



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:41 AM UTC

PDB ID : 3NTD / pdb_00003ntd
Title : Structure of the Shewanella loihica PV-4 NADH-dependent persulfide reductase C531S Mutant
Authors : Sazinsky, M.H.; Warner, M.D.; Lukose, V.; Lee, K.H.; Crane, E.J.
Deposited on : 2010-07-03
Resolution : 1.99 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

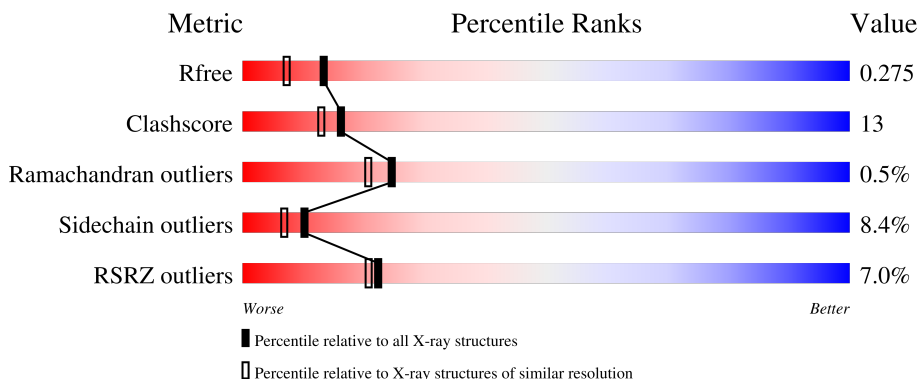
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	565	8% 71% 24% • •
1	B	565	6% 68% 27% 5% •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9400 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.

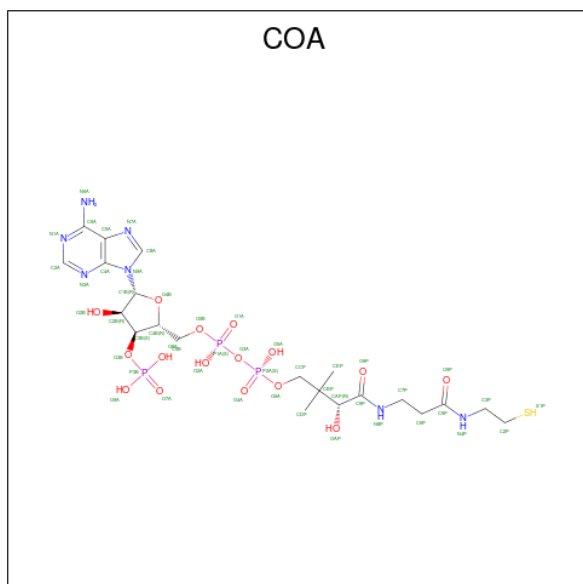
- Molecule 1 is a protein called FAD-dependent pyridine nucleotide-disulphide oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4295	2694	762	820	19			
1	B	565	Total	C	N	O	S	0	0	0
			4294	2694	763	819	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	SER	CYS	engineered mutation	UNP A3QAV3
B	531	SER	CYS	engineered mutation	UNP A3QAV3

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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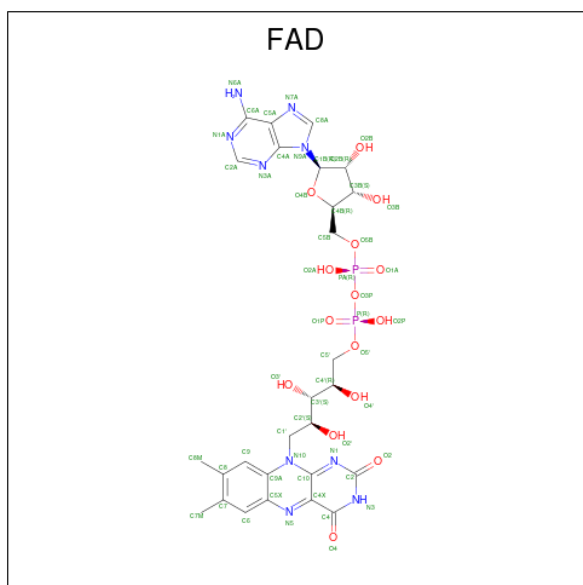
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	300	Total	O	0	0
			300	300		
5	B	307	Total	O	0	0
			307	307		

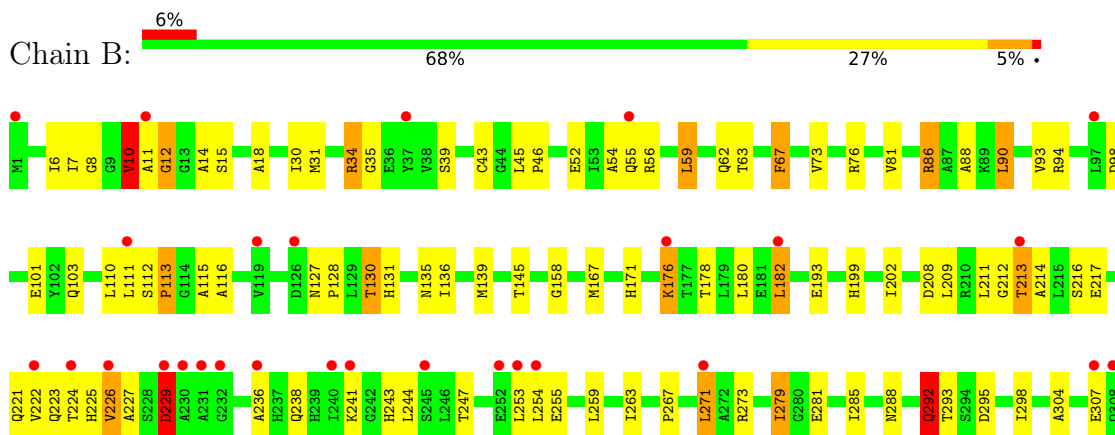
3 Residue-property plots

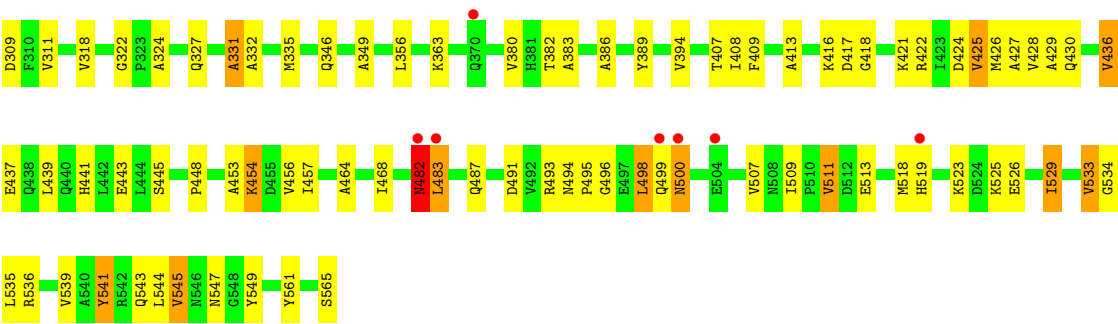
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: FAD-dependent pyridine nucleotide-disulphide oxidoreductase



- Molecule 1: FAD-dependent pyridine nucleotide-disulphide oxidoreductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	133.74Å 133.74Å 79.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	115.85 – 1.99 115.82 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (115.85-1.99) 99.9 (115.82-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.158 , 0.185 0.239 , 0.275	Depositor DCC
R_{free} test set	5561 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.026 for H, K, L 0.323 for K, H, -L 0.651 for -h,-k,l	Depositor
Outliers	0 of 109330 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9400	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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, CL, COA

