



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:39 PM UTC

PDB ID : 3NTA / pdb_00003nta
Title : Structure of the Shewanella loihica PV-4 NADH-dependent persulfide reductase
Authors : Sazinsky, M.H.; Crane, E.J.; Warner, M.D.; Lukose, V.; Lee, K.H.
Deposited on : 2010-07-03
Resolution : 2.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

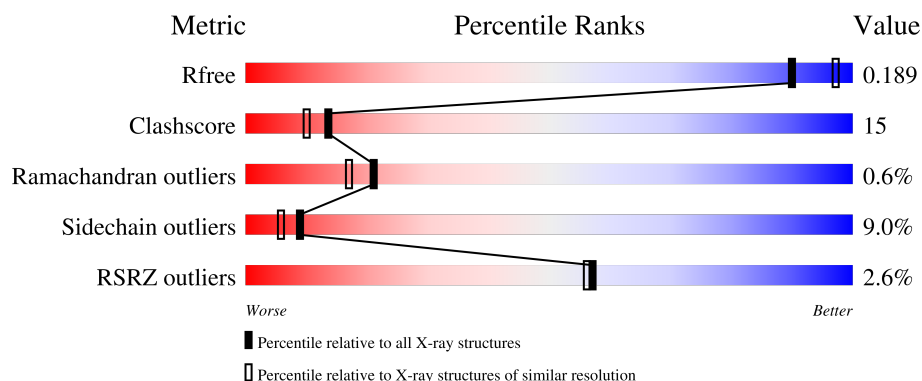
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	574	2% 57% 34% 6% ..
1	B	574	3% 52% 37% 8% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	575	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9344 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	Se	0	1	0
			4301	2698	762	821	4	16			
1	B	565	Total	C	N	O	S	Se	0	0	0
			4294	2694	763	818	4	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	LEU	-	expression tag	UNP A3QAV3
A	568	GLU	-	expression tag	UNP A3QAV3
A	569	HIS	-	expression tag	UNP A3QAV3
A	570	HIS	-	expression tag	UNP A3QAV3
A	571	HIS	-	expression tag	UNP A3QAV3
A	572	HIS	-	expression tag	UNP A3QAV3
A	573	HIS	-	expression tag	UNP A3QAV3
A	574	HIS	-	expression tag	UNP A3QAV3
B	567	LEU	-	expression tag	UNP A3QAV3
B	568	GLU	-	expression tag	UNP A3QAV3
B	569	HIS	-	expression tag	UNP A3QAV3
B	570	HIS	-	expression tag	UNP A3QAV3
B	571	HIS	-	expression tag	UNP A3QAV3
B	572	HIS	-	expression tag	UNP A3QAV3
B	573	HIS	-	expression tag	UNP A3QAV3
B	574	HIS	-	expression tag	UNP A3QAV3

