C5'-C4'	-2.07	103.83	109.36
2	B	1000	FAD	C4X-C10-N10	2.03	119.39	116.48
2	B	1000	FAD	C4X-C10-N1	-2.03	119.61	124.59
2	A	1000	FAD	C5A-C4A-N9A	2.01	108.00	105.81

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	FAD	C5B-O5B-PA-O1A
2	A	1000	FAD	C5B-O5B-PA-O2A
2	A	1000	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	A	1000	FAD	O4'-C4'-C5'-O5'
2	B	1000	FAD	C5B-O5B-PA-O1A
2	B	1000	FAD	C5B-O5B-PA-O3P
2	B	1000	FAD	O4'-C4'-C5'-O5'
2	C	1000	FAD	C5B-O5B-PA-O1A
2	C	1000	FAD	C5B-O5B-PA-O2A
2	C	1000	FAD	C5B-O5B-PA-O3P
2	C	1000	FAD	O4'-C4'-C5'-O5'
2	C	1000	FAD	C5'-O5'-P-O1P
2	C	1000	FAD	C5'-O5'-P-O2P
2	C	1000	FAD	C5'-O5'-P-O3P
2	D	1000	FAD	N10-C1'-C2'-O2'
2	D	1000	FAD	C2'-C3'-C4'-O4'
2	D	1000	FAD	O3'-C3'-C4'-O4'
2	D	1000	FAD	C5'-O5'-P-O2P
2	D	1000	FAD	C5'-O5'-P-O3P
2	A	1000	FAD	C3B-C4B-C5B-O5B
2	D	1000	FAD	O3'-C3'-C4'-C5'
2	D	1000	FAD	C2'-C3'-C4'-C5'
2	A	1000	FAD	O4B-C4B-C5B-O5B
2	B	1000	FAD	O4B-C4B-C5B-O5B
2	C	1000	FAD	O4B-C4B-C5B-O5B
2	B	1000	FAD	C3B-C4B-C5B-O5B
2	C	1000	FAD	C3B-C4B-C5B-O5B
2	A	1000	FAD	C3'-C4'-C5'-O5'
2	B	1000	FAD	C3'-C4'-C5'-O5'
2	C	1000	FAD	C3'-C4'-C5'-O5'
2	A	1000	FAD	C2B-C1B-N9A-C8A
2	D	1000	FAD	N10-C1'-C2'-C3'
2	B	1000	FAD	C5B-O5B-PA-O2A
2	D	1000	FAD	C5'-O5'-P-O1P
2	C	1000	FAD	O2'-C2'-C3'-O3'
2	C	1000	FAD	O2'-C2'-C3'-C4'
2	B	1000	FAD	C2B-C1B-N9A-C8A

There are no ring outliers.

4 monomers are involved in 10 short contacts:

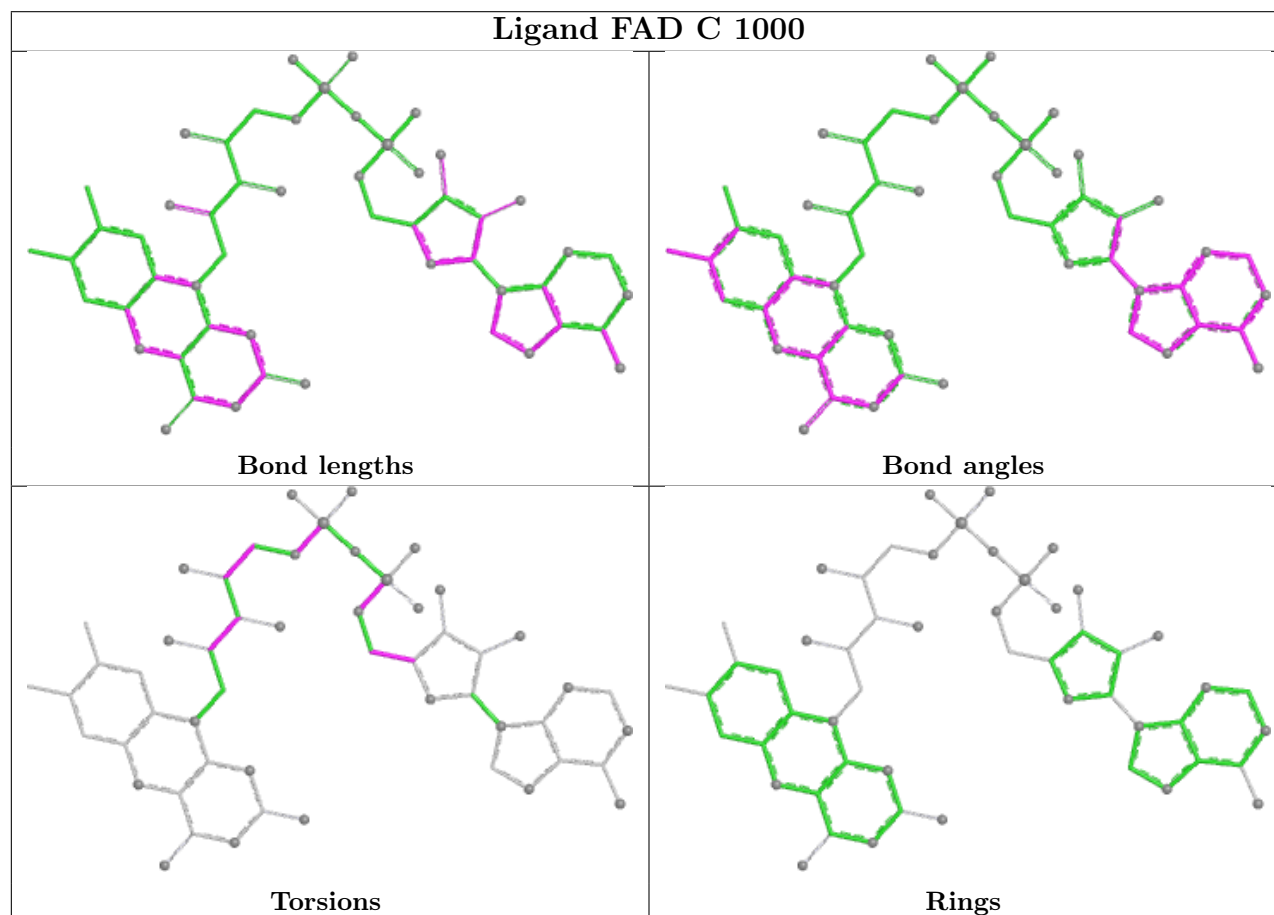
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1000	FAD	1	0
2	A	1000	FAD	3	0
2	D	1000	FAD	4	0