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	1.65	42/4365 (1.0%)	1.39	26/5910 (0.4%)
1	B	1.72	51/4364 (1.2%)	1.46	28/5908 (0.5%)
All	All	1.68	93/8729 (1.1%)	1.43	54/11818 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	453	ALA	CA-CB	9.29	1.67	1.53
1	A	394	VAL	CA-CB	8.76	1.64	1.54
1	A	353	VAL	CA-CB	8.27	1.62	1.53
1	B	30	ILE	C-N	-7.97	1.23	1.33
1	A	518	MET	SD-CE	-7.88	1.59	1.79
1	B	331	ALA	CA-CB	7.27	1.64	1.53
1	B	394	VAL	CA-CB	7.17	1.62	1.54
1	A	69	ALA	CA-CB	-7.13	1.42	1.53
1	B	429	ALA	CA-CB	6.97	1.64	1.53
1	A	321	ALA	CA-CB	6.84	1.64	1.53
1	A	292	GLN	CB-CG	-6.81	1.32	1.52
1	A	429	ALA	N-CA	6.74	1.54	1.46
1	A	474	PRO	CA-C	6.72	1.59	1.52
1	B	324	ALA	CA-C	6.67	1.61	1.52
1	B	386	ALA	CA-CB	6.46	1.64	1.53
1	A	542	ARG	N-CA	-6.39	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	539	VAL	CA-C	6.35	1.60	1.52
1	A	92	THR	CA-CB	6.33	1.63	1.53
1	B	424	ASP	N-CA	6.31	1.53	1.46
1	B	226	VAL	C-O	-6.28	1.17	1.24
1	A	158	GLY	CA-C	6.27	1.56	1.52
1	B	533	VAL	N-CA	6.22	1.54	1.46
1	B	332	ALA	CA-CB	6.22	1.63	1.53
1	A	301	VAL	CA-C	6.15	1.59	1.52
1	B	263	ILE	CA-CB	6.15	1.61	1.54
1	A	554	LEU	C-O	-6.15	1.16	1.23
1	B	436	VAL	CA-CB	6.13	1.61	1.54
1	A	332	ALA	N-CA	6.10	1.53	1.46
1	B	425	VAL	CA-CB	6.10	1.61	1.54
1	B	417	ASP	N-CA	6.03	1.53	1.46
1	A	560	THR	C-O	5.98	1.30	1.24
1	B	229	ASP	CA-C	-5.97	1.45	1.52
1	A	559	ARG	N-CA	5.92	1.53	1.46
1	B	349	ALA	CA-CB	5.90	1.65	1.54
1	A	461	ALA	C-O	-5.86	1.17	1.24
1	B	456	VAL	N-CA	5.85	1.53	1.46
1	B	18	ALA	CA-CB	5.82	1.62	1.53
1	B	541	TYR	C-O	5.79	1.30	1.24
1	A	419	ILE	N-CA	5.78	1.53	1.46
1	B	543	GLN	C-O	-5.77	1.17	1.24
1	A	472	ALA	CA-CB	5.76	1.64	1.53
1	B	318	VAL	CA-CB	5.76	1.61	1.54
1	A	105	SER	C-O	5.75	1.31	1.23
1	A	331	ALA	CA-CB	5.74	1.62	1.53
1	B	426	MET	N-CA	5.72	1.53	1.46
1	B	383	ALA	CA-C	5.71	1.60	1.52
1	B	436	VAL	N-CA	-5.60	1.40	1.46
1	B	382	THR	N-CA	5.59	1.52	1.46
1	A	379	TYR	C-O	5.59	1.31	1.24
1	A	69	ALA	C-O	5.57	1.30	1.24
1	B	536	ARG	CA-C	5.55	1.60	1.52
1	A	533	VAL	CA-CB	5.52	1.60	1.54
1	B	59	LEU	CA-C	5.52	1.60	1.52
1	A	413	ALA	CA-C	-5.51	1.45	1.52
1	A	417	ASP	C-O	5.51	1.30	1.23
1	A	456	VAL	N-CA	5.50	1.53	1.46
1	B	208	ASP	CA-CB	5.49	1.59	1.52
1	B	10	VAL	CA-CB	5.48	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	ALA	CA-CB	5.47	1.63	1.53
1	A	561	TYR	C-O	-5.45	1.17	1.24
1	B	408	ILE	CA-CB	5.45	1.59	1.53
1	A	349	ALA	CA-CB	5.44	1.63	1.53
1	A	327	GLN	N-CA	5.40	1.52	1.46
1	A	333	ASP	N-CA	5.39	1.52	1.46
1	A	426	MET	N-CA	5.38	1.52	1.46
1	A	63	THR	N-CA	5.36	1.49	1.46
1	B	63	THR	C-O	5.35	1.31	1.24
1	B	322	GLY	N-CA	5.35	1.52	1.44
1	A	272	ALA	CA-CB	5.34	1.61	1.53
1	B	193	GLU	N-CA	5.31	1.53	1.46
1	A	333	ASP	C-O	5.31	1.30	1.24
1	B	115	ALA	CA-CB	-5.31	1.43	1.53
1	B	8	GLY	N-CA	5.29	1.53	1.45
1	B	46	PRO	N-CA	5.23	1.54	1.47
1	A	238	GLN	N-CA	-5.21	1.39	1.45
1	A	412	GLN	C-O	-5.19	1.17	1.23
1	B	394	VAL	C-O	5.18	1.29	1.24
1	A	365	GLU	C-O	5.18	1.30	1.24
1	B	12	GLY	N-CA	5.16	1.52	1.45
1	B	116	ALA	CA-CB	5.16	1.61	1.53
1	B	93	VAL	CA-C	-5.15	1.46	1.52
1	B	448	PRO	CA-C	5.13	1.56	1.52
1	B	443	GLU	C-O	5.11	1.29	1.23
1	B	199	HIS	N-CA	5.11	1.52	1.46
1	B	76	ARG	C-O	5.09	1.29	1.24
1	B	409	PHE	N-CA	5.08	1.52	1.46
1	A	457	ILE	CA-CB	5.08	1.60	1.54
1	A	523	LYS	CA-C	5.06	1.59	1.52
1	B	535	LEU	N-CA	5.05	1.52	1.46
1	B	135	ASN	CA-C	-5.04	1.46	1.53
1	B	113	PRO	CA-C	5.02	1.58	1.52
1	A	483	LEU	CA-C	5.01	1.59	1.52
1	B	46	PRO	CG-CD	5.00	1.67	1.50