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- # FAD

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

- # COA

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



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

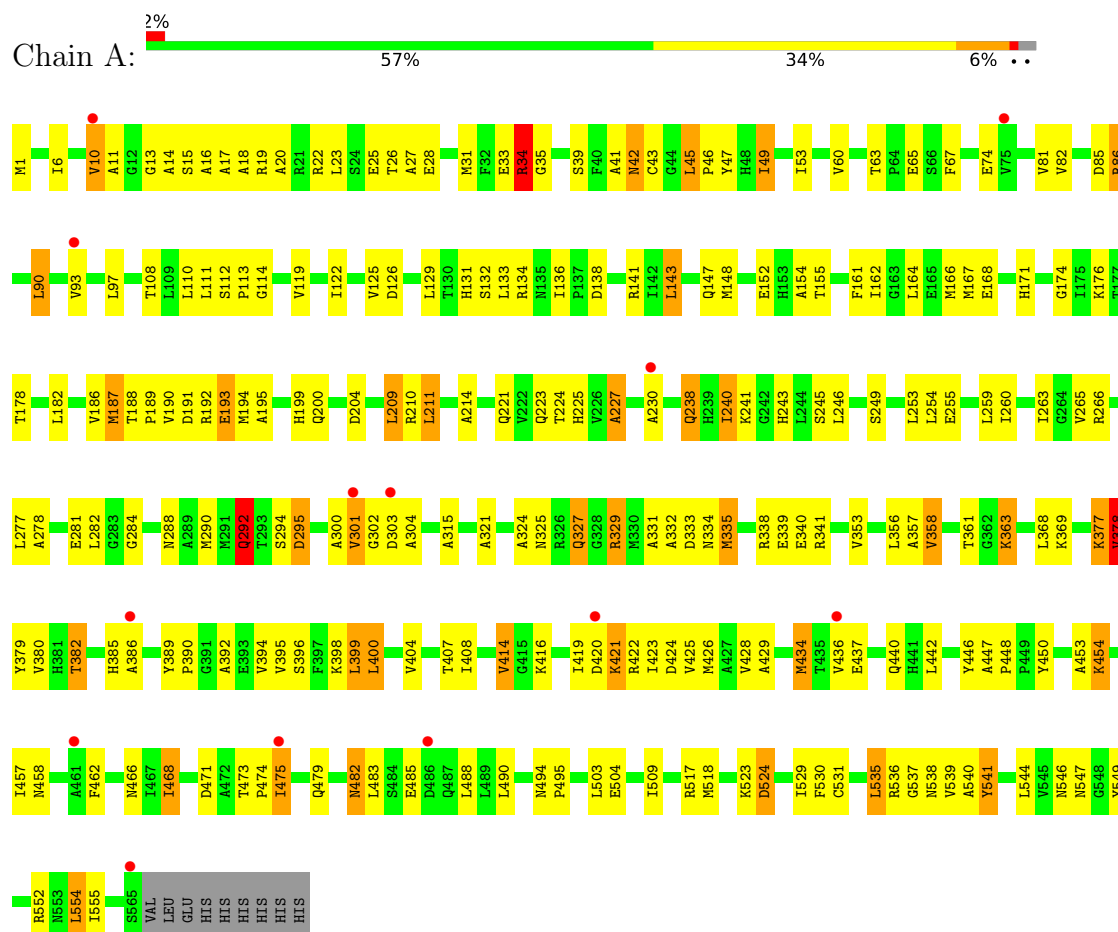
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	264	Total	O	0	0
			264	264		
5	B	281	Total	O	0	0
			281	281		

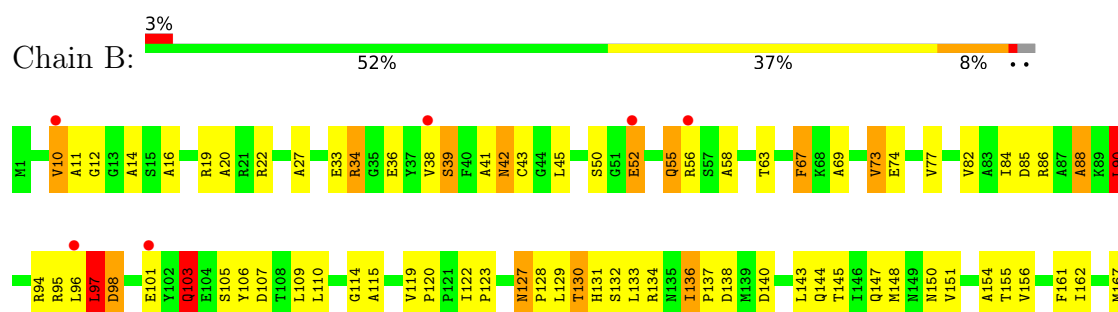
3 Residue-property plots

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



L498	Q499	R500	G501	V507	N508	I509	P510	V511	R517	M518	H519	E520	L521	K525	I528	I529	F530	C531	Q532	V533	G534	L535	R536	V539	A540	Y541	R542	Q543	L544	V545	N546	N547	G548	Y549	I555	T560	Y561	S565	VAL	LEU	GLU	HIS	HIS	HIS	HIS	HIS						
D417	G418	D420	K421	R422	I423	D424	V425	V428	A429	Q430	R431	M434	T435	V436	E437	S445	Y446	A447	P448	P449	Y450	G451	S452	A453	K454	N458	Q459	A460	V463	A464	S465	R466	I467	I468	K469	I475	H476	F477	D478	Q479	R482	L483	S484	E485	D486	Q487	L488	L489	L490	E497		
L320	A321	G322	P323	A324	N325	R326	Q327	G328	R329	A332	L258	D333	N334	R335	R338	V342	Q343	Q346	A349	I350	V353	L356	A357	V358	G359	A360	T361	G362	K363	I373	E376	K377	V378	V379	V380	A383	S384	H385	L400	F401	D402	P403	V404	T407	G410	K416						
L246	N250	G251	E252	L253	L254	E255	T256	D257	L258	L259	L260	R261	A262	L263	G264	V265	R266	P267	E268	T269	Q270	L271	A272	R273	L279	Q280	E281	L282	G283	G284	L285	K286	V287	N288	A289	M290	M291	Q292	D295	A300	V301	G302	D303	A304	V305	E306	E307	Q308	D309	T312	V318	P319
H171	I175	K176	T177	T178	L179	L180	E181	L182	A183	D184	Q185	V186	M187	T188	P189	V190	D191	R192	E193	M194	A195	A201	L202	R203	D204	V207	D208	L209	R210	L211	G212	T213	A214	L215	V218	Q221	V222	Q223	T224	H225	S228	D229	A230	A231	G232	E233	Q238	K241	G242	H243		