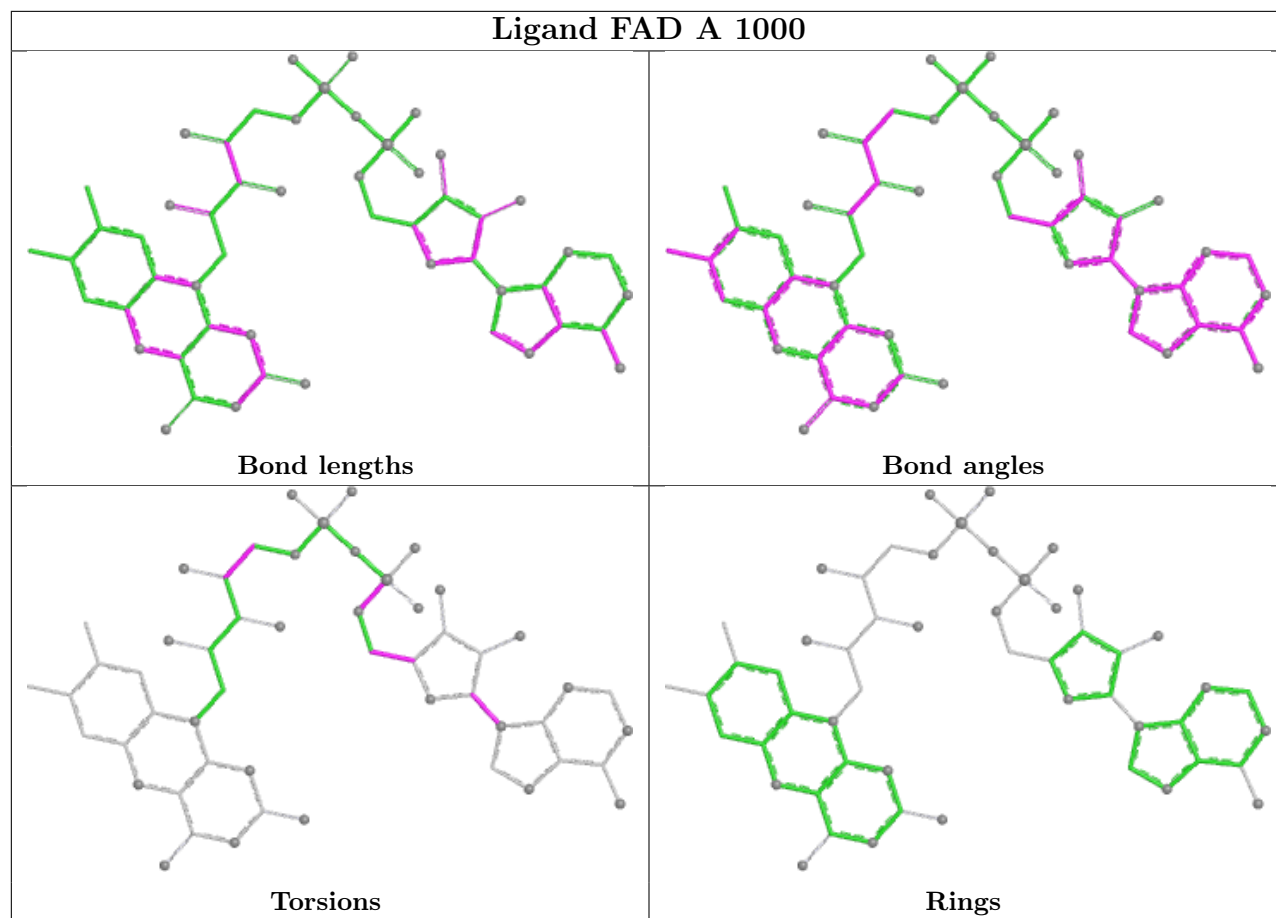
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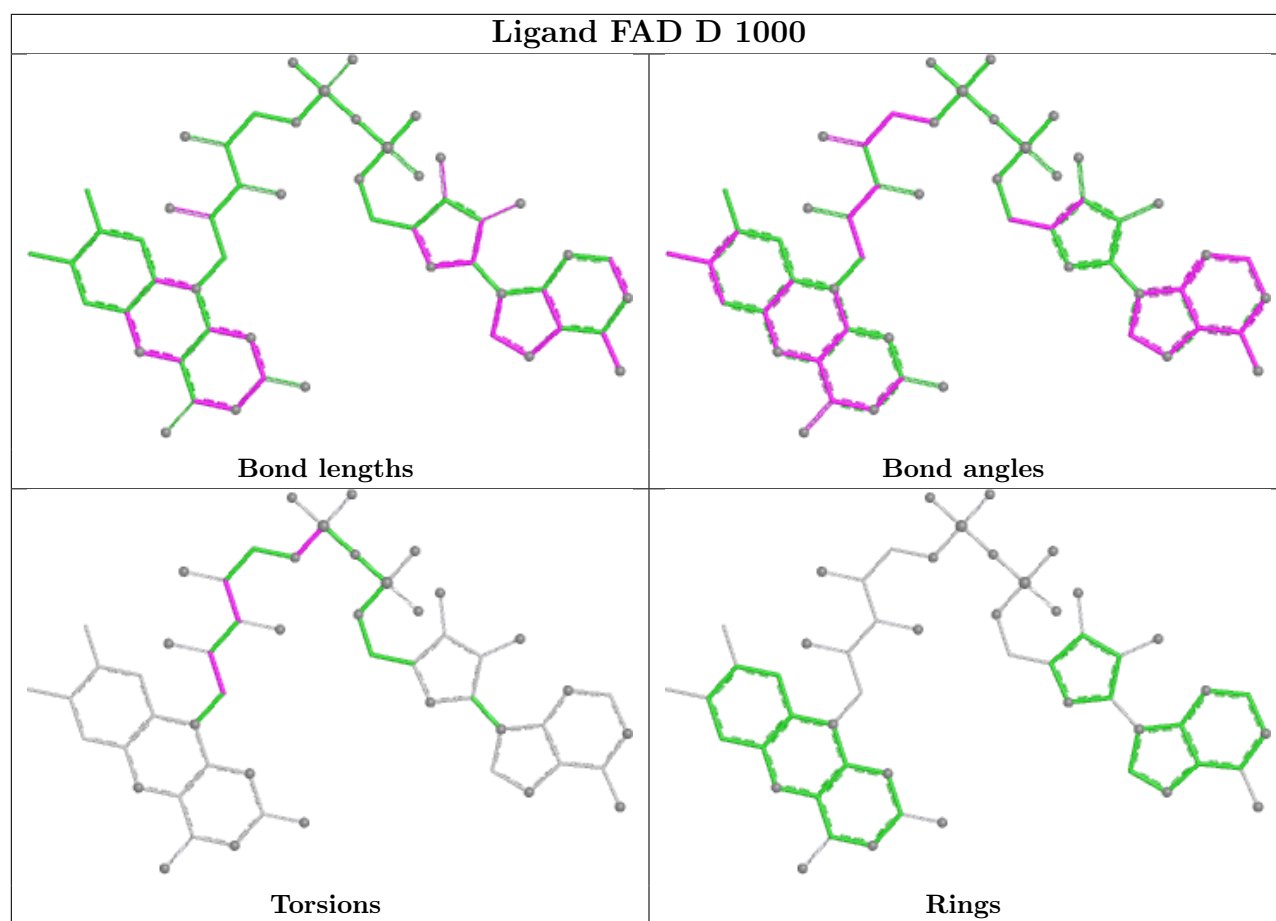
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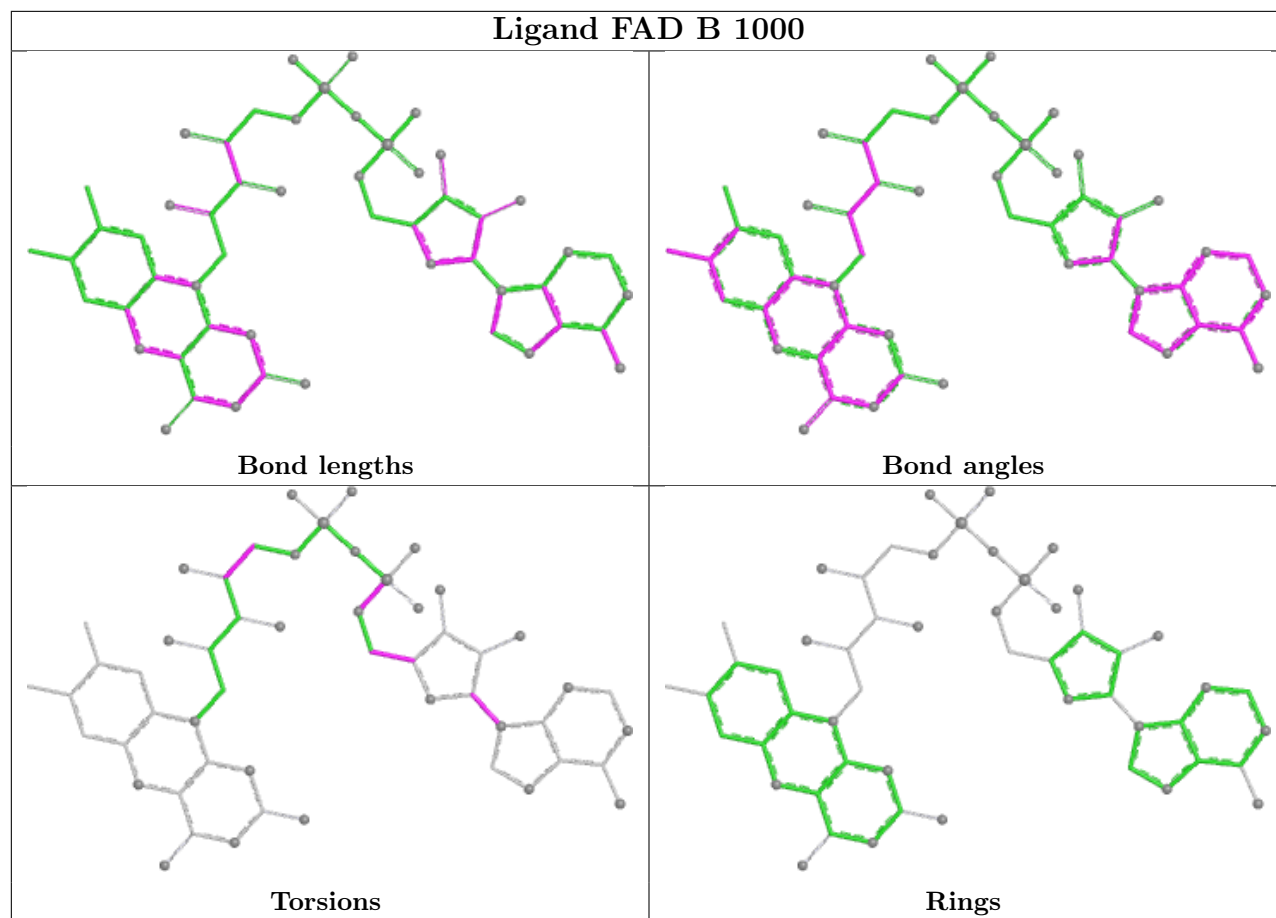
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	FAD	2	0