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	511	VAL	CB-CA-C	-9.99	98.96	112.04
1	B	31	MET	O-C-N	-8.04	113.94	123.27
1	B	509	ILE	CA-C-N	-7.58	112.19	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	509	ILE	C-N-CA	-7.58	112.19	119.85
1	A	119	VAL	CA-C-N	-7.46	112.70	120.38
1	A	119	VAL	C-N-CA	-7.46	112.70	120.38
1	A	118	ILE	CA-C-N	-7.21	117.40	122.59
1	A	118	ILE	C-N-CA	-7.21	117.40	122.59
1	B	298	ILE	N-CA-C	6.83	117.68	108.11
1	A	485	GLU	CA-C-N	-6.74	112.45	122.83
1	A	485	GLU	C-N-CA	-6.74	112.45	122.83
1	A	311	VAL	N-CA-C	6.67	116.80	110.53
1	B	54	ALA	N-CA-C	6.66	118.54	111.28
1	A	327	GLN	N-CA-C	6.62	118.49	111.28
1	A	23	LEU	N-CA-C	6.40	119.25	111.82
1	A	448	PRO	N-CA-C	6.31	118.40	110.70
1	B	422	ARG	N-CA-C	6.27	118.12	111.28
1	B	511	VAL	N-CA-C	6.27	117.77	110.62
1	B	436	VAL	N-CA-CB	6.17	117.77	110.55
1	A	246	LEU	CA-C-N	-6.15	114.23	122.72
1	A	246	LEU	C-N-CA	-6.15	114.23	122.72
1	B	439	LEU	N-CA-C	6.11	119.57	111.75
1	A	344	GLY	N-CA-C	6.04	120.50	112.65
1	A	135	ASN	N-CA-C	6.03	117.74	109.18
1	A	475	ILE	CB-CA-C	-5.91	101.56	110.55
1	B	394	VAL	N-CA-C	5.81	116.56	109.30
1	B	464	ALA	N-CA-C	5.77	117.57	111.28
1	A	152	GLU	N-CA-C	-5.73	106.94	114.04
1	A	448	PRO	CA-C-N	-5.52	113.93	119.56
1	A	448	PRO	C-N-CA	-5.52	113.93	119.56
1	B	533	VAL	CA-CB-CG2	5.49	119.72	110.40
1	A	196	GLY	N-CA-C	-5.48	106.03	113.37
1	B	45	LEU	CA-C-N	-5.47	113.27	119.28
1	B	45	LEU	C-N-CA	-5.47	113.27	119.28
1	B	171	HIS	CA-C-O	5.42	126.48	120.63
1	A	266	ARG	N-CA-C	5.39	118.28	110.14
1	B	413	ALA	N-CA-C	5.37	117.93	108.75
1	B	292	GLN	CB-CA-C	5.34	118.56	109.75
1	B	15	SER	N-CA-C	-5.31	105.16	111.69
1	B	427	ALA	N-CA-C	-5.28	105.60	111.36
1	B	158	GLY	N-CA-C	-5.25	100.73	113.18
1	A	160	GLY	N-CA-C	-5.24	103.97	112.31
1	B	491	ASP	N-CA-C	-5.20	100.26	108.73
1	A	473	THR	CA-C-N	-5.18	115.01	120.66
1	A	473	THR	C-N-CA	-5.18	115.01	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	ARG	CB-CG-CD	-5.18	99.38	111.30
1	B	511	VAL	CG1-CB-CG2	5.18	122.19	110.80
1	A	70	ARG	N-CA-C	5.16	116.75	111.03
1	B	389	TYR	N-CA-C	-5.09	103.29	110.31
1	B	236	ALA	N-CA-C	5.08	117.71	111.82
1	A	482	ASN	N-CA-C	5.05	116.28	109.11
1	B	494	ASN	CA-C-N	5.01	124.61	119.05
1	B	494	ASN	C-N-CA	5.01	124.61	119.05
1	A	446	TYR	N-CA-C	5.01	116.78	108.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	474	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4295	0	4296	117	1
1	B	4294	0	4300	116	1
2	A	48	0	31	2	0
2	B	48	0	32	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	31	3	0
4	B	53	0	31	2	0
5	A	300	0	0	25	0
5	B	307	0	0	32	0
All	All	9400	0	8721	230	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (230) 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:229:ASP:HB3	5:B:745:HOH:O	1.41	1.18
1:B:500:ASN:HB3	5:B:803:HOH:O	1.46	1.16
1:A:266:ARG:HG3	1:A:266:ARG:HH11	1.11	1.11
1:A:474:PRO:CB	1:A:555:ILE:HD11	1.83	1.08
1:A:227:ALA:H	1:A:238:GLN:NE2	1.55	1.02
1:A:227:ALA:N	1:A:238:GLN:NE2	2.09	1.00
1:A:382:THR:HG23	1:A:456:VAL:HG22	1.44	1.00
1:A:266:ARG:HG3	1:A:266:ARG:NH1	1.68	0.99
1:A:437:GLU:HG2	5:A:618:HOH:O	1.62	0.98
1:B:55:GLN:HG2	5:B:878:HOH:O	1.65	0.96
1:A:290:MET:HE3	1:A:339:GLU:HA	1.44	0.95
1:B:223:GLN:HE21	1:B:225:HIS:H	1.09	0.94
1:B:346:GLN:HE21	1:B:430:GLN:HE21	1.09	0.93
1:A:85:ASP:HB3	5:A:733:HOH:O	1.67	0.92
1:A:1:MET:HB3	5:A:820:HOH:O	1.68	0.91
1:A:227:ALA:HB3	1:A:238:GLN:NE2	1.85	0.91
1:B:67:PHE:CD1	1:B:73:VAL:HG11	2.06	0.90
1:A:227:ALA:H	1:A:238:GLN:HE21	1.21	0.89
1:A:474:PRO:HB2	1:A:555:ILE:HD11	1.54	0.87
1:B:288:ASN:HD21	1:B:292:GLN:HE21	1.17	0.87
1:A:241:LYS:HE3	5:A:1106:HOH:O	1.73	0.86
1:A:418:GLY:HA2	5:A:1092:HOH:O	1.75	0.86
1:A:499:GLN:HB2	5:A:759:HOH:O	1.74	0.85
1:A:474:PRO:HB3	1:A:555:ILE:HD11	1.57	0.84
1:B:523:LYS:HE3	5:B:969:HOH:O	1.77	0.84
1:B:482:ASN:O	1:B:483:LEU:HB2	1.77	0.83
1:A:266:ARG:HH11	1:A:266:ARG:CG	1.90	0.82
1:A:241:LYS:HD3	5:A:1106:HOH:O	1.80	0.81
1:B:86:ARG:HD2	1:B:295:ASP:OD1	1.80	0.81
1:A:382:THR:HG21	1:A:456:VAL:HA	1.63	0.79
1:A:227:ALA:CB	1:A:238:GLN:HE21	1.96	0.79
5:A:814:HOH:O	1:B:441:HIS:HE1	1.66	0.78
1:B:223:GLN:NE2	1:B:225:HIS:H	1.80	0.78
1:B:243:HIS:HE1	1:B:255:GLU:HG3	1.49	0.78
1:B:127:ASN:OD1	1:B:130:THR:HG23	1.84	0.77
1:B:243:HIS:HE1	1:B:255:GLU:CG	1.98	0.77
5:A:814:HOH:O	1:B:441:HIS:CE1	2.36	0.77
1:A:227:ALA:N	1:A:238:GLN:HE22	1.82	0.77
1:A:227:ALA:CB	1:A:238:GLN:NE2	2.47	0.77
1:A:474:PRO:HB2	1:A:555:ILE:CD1	2.14	0.76
1:A:223:GLN:HE21	1:A:225:HIS:H	1.29	0.76
1:B:518:MET:HE1	1:B:547:ASN:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:O	1:B:213:THR:HG22	1.86	0.74
1:B:496:GLY:O	1:B:499:GLN:HB2	1.88	0.74
1:A:436:VAL:HG21	1:A:468:ILE:CD1	2.19	0.73
1:A:518:MET:HE3	1:A:544:LEU:HD23	1.71	0.73
1:B:518:MET:HE3	1:B:544:LEU:HD23	1.70	0.72
1:B:519:HIS:CD2	5:B:757:HOH:O	2.41	0.72
1:A:476:HIS:CE1	1:A:555:ILE:HD13	2.25	0.71
1:A:241:LYS:CE	5:A:1106:HOH:O	2.35	0.69
1:B:67:PHE:HD1	1:B:73:VAL:HG11	1.55	0.69
1:B:518:MET:HE1	1:B:547:ASN:CB	2.23	0.68
1:B:518:MET:HE2	1:B:549:TYR:HE1	1.58	0.68
1:B:67:PHE:CD1	1:B:73:VAL:CG1	2.77	0.68
1:A:227:ALA:CA	1:A:238:GLN:NE2	2.57	0.67
1:A:209:LEU:HD13	1:A:211:LEU:HD11	1.75	0.66
1:B:519:HIS:HE1	5:B:754:HOH:O	1.77	0.66
1:A:499:GLN:CB	5:A:759:HOH:O	2.38	0.66
1:A:288:ASN:HD21	1:A:292:GLN:HE21	1.43	0.65
1:B:94:ARG:CZ	5:B:674:HOH:O	2.44	0.65
1:B:67:PHE:HD1	1:B:73:VAL:CG1	2.09	0.65
1:A:243:HIS:HE1	1:A:255:GLU:OE2	1.79	0.65
1:A:187:MET:HE3	1:A:351:CYS:HB3	1.79	0.64
1:B:519:HIS:CE1	5:B:754:HOH:O	2.51	0.63
1:A:436:VAL:HG21	1:A:468:ILE:HD12	1.79	0.63
1:B:518:MET:HE2	1:B:549:TYR:CE1	2.33	0.63
1:A:116:ALA:HB3	1:A:266:ARG:HH12	1.64	0.62
1:B:127:ASN:CG	1:B:130:THR:HG23	2.24	0.62
1:A:164:LEU:HD12	1:A:187:MET:HE2	1.80	0.62
1:B:243:HIS:HD2	5:B:753:HOH:O	1.82	0.62
1:A:168:GLU:HG2	5:A:922:HOH:O	1.99	0.62
1:B:55:GLN:HG3	5:B:967:HOH:O	2.00	0.61
1:A:425:VAL:HG13	1:B:428:VAL:HG21	1.82	0.61
1:A:227:ALA:N	1:A:238:GLN:HE21	1.87	0.61
1:A:382:THR:CG2	1:A:456:VAL:HG22	2.26	0.61
1:A:211:LEU:HD12	1:A:211:LEU:N	2.16	0.60
1:B:346:GLN:NE2	1:B:430:GLN:HE21	1.92	0.59
1:B:130:THR:HG21	1:B:259:LEU:HD23	1.85	0.59
1:B:94:ARG:HD2	5:B:839:HOH:O	2.03	0.59
1:B:436:VAL:HG21	1:B:468:ILE:HD12	1.84	0.59
1:B:130:THR:HB	1:B:259:LEU:HB3	1.85	0.58
1:A:266:ARG:NH1	1:A:266:ARG:CG	2.51	0.58
1:B:211:LEU:O	1:B:213:THR:CG2	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:MET:CE	1:A:339:GLU:HA	2.27	0.57
1:B:223:GLN:HE21	1:B:225:HIS:N	1.90	0.57
1:A:90:LEU:HD12	1:A:105:SER:HA	1.87	0.56
1:A:355:ASP:HB2	5:A:965:HOH:O	2.04	0.56
1:B:110:LEU:HB2	1:B:335:MET:HE1	1.87	0.56
1:B:273:ARG:HG2	1:B:279:ILE:CD1	2.34	0.56
1:B:436:VAL:CG2	1:B:468:ILE:HD12	2.36	0.56