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	134.34Å 134.34Å 81.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	116.37 – 2.01 116.34 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.8 (116.37-2.01) 98.9 (116.34-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.137 , 0.173 0.167 , 0.189	Depositor DCC
R_{free} test set	5482 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.018 for h,-h-k,-l 0.008 for -k,-h,-l	Xtriage
Reported twinning fraction	0.479 for H, K, L 0.521 for h,-h-k,-l	Depositor
Outliers	0 of 108118 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9344	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, COA, 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	2.08	120/4359 (2.8%)	1.59	48/5877 (0.8%)
1	B	2.04	121/4349 (2.8%)	1.57	47/5863 (0.8%)
All	All	2.06	241/8708 (2.8%)	1.58	95/11740 (0.8%)

All (241) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	ILE	CA-CB	16.34	1.63	1.54
1	A	434	MSE	SE-CE	-11.56	1.60	1.95
1	A	63	THR	N-CA	11.35	1.53	1.46
1	A	324	ALA	CA-C	11.14	1.67	1.52
1	A	394	VAL	CA-CB	10.66	1.66	1.53
1	A	458	ASN	CA-C	10.06	1.65	1.52
1	A	358	VAL	CA-CB	9.66	1.66	1.54
1	A	284	GLY	N-CA	9.34	1.54	1.44
1	A	260	ILE	CA-CB	9.18	1.65	1.54
1	A	136	ILE	CA-CB	9.18	1.66	1.54
1	A	41	ALA	CA-C	8.99	1.63	1.53
1	B	156	VAL	CA-CB	8.96	1.65	1.54
1	B	179	LEU	C-O	8.81	1.34	1.24
1	A	361	THR	C-O	-8.70	1.13	1.23
1	A	419	ILE	CA-CB	8.53	1.67	1.54
1	B	233	GLU	N-CA	8.48	1.55	1.45
1	B	332	ALA	N-CA	8.40	1.56	1.46
1	A	357	ALA	C-O	-8.28	1.13	1.23
1	A	447	ALA	N-CA	8.28	1.52	1.45
1	A	45	LEU	C-O	-8.19	1.16	1.24
1	A	380	VAL	CA-CB	8.14	1.67	1.54
1	B	320	LEU	CA-C	8.13	1.62	1.52
1	A	341	ARG	N-CA	8.05	1.56	1.46
1	B	509	ILE	CA-C	8.04	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	ILE	CA-CB	8.03	1.64	1.54
1	A	329	ARG	CA-C	7.95	1.63	1.52
1	B	132	SER	CA-C	7.88	1.63	1.53
1	A	18	ALA	CA-CB	-7.86	1.41	1.53
1	A	155	THR	CA-CB	7.84	1.67	1.53
1	A	148	MSE	SE-CE	-7.75	1.72	1.95
1	B	175	ILE	CA-C	7.73	1.61	1.52
1	A	74	GLU	CA-C	7.71	1.62	1.52
1	A	421	LYS	N-CA	7.64	1.55	1.46
1	A	224	THR	CA-CB	7.62	1.65	1.54
1	A	16	ALA	CA-CB	-7.60	1.41	1.53
1	B	528	ILE	CA-CB	7.59	1.63	1.54
1	A	554	LEU	CA-C	7.55	1.62	1.52
1	B	324	ALA	CA-C	7.53	1.62	1.52
1	B	42	ASN	N-CA	7.48	1.55	1.46