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	615/649 (94%)	-0.19	7 (1%) 78 65	23, 33, 52, 72	0
1	B	607/649 (93%)	-0.12	8 (1%) 75 61	23, 36, 70, 104	0
1	C	619/649 (95%)	-0.00	17 (2%) 56 41	29, 41, 65, 109	0
1	D	609/649 (93%)	0.09	10 (1%) 70 55	37, 55, 72, 121	0
All	All	2450/2596 (94%)	-0.06	42 (1%) 69 53	23, 41, 67, 121	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	637	PRO	4.5
1	A	636	ALA	4.4
1	B	61	ASN	3.8
1	B	59	VAL	3.8
1	C	638	VAL	3.6
1	D	338	GLN	3.4
1	C	47	PRO	3.3
1	C	639	PRO	3.1
1	C	58	ASN	3.1
1	D	350	ASN	3.0
1	C	56	VAL	3.0
1	A	518	GLY	3.0
1	C	518	GLY	3.0
1	B	530	SER	2.9
1	C	62	ASP	2.9
1	C	636	ALA	2.8
1	D	355	SER	2.8
1	C	643	PRO	2.7
1	B	322	ASN	2.7
1	D	349	PRO	2.7
1	C	64	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	642	LYS	2.6
1	C	45	ASP	2.6
1	C	338	GLN	2.6
1	D	354	LEU	2.6
1	A	336	ASP	2.5
1	C	516	HIS	2.4
1	A	65	ASN	2.4
1	B	527	PHE	2.4
1	B	47	PRO	2.4
1	B	46	ASP	2.3
1	B	62	ASP	2.3
1	D	184	LYS	2.3
1	C	205	ASP	2.3
1	D	3	HIS	2.2
1	A	520	TRP	2.2
1	D	527	PHE	2.1
1	D	205	ASP	2.1
1	C	374	GLU	2.1
1	D	341	LEU	2.0
1	C	61	ASN	2.0
1	A	45	ASP	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.