1:B:534:GLY:HA2	5:B:767:HOH:O	2.06	0.56
1:A:223:GLN:NE2	1:A:225:HIS:H	2.02	0.56
1:A:474:PRO:CB	1:A:555:ILE:CD1	2.68	0.56
1:B:227:ALA:H	1:B:238:GLN:NE2	2.02	0.56
1:A:209:LEU:HD22	1:A:211:LEU:CD1	2.36	0.56
1:B:523:LYS:CE	5:B:969:HOH:O	2.43	0.56
1:B:498:LEU:HD23	1:B:498:LEU:H	1.71	0.56
1:A:437:GLU:CG	5:A:618:HOH:O	2.35	0.56
1:B:222:VAL:HG22	5:B:749:HOH:O	2.05	0.55
1:B:182:LEU:O	1:B:212:GLY:HA2	2.05	0.55
1:B:101:GLU:HG3	5:B:893:HOH:O	2.06	0.55
1:A:7:ILE:HD12	1:A:111:LEU:CD2	2.35	0.55
1:A:97:LEU:HD23	1:A:98:ASP:CG	2.30	0.55
1:A:34:ARG:CD	4:A:900:FAD:O2B	2.56	0.54
1:A:424:ASP:O	1:A:428:VAL:HG23	2.08	0.54
1:B:94:ARG:CD	5:B:839:HOH:O	2.55	0.54
1:A:36:GLU:HG3	1:A:78:LYS:HE3	1.90	0.54
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.71	0.54
1:A:68:LYS:NZ	5:A:674:HOH:O	2.39	0.54
1:B:498:LEU:HD23	1:B:498:LEU:N	2.23	0.53
1:A:329:ARG:HH11	1:A:329:ARG:CG	2.22	0.53
1:A:34:ARG:HD2	4:A:900:FAD:O2B	2.09	0.53
1:B:176:LYS:HG2	5:B:1025:HOH:O	2.10	0.52
1:B:243:HIS:CE1	1:B:255:GLU:HG3	2.38	0.52
1:B:425:VAL:CG1	1:B:457:ILE:HD13	2.39	0.52
1:A:11:ALA:HB2	2:A:901:COA:H32	1.92	0.51
1:A:436:VAL:CG2	1:A:468:ILE:CD1	2.86	0.51
1:A:436:VAL:HG21	1:A:468:ILE:HD11	1.91	0.51
1:A:402:ASP:OD1	1:A:404:VAL:HG23	2.10	0.51
1:A:436:VAL:CG2	1:A:468:ILE:HD12	2.40	0.51
1:B:273:ARG:HG2	1:B:279:ILE:HD13	1.93	0.51
1:B:307:GLU:CD	1:B:327:GLN:HE22	2.18	0.51
1:B:243:HIS:CE1	1:B:255:GLU:CG	2.88	0.51
1:A:378:VAL:HG12	1:A:399:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLY:HA2	5:B:721:HOH:O	2.10	0.50
1:B:418:GLY:N	5:B:721:HOH:O	2.34	0.50
1:B:167:MET:HE1	1:B:202:ILE:HG12	1.94	0.49
1:B:541:TYR:O	1:B:545:VAL:HB	2.12	0.49
1:B:513:GLU:CG	5:B:1065:HOH:O	2.60	0.49
1:A:241:LYS:CD	5:A:1106:HOH:O	2.40	0.49
1:B:513:GLU:HG3	5:B:1065:HOH:O	2.13	0.49
1:B:43:CYS:SG	4:B:900:FAD:C4X	3.01	0.49
1:A:108:THR:HG23	1:A:297:ALA:O	2.12	0.48
1:A:168:GLU:CG	5:A:922:HOH:O	2.57	0.48
1:B:56:ARG:HD2	5:B:659:HOH:O	2.12	0.48
1:A:545:VAL:HG12	5:A:649:HOH:O	2.13	0.48
1:A:535:LEU:HD23	1:A:536:ARG:N	2.28	0.48
1:B:131:HIS:HE1	1:B:145:THR:OG1	1.97	0.48
1:A:454:LYS:HE3	5:B:652:HOH:O	2.13	0.48
1:B:311:VAL:HG13	5:B:1060:HOH:O	2.13	0.48
1:B:493:ARG:HH12	1:B:500:ASN:HD21	1.60	0.48
1:A:288:ASN:HD21	1:A:292:GLN:HG2	1.79	0.48
1:A:7:ILE:HD12	1:A:111:LEU:HD23	1.95	0.48
1:A:209:LEU:HD22	1:A:211:LEU:HD12	1.96	0.48
1:A:288:ASN:ND2	1:A:292:GLN:HG2	2.29	0.47
1:A:211:LEU:N	1:A:211:LEU:CD1	2.77	0.47
1:B:483:LEU:HA	1:B:487:GLN:OE1	2.14	0.47
1:B:182:LEU:HG	1:B:214:ALA:HB2	1.94	0.47
1:A:227:ALA:HB3	1:A:238:GLN:HE21	1.54	0.47
1:B:88:ALA:HB1	1:B:90:LEU:HD22	1.96	0.47
1:B:500:ASN:C	1:B:500:ASN:HD22	2.22	0.47
1:B:561:TYR:C	1:B:561:TYR:CD2	2.92	0.47
1:A:243:HIS:HD2	5:A:591:HOH:O	1.97	0.47
1:A:402:ASP:OD1	1:A:404:VAL:CG2	2.62	0.47
1:A:209:LEU:HD22	1:A:211:LEU:HD11	1.97	0.47
1:A:197:PHE:HB2	1:A:414:VAL:HG11	1.97	0.47
1:B:6:ILE:HG23	1:B:110:LEU:HD23	1.97	0.46
1:B:418:GLY:CA	5:B:721:HOH:O	2.62	0.46
1:B:529:ILE:HD11	1:B:544:LEU:HD12	1.97	0.46
1:B:226:VAL:HA	1:B:238:GLN:HE22	1.80	0.46
1:A:114:GLY:HA2	1:A:303:ASP:HB2	1.98	0.46
1:A:209:LEU:CD1	1:A:211:LEU:HD11	2.44	0.46
1:B:34:ARG:HG2	1:B:35:GLY:N	2.30	0.46
1:B:39:SER:HB2	1:B:62:GLN:HB2	1.96	0.46
1:B:519:HIS:HD2	5:B:757:HOH:O	1.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:HIS:CD2	5:B:753:HOH:O	2.62	0.46
1:B:222:VAL:CG2	5:B:749:HOH:O	2.63	0.45
1:A:37:TYR:CD2	1:A:136:ILE:HD12	2.52	0.45
1:A:120:PRO:HG3	1:A:261:MET:HE2	1.98	0.45
1:A:240:ILE:HD13	1:A:240:ILE:HG21	1.63	0.45
1:B:59:LEU:CD1	1:B:139:MET:HE1	2.46	0.45
1:B:130:THR:HG22	1:B:244:LEU:HD11	1.98	0.45
1:A:182:LEU:O	1:A:212:GLY:HA2	2.16	0.45
1:B:127:ASN:ND2	1:B:130:THR:HG23	2.32	0.45
1:B:271:LEU:HB2	5:B:699:HOH:O	2.17	0.45
1:A:136:ILE:HB	1:A:137:PRO:HD3	1.99	0.45
1:A:333:ASP:OD2	1:A:340:GLU:OE1	2.35	0.45
1:B:507:VAL:HG23	5:B:758:HOH:O	2.17	0.45
1:A:386:ALA:HB1	1:A:388:TYR:CE2	2.52	0.44
1:A:454:LYS:HZ2	1:A:454:LYS:HG3	1.47	0.44
1:B:454:LYS:HB2	1:B:454:LYS:HE3	1.73	0.44
1:A:243:HIS:HA	5:A:591:HOH:O	2.16	0.44
1:B:127:ASN:HD21	1:B:130:THR:CG2	2.31	0.44
1:B:331:ALA:O	1:B:335:MET:HG3	2.16	0.44
1:B:7:ILE:HG12	1:B:81:VAL:HG21	2.00	0.43
1:B:178:THR:HG21	1:B:254:LEU:HD11	2.00	0.43
1:A:112:SER:O	4:A:900:FAD:H52A	2.18	0.43
1:B:11:ALA:HB2	2:B:901:COA:H32	1.99	0.43
1:A:5:LEU:HD22	1:A:30:ILE:HB	2.00	0.43
1:A:500:ASN:HD22	1:A:500:ASN:N	2.16	0.43
1:B:309:ASP:OD2	1:B:363:LYS:HE3	2.19	0.43
1:A:416:LYS:N	5:A:821:HOH:O	2.50	0.43
1:B:43:CYS:SG	2:B:901:COA:S1P	3.16	0.43
1:B:217:GLU:HB2	1:B:247:THR:HB	2.00	0.43
1:B:518:MET:CE	1:B:547:ASN:HB2	2.44	0.43
1:A:475:ILE:H	1:A:475:ILE:HG13	1.54	0.43
1:A:515:ARG:N	5:A:779:HOH:O	2.44	0.43
1:B:130:THR:CG2	1:B:259:LEU:HD23	2.47	0.43
1:A:240:ILE:HG22	5:A:675:HOH:O	2.19	0.43
1:A:97:LEU:HD23	1:A:98:ASP:CB	2.49	0.43
1:B:223:GLN:HE21	1:B:224:THR:N	2.15	0.43
1:B:500:ASN:C	1:B:500:ASN:ND2	2.77	0.43
1:B:529:ILE:HD11	1:B:544:LEU:CD1	2.49	0.42
1:A:175:ILE:O	1:A:177:THR:HG23	2.19	0.42
1:B:12:GLY:HA3	1:B:112:SER:OG	2.19	0.42
1:B:518:MET:CE	1:B:547:ASN:CB	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:GLN:HG2	1:B:526:GLU:HG3	2.01	0.42
1:A:377:LYS:HE3	1:A:377:LYS:HB3	1.76	0.42
1:A:424:ASP:OD2	1:B:421:LYS:HD2	2.19	0.42
1:B:285:ILE:HD12	1:B:304:ALA:HB1	2.02	0.42
1:A:518:MET:HE2	1:A:549:TYR:HE1	1.85	0.42
1:B:495:PRO:HD2	5:B:1022:HOH:O	2.19	0.42
1:A:144:GLN:HB2	5:A:1066:HOH:O	2.20	0.41
1:B:436:VAL:HG21	1:B:468:ILE:CD1	2.50	0.41
1:A:11:ALA:O	1:A:15:SER:HB3	2.20	0.41
1:A:34:ARG:HG2	1:A:35:GLY:N	2.35	0.41
1:A:475:ILE:CD1	1:A:480:ILE:HD12	2.50	0.41
1:B:127:ASN:HB2	1:B:128:PRO:CD	2.50	0.41
1:A:442:LEU:HD22	1:B:428:VAL:HG22	2.02	0.41
1:B:34:ARG:HD2	4:B:900:FAD:C4A	2.50	0.41
1:B:111:LEU:C	1:B:113:PRO:HD3	2.46	0.41
1:A:42:ASN:OD1	2:A:901:COA:H22	2.21	0.41
1:A:542:ARG:HH21	1:A:546:ASN:HD21	1.68	0.41
1:B:34:ARG:NH2	5:B:894:HOH:O	2.40	0.41
1:A:40:PHE:HA	1:A:59:LEU:O	2.21	0.41
1:A:71:PHE:O	1:A:72:ASN:C	2.63	0.41
1:A:378:VAL:HA	1:A:555:ILE:HG21	2.02	0.41
1:B:10:VAL:O	1:B:14:ALA:HB3	2.21	0.41
1:A:382:THR:HA	5:A:979:HOH:O	2.20	0.41
1:A:243:HIS:CE1	1:A:255:GLU:HB3	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ASN:OD1	1:B:482:ASN:ND2[1_554]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	563/565 (100%)	547 (97%)	14 (2%)	2 (0%)	30	27
1	B	563/565 (100%)	544 (97%)	15 (3%)	4 (1%)	18	14
All	All	1126/1130 (100%)	1091 (97%)	29 (3%)	6 (0%)	24	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	ASN
1	B	10	VAL
1	B	293	THR
1	A	10	VAL
1	B	483	LEU
1	A	456	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	449/450 (100%)	414 (92%)	35 (8%)	11	8
1	B	449/450 (100%)	409 (91%)	40 (9%)	9	6
All	All	898/900 (100%)	823 (92%)	75 (8%)	10	7