1	A	161	PHE	N-CA	7.45	1.55	1.46
1	B	285	ILE	C-O	-7.32	1.16	1.24
1	B	416	LYS	CA-C	7.31	1.62	1.52
1	A	332	ALA	N-CA	7.27	1.54	1.46
1	A	368	LEU	CA-C	7.22	1.61	1.52
1	B	431	ARG	N-CA	7.22	1.55	1.46
1	A	138	ASP	N-CA	7.13	1.54	1.46
1	B	424	ASP	N-CA	7.12	1.54	1.46
1	B	467	ILE	CA-CB	7.12	1.62	1.54
1	B	490	LEU	CA-C	7.11	1.60	1.52
1	A	90	LEU	C-O	7.09	1.32	1.23
1	A	263	ILE	CA-CB	7.05	1.62	1.54
1	B	333	ASP	C-O	6.98	1.32	1.24
1	A	60	VAL	CA-CB	6.97	1.62	1.54
1	A	19	ARG	C-O	6.93	1.32	1.24
1	A	488	LEU	CA-C	6.93	1.61	1.52
1	B	109	LEU	N-CA	6.92	1.54	1.46
1	B	292	GLN	CA-C	6.90	1.61	1.52
1	B	436	VAL	CA-CB	6.89	1.63	1.54
1	B	518	MSE	SE-CE	-6.89	1.74	1.95
1	A	407	THR	C-O	6.86	1.31	1.23
1	B	434	MSE	SE-CE	-6.85	1.75	1.95
1	B	373	ILE	CA-CB	6.81	1.62	1.54
1	A	111	LEU	N-CA	6.77	1.54	1.46
1	A	16	ALA	CA-C	6.71	1.61	1.52
1	A	334	ASN	N-CA	-6.69	1.37	1.46
1	A	546	ASN	C-O	-6.69	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	GLY	N-CA	6.69	1.51	1.45
1	A	392	ALA	CA-C	6.68	1.61	1.52
1	B	541	TYR	C-O	6.66	1.31	1.24
1	B	207	VAL	CA-CB	-6.65	1.46	1.54
1	B	138	ASP	N-CA	6.64	1.54	1.46
1	A	395	VAL	CA-CB	6.61	1.61	1.53
1	A	193	GLU	CA-C	6.53	1.61	1.52
1	A	134	ARG	CA-C	6.51	1.60	1.52
1	A	155	THR	C-O	-6.49	1.16	1.24
1	B	446	TYR	C-O	-6.48	1.16	1.24
1	A	327	GLN	CA-C	-6.47	1.44	1.52
1	B	19	ARG	C-O	6.45	1.31	1.24
1	A	278	ALA	CA-CB	6.41	1.64	1.53
1	B	45	LEU	CA-CB	6.40	1.61	1.53
1	A	210	ARG	CA-C	-6.40	1.45	1.53
1	A	138	ASP	CA-CB	6.39	1.63	1.53
1	B	322	GLY	N-CA	6.37	1.53	1.44
1	A	42	ASN	N-CA	6.35	1.54	1.46
1	B	20	ALA	CA-C	6.33	1.60	1.52
1	A	14	ALA	C-O	6.31	1.31	1.24
1	B	74	GLU	CA-C	6.29	1.60	1.52
1	B	383	ALA	CA-C	6.29	1.60	1.52
1	B	353	VAL	CA-CB	6.27	1.60	1.53
1	B	192	ARG	CA-CB	6.25	1.63	1.53
1	B	404	VAL	CA-C	6.25	1.59	1.52
1	A	473	THR	C-O	-6.25	1.16	1.24
1	B	532	GLN	C-O	-6.22	1.17	1.24
1	B	162	ILE	C-O	-6.22	1.16	1.24
1	A	400	LEU	N-CA	6.21	1.53	1.46
1	B	148	MSE	N-CA	-6.17	1.38	1.46
1	A	440	GLN	N-CA	-6.16	1.38	1.46
1	B	477	PHE	N-CA	6.15	1.54	1.46
1	B	303	ASP	N-CA	6.14	1.53	1.46
1	B	202	ILE	CA-C	6.12	1.60	1.52
1	B	194	MSE	N-CA	6.10	1.53	1.46
1	B	465	SER	C-O	-6.07	1.16	1.24
1	A	204	ASP	N-CA	6.05	1.54	1.46
1	A	529	ILE	C-O	-6.05	1.16	1.24
1	A	466	ASN	C-O	-6.01	1.17	1.24
1	A	353	VAL	CA-CB	6.01	1.62	1.54
1	B	127	ASN