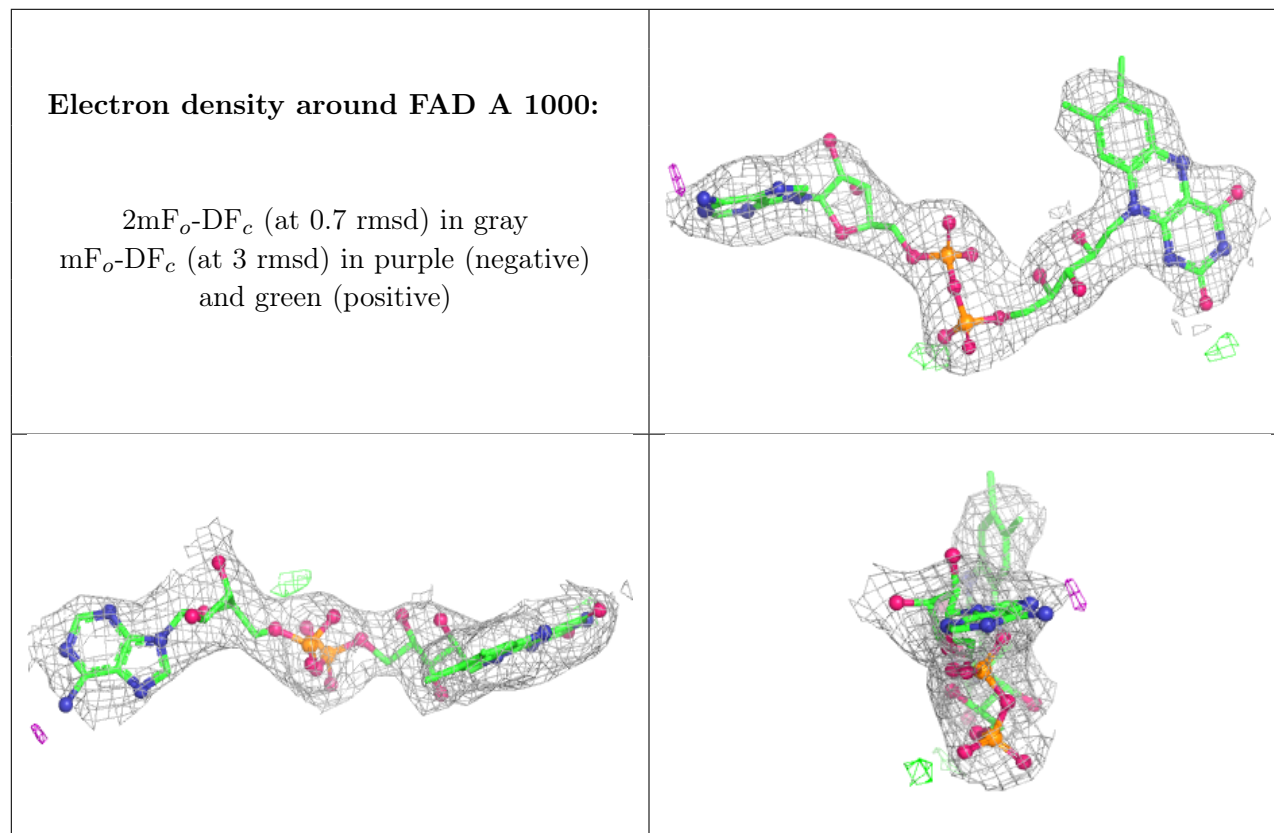
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	1000	53/53	0.95	0.10	31,31,31,31	0
2	FAD	B	1000	53/53	0.95	0.15	58,58,58,58	0