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	VAL
1	A	15	SER
1	A	42	ASN
1	A	43	CYS
1	A	64	PRO
1	A	90	LEU
1	A	97	LEU

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Mol	Chain	Res	Type
1	A	129	LEU
1	A	132	SER
1	A	143	LEU
1	A	192	ARG
1	A	209	LEU
1	A	221	GLN
1	A	224	THR
1	A	241	LYS
1	A	253	LEU
1	A	254	LEU
1	A	259	LEU
1	A	266	ARG
1	A	282	LEU
1	A	329	ARG
1	A	356	LEU
1	A	363	LYS
1	A	377	LYS
1	A	378	VAL
1	A	382	THR
1	A	454	LYS
1	A	475	ILE
1	A	483	LEU
1	A	485	GLU
1	A	486	ASP
1	A	490	LEU
1	A	500	ASN
1	A	523	LYS
1	B	10	VAL
1	B	34	ARG
1	B	52	GLU
1	B	67	PHE
1	B	90	LEU
1	B	98	ASP
1	B	103	GLN
1	B	130	THR
1	B	136	ILE
1	B	176	LYS
1	B	180	LEU
1	B	182	LEU
1	B	209	LEU
1	B	213	THR
1	B	216	SER

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Mol	Chain	Res	Type
1	B	221	GLN
1	B	229	ASP
1	B	241	LYS
1	B	253	LEU
1	B	267	PRO
1	B	271	LEU
1	B	279	ILE
1	B	281	GLU
1	B	292	GLN
1	B	356	LEU
1	B	380	VAL
1	B	407	THR
1	B	416	LYS
1	B	437	GLU
1	B	445	SER
1	B	454	LYS
1	B	482	ASN
1	B	498	LEU
1	B	500	ASN
1	B	511	VAL
1	B	525	LYS
1	B	529	ILE
1	B	533	VAL
1	B	545	VAL
1	B	565	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	HIS
1	A	200	GLN
1	A	223	GLN
1	A	238	GLN
1	A	243	HIS
1	A	292	GLN
1	A	343	GLN
1	A	500	ASN
1	A	543	GLN
1	A	546	ASN
1	B	55	GLN
1	B	62	GLN
1	B	131	HIS

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Mol	Chain	Res	Type
1	B	172	HIS
1	B	205	GLN
1	B	221	GLN
1	B	223	GLN
1	B	238	GLN
1	B	243	HIS
1	B	292	GLN
1	B	346	GLN
1	B	370	GLN
1	B	430	GLN
1	B	441	HIS
1	B	482	ASN
1	B	494	ASN
1	B	500	ASN
1	B	519	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	B	901	-	47,50,50	1.57	7 (14%)	69,75,75	2.85	23 (33%)
4	FAD	B	900	-	58,58,58	1.70	9 (15%)	85,89,89	1.65	19 (22%)
2	COA	A	901	-	47,50,50	1.51	5 (10%)	69,75,75	1.94	19 (27%)
4	FAD	A	900	-	58,58,58	1.42	8 (13%)	85,89,89	1.81	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	COA	B	901	-	-	5/48/64/64	0/3/3/3
4	FAD	B	900	-	-	1/34/50/50	0/6/6/6
2	COA	A	901	-	-	3/48/64/64	0/3/3/3
4	FAD	A	900	-	-	1/34/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	COA	O9P-C9P	6.43	1.35	1.23
4	B	900	FAD	PA-O3P	4.70	1.64	1.59
4	B	900	FAD	C4X-N5	4.36	1.40	1.30
2	B	901	COA	O9P-C9P	4.26	1.31	1.23
4	A	900	FAD	C4X-N5	4.21	1.39	1.30
2	B	901	COA	O5P-C5P	4.20	1.31	1.23
4	B	900	FAD	C5A-N7A	-3.98	1.31	1.39
4	B	900	FAD	C2A-N3A	3.83	1.40	1.33
2	A	901	COA	P2A-O3A	3.80	1.63	1.59
2	B	901	COA	P1A-O3A	-3.74	1.55	1.59
4	A	900	FAD	C2A-N1A	3.66	1.40	1.33
4	A	900	FAD	O2-C2	-3.56	1.17	1.24
4	B	900	FAD	C10-N1	3.39	1.40	1.33
4	B	900	FAD	C2A-N1A	3.30	1.39	1.33
2	B	901	COA	CCP-CBP	3.06	1.57	1.52
4	B	900	FAD	O2'-C2'	-3.02	1.37	1.43
2	B	901	COA	C2A-N3A	2.94	1.39	1.33
2	A	901	COA	P1A-O2A	-2.88	1.42	1.55
4	A	900	FAD	PA-O3P	-2.82	1.56	1.59
4	A	900	FAD	C4A-N3A	2.77	1.39	1.34
4	B	900	FAD	C9A-N10	-2.72	1.36	1.41
4	A	900	FAD	C10-N10	2.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	COA	C2A-N3A	2.44	1.38	1.33
4	A	900	FAD	C2A-N3A	2.39	1.38	1.33
2	B	901	COA	C6P-C5P	2.26	1.55	1.51
2	A	901	COA	C5A-N7A	-2.26	1.35	1.39
2	B	901	COA	C8A-N7A	2.10	1.35	1.31
4	A	900	FAD	C6-C5X	2.06	1.43	1.40
4	B	900	FAD	O5B-C5B	-2.01	1.37	1.44

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	COA	C3P-N4P-C5P	-11.34	101.71	122.82
2	B	901	COA	N3A-C2A-N1A	-8.04	116.40	128.58
2	B	901	COA	C7P-C6P-C5P	-7.80	99.41	112.39
2	B	901	COA	CEP-CBP-CDP	-5.73	97.78	109.20
2	A	901	COA	CDP-CBP-CAP	5.46	118.08	108.77
2	B	901	COA	O5A-P2A-O3A	5.19	121.30	107.27
2	A	901	COA	N3A-C2A-N1A	-4.96	121.07	128.58
4	A	900	FAD	C4-N3-C2	-4.79	117.13	125.64
2	A	901	COA	O2A-P1A-O3A	4.74	120.09	107.27
4	A	900	FAD	N3A-C2A-N1A	-4.65	121.55	128.58
4	A	900	FAD	O2-C2-N1	-4.61	114.14	121.80
2	B	901	COA	CDP-CBP-CAP	4.60	116.62	108.77
2	B	901	COA	C2A-N3A-C4A	4.41	122.60	111.83
2	B	901	COA	C6P-C5P-N4P	-4.26	108.57	116.34
4	A	900	FAD	N9A-C8A-N7A	-4.23	107.94	113.94
2	B	901	COA	N9A-C8A-N7A	-4.18	108.01	113.94
2	B	901	COA	CEP-CBP-CCP	4.10	115.00	108.22
2	B	901	COA	C5A-C4A-N3A	-4.09	121.08	126.72
4	B	900	FAD	C5'-C4'-C3'	-4.02	104.63	112.22
4	A	900	FAD	C4X-C10-N10	3.99	122.19	116.48
4	A	900	FAD	C4A-N9A-C8A	3.98	109.91	105.74
4	B	900	FAD	N3A-C2A-N1A	-3.87	122.72	128.58
4	B	900	FAD	C5A-N7A-C8A	3.81	109.43	103.45
2	A	901	COA	C5A-C4A-N3A	-3.77	121.52	126.72
2	A	901	COA	N9A-C8A-N7A	-3.74	108.62	113.94
4	A	900	FAD	C5A-C4A-N3A	-3.71	121.61	126.72
2	A	901	COA	CEP-CBP-CDP	-3.70	101.82	109.20
4	A	900	FAD	N3A-C4A-N9A	3.69	133.45	127.17
4	B	900	FAD	C4A-C5A-N7A	-3.61	106.46	110.58
2	B	901	COA	CAP-C9P-N8P	3.55	123.22	116.48
2	A	901	COA	C6P-C7P-N8P	-3.40	104.76	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	COA	C5B-C4B-C3B	-3.39	103.10	114.38
2	B	901	COA	N3A-C4A-N9A	3.39	132.93	127.17
4	B	900	FAD	O2A-PA-O3P	3.36	116.34	107.27
4	B	900	FAD	C5X-C9A-N10	3.31	120.96	117.97
2	A	901	COA	O3A-P1A-O1A	-3.30	100.79	110.70
2	B	901	COA	C6P-C7P-N8P	-3.28	105.02	112.00
4	B	900	FAD	N9A-C8A-N7A	-3.24	109.34	113.94
2	A	901	COA	C2A-N3A-C4A	3.15	119.53	111.83
4	B	900	FAD	O4B-C1B-N9A	-3.14	102.06	108.09
4	A	900	FAD	O4B-C1B-N9A	-2.98	102.37	108.09
2	B	901	COA	C2P-C3P-N4P	2.92	118.93	112.31
4	B	900	FAD	O4B-C4B-C3B	2.90	110.92	105.15
2	B	901	COA	O2A-P1A-O3A	2.87	115.04	107.27
4	B	900	FAD	C9-C9A-N10	-2.87	117.99	121.85
2	B	901	COA	O9P-C9P-CAP	-2.86	112.90	120.89
2	A	901	COA	O5A-P2A-O3A	2.86	114.99	107.27
4	B	900	FAD	C5A-C4A-N3A	-2.71	122.99	126.72
4	A	900	FAD	O2A-PA-O3P	2.68	114.51	107.27
2	A	901	COA	C5A-N7A-C8A	2.65	107.61	103.45
2	B	901	COA	C4A-N9A-C8A	2.64	108.51	105.74
4	A	900	FAD	C2A-N3A-C4A	2.63	118.27	111.83
4	B	900	FAD	O4-C4-C4X	-2.60	119.66	126.53
4	A	900	FAD	C4-C4X-C10	2.60	121.39	116.93
2	B	901	COA	C5A-N7A-C8A	2.58	107.50	103.45
4	A	900	FAD	C10-C4X-N5	-2.55	119.59	124.81
4	B	900	FAD	C4X-C10-N10	2.54	120.11	116.48
4	A	900	FAD	C9A-N10-C10	-2.48	116.97	120.75
4	A	900	FAD	O4'-C4'-C5'	-2.47	104.53	109.99
4	B	900	FAD	O3B-C3B-C4B	2.45	118.12	111.08
4	A	900	FAD	C5A-N7A-C8A	2.43	107.27	103.45
2	A	901	COA	C2P-C3P-N4P	-2.41	106.83	112.31
2	A	901	COA	CEP-CBP-CCP	2.39	112.17	108.22
4	B	900	FAD	O4'-C4'-C3'	2.34	114.72	109.25
4	A	900	FAD	O3B-C3B-C2B	-2.30	104.44	111.82
4	A	900	FAD	O4-C4-C4X	-2.28	120.51	126.53
4	A	900	FAD	O2'-C2'-C3'	2.27	114.55	109.25
2	A	901	COA	O6A-P2A-O4A	2.26	117.90	108.94
4	A	900	FAD	N3-C2-N1	2.25	124.28	119.50
4	A	900	FAD	C5X-C9A-N10	2.24	119.99	117.97
2	B	901	COA	O3A-P1A-O1A	-2.20	104.08	110.70
2	A	901	COA	N3A-C4A-N9A	2.13	130.79	127.17
4	A	900	FAD	O4B-C1B-C2B	-2.10	102.11	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	FAD	C4X-C4-N3	2.10	118.60	113.25
2	A	901	COA	N6A-C6A-N1A	2.07	123.00	118.38
4	B	900	FAD	O4'-C4'-C5'	-2.07	105.42	109.99
2	A	901	COA	O5P-C5P-C6P	2.05	125.74	122.02
4	B	900	FAD	C9A-C5X-N5	-2.05	120.28	122.45
2	B	901	COA	C2A-N1A-C6A	2.05	122.10	118.73
4	B	900	FAD	O3'-C3'-C4'	2.03	113.53	108.93
2	A	901	COA	CAP-C9P-N8P	2.02	120.32	116.48
2	A	901	COA	C5A-C6A-N6A	-2.02	118.29	123.29
4	B	900	FAD	C4X-C4-N3	2.01	118.36	113.25
2	B	901	COA	C2B-C1B-N9A	-2.00	108.33	113.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	COA	P2A-O3A-P1A-O5B
2	B	901	COA	P2A-O3A-P1A-O5B
4	A	900	FAD	PA-O3P-P-O5'
2	B	901	COA	O5P-C5P-N4P-C3P
2	B	901	COA	S1P-C2P-C3P-N4P
2	A	901	COA	P1A-O3A-P2A-O5A
2	B	901	COA	P1A-O3A-P2A-O4A
4	B	900	FAD	O4B-C4B-C5B-O5B
2	B	901	COA	C3B-O3B-P3B-O9A
2	A	901	COA	P1A-O3A-P2A-O4A