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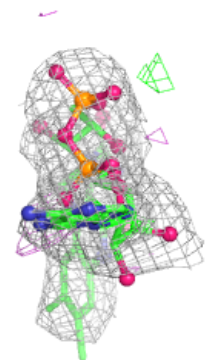
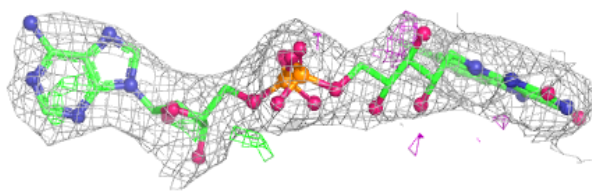
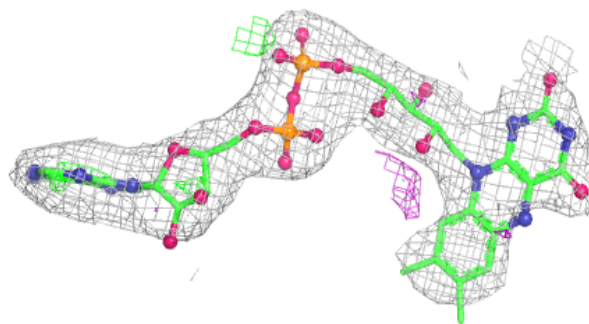
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	C	1000	53/53	0.95	0.09	25,25,25,25	0
2	FAD	D	1000	53/53	0.95	0.09	31,31,31,31	0

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.