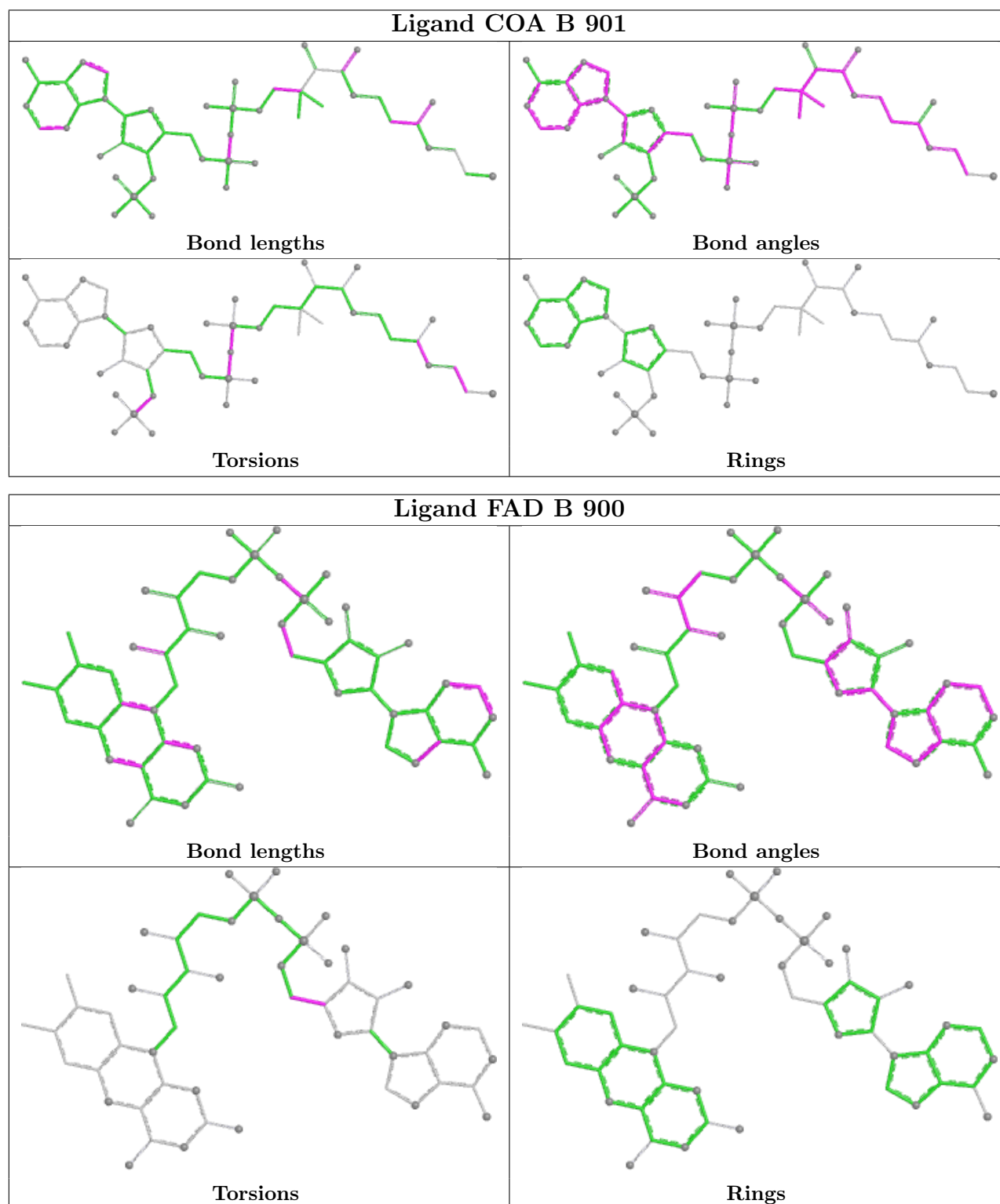
There are no ring outliers.

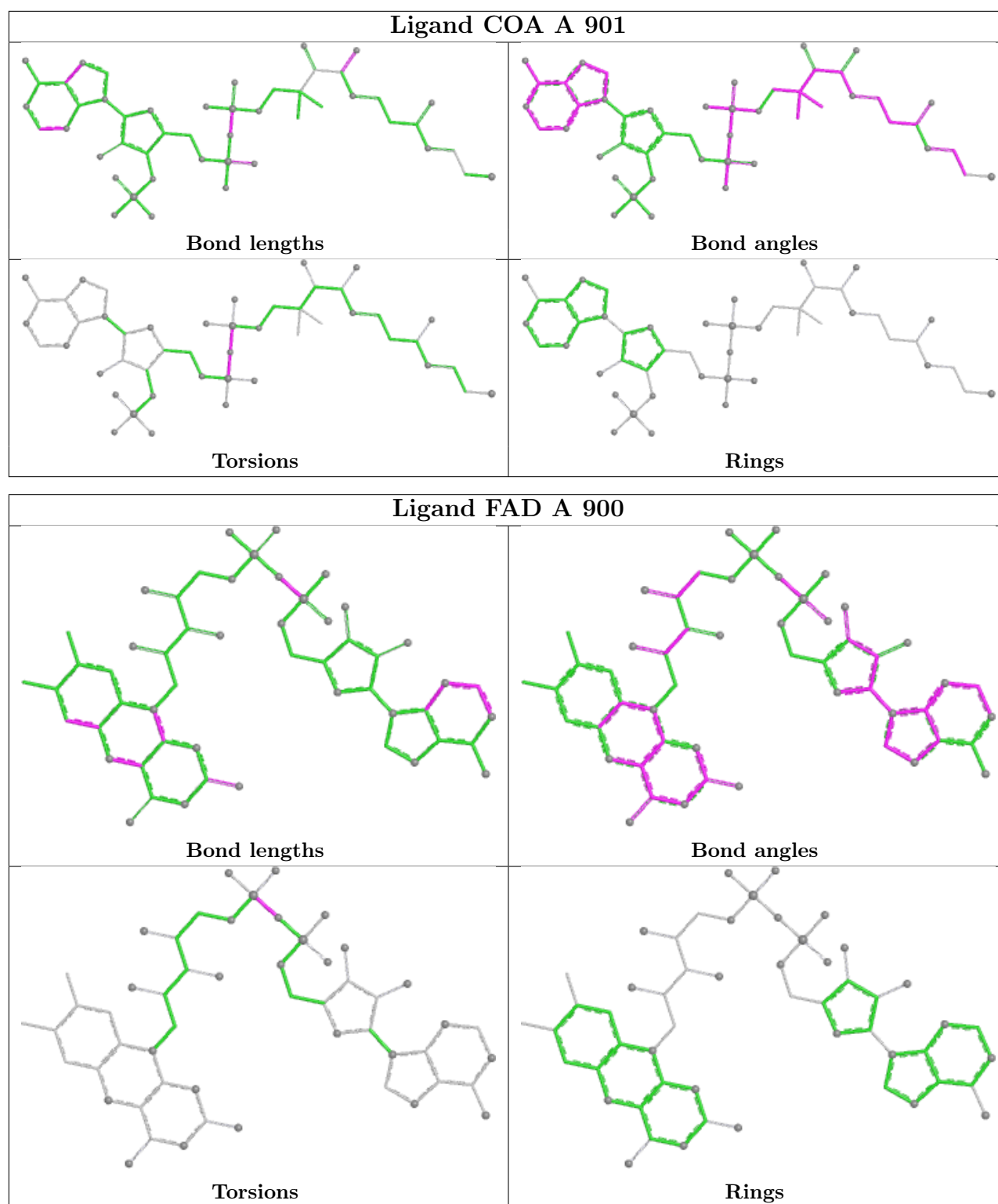
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	COA	2	0
4	B	900	FAD	2	0
2	A	901	COA	2	0
4	A	900	FAD	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	565/565 (100%)	0.77	44 (7%)	19 18	20, 33, 49, 74	0
1	B	565/565 (100%)	0.68	35 (6%)	26 25	23, 32, 49, 65	0
All	All	1130/1130 (100%)	0.73	79 (6%)	22 21	20, 32, 49, 74	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	565	SER	7.3
1	A	230	ALA	5.8
1	A	236	ALA	5.6
1	A	564	ALA	5.3
1	B	230	ALA	4.7
1	A	231	ALA	4.5
1	A	229	ASP	4.2
1	A	232	GLY	4.0
1	B	231	ALA	4.0
1	B	482	ASN	3.8
1	A	224	THR	3.7
1	B	500	ASN	3.7
1	B	97	LEU	3.6
1	A	240	ILE	3.6
1	A	266	ARG	3.6
1	A	226	VAL	3.6
1	A	235	THR	3.6
1	A	97	LEU	3.5
1	A	500	ASN	3.5
1	A	563	PHE	3.4
1	A	228	SER	3.4
1	A	475	ILE	3.4
1	B	232	GLY	3.3
1	B	253	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	519	HIS	3.2
1	B	229	ASP	3.2
1	A	482	ASN	3.1
1	B	111	LEU	3.1
1	A	437	GLU	3.1
1	B	499	GLN	3.1
1	B	1	MET	2.9
1	B	252	GLU	2.9
1	A	225	HIS	2.8
1	A	85	ASP	2.8
1	A	382	THR	2.7
1	A	55	GLN	2.7
1	B	226	VAL	2.7
1	A	200	GLN	2.7
1	B	55	GLN	2.6
1	A	488	LEU	2.6
1	A	188	THR	2.6
1	A	504	GLU	2.6
1	A	119	VAL	2.6
1	A	507	VAL	2.5
1	A	57	SER	2.5
1	B	245	SER	2.5
1	A	227	ALA	2.4
1	B	119	VAL	2.4
1	B	236	ALA	2.4
1	A	1	MET	2.4
1	A	43	CYS	2.4
1	B	254	LEU	2.3
1	B	307	GLU	2.3
1	A	371	ALA	2.3
1	A	562	LYS	2.3
1	A	211	LEU	2.3
1	B	176	LYS	2.3
1	B	483	LEU	2.3
1	B	519	HIS	2.3
1	B	11	ALA	2.3
1	B	182	LEU	2.3
1	B	240	ILE	2.2
1	B	224	THR	2.2
1	B	370	GLN	2.2
1	A	238	GLN	2.2
1	B	308	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	234	ASP	2.2
1	B	126	ASP	2.1
1	B	271	LEU	2.1
1	B	504	GLU	2.1
1	B	37	TYR	2.1
1	B	241	LYS	2.1
1	A	483	LEU	2.1
1	A	498	LEU	2.1
1	A	58	ALA	2.1
1	A	60	VAL	2.0
1	B	222	VAL	2.0
1	A	15	SER	2.0
1	B	213	THR	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](#)

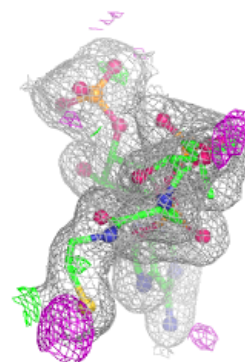
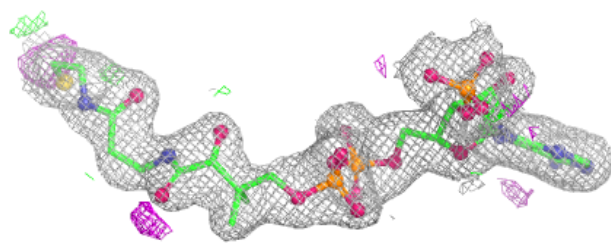
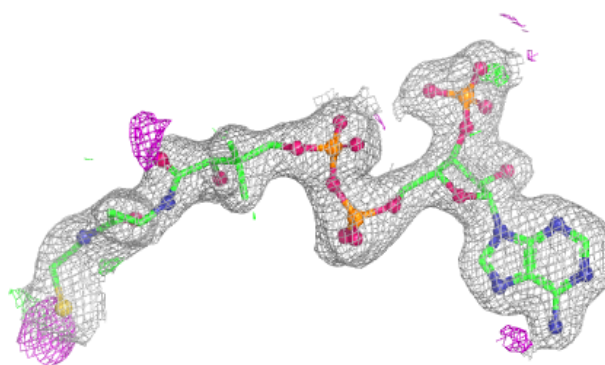
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	COA	A	901	48/48	0.95	0.09	22,33,45,53	0
2	COA	B	901	48/48	0.95	0.08	23,31,44,54	0
4	FAD	A	900	53/53	0.96	0.07	19,29,34,39	0
4	FAD	B	900	53/53	0.96	0.07	23,28,32,34	0
3	CL	A	566	1/1	0.97	0.05	29,29,29,29	0
3	CL	B	566	1/1	0.99	0.05	28,28,28,28	0

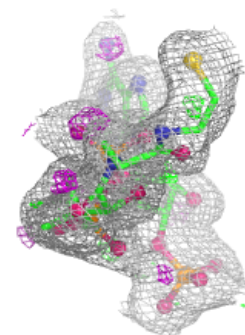
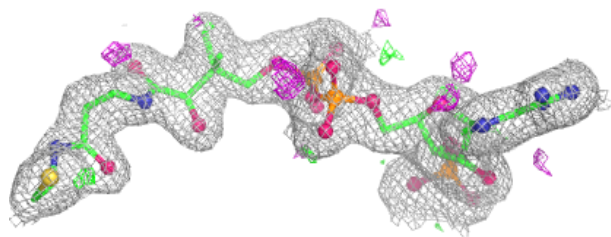
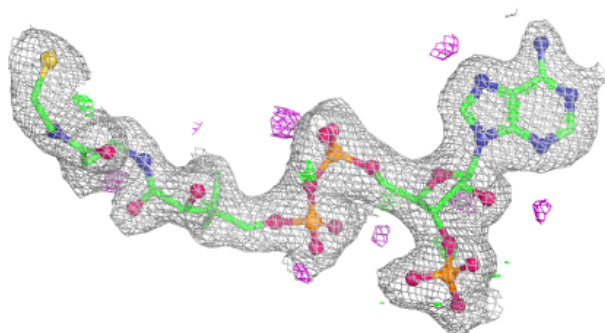
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA A 901:

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

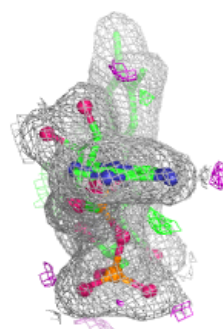
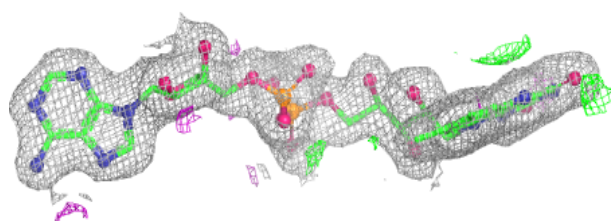
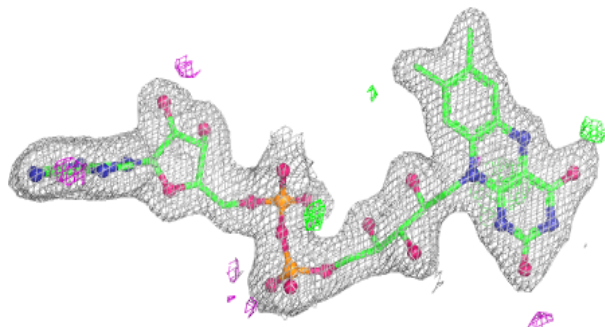
**Electron density around COA B 901:**

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

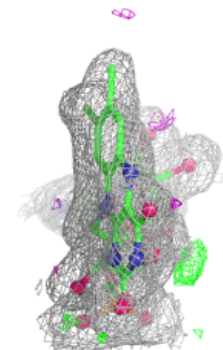
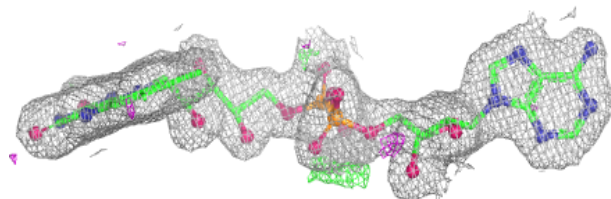
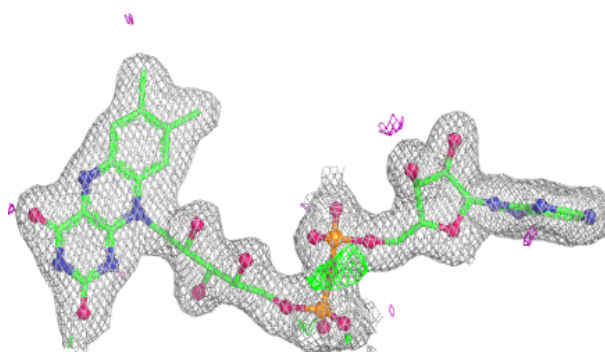


Electron density around FAD A 900:

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

**Electron density around FAD B 900:**

$2mF_o-DF_c$ (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.