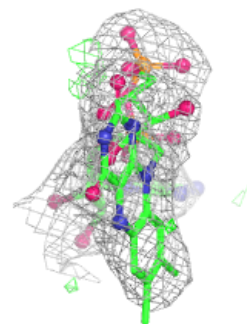
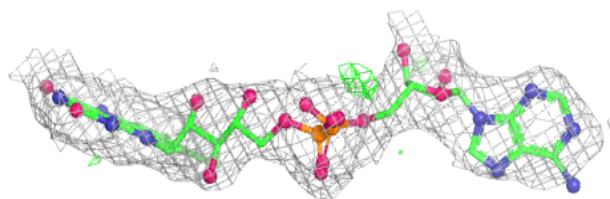
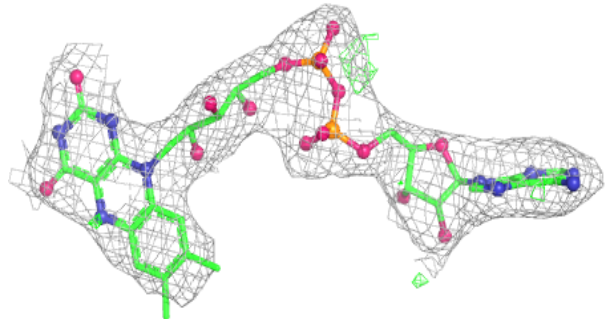


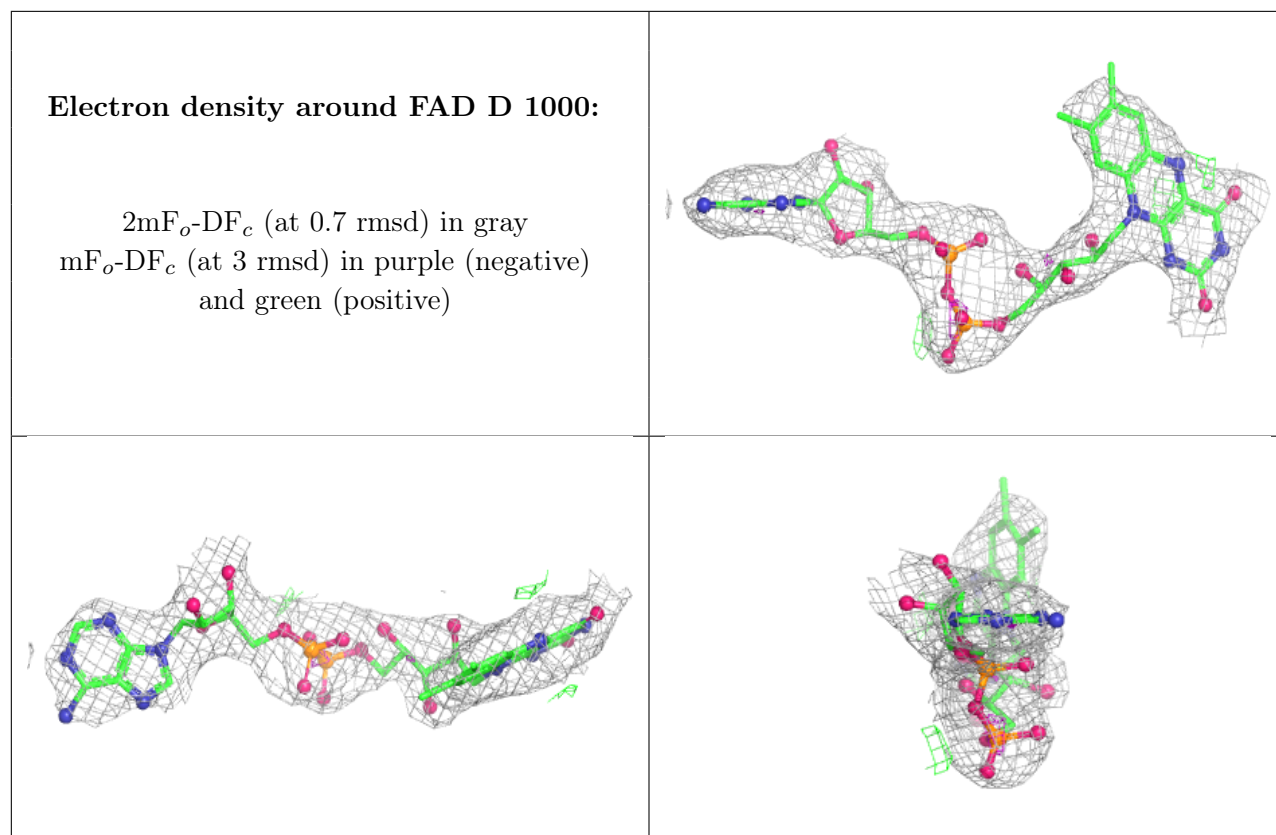
Electron density around FAD B 1000:

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

**Electron density around FAD C 1000:**

$2mF_o-DF_c$ (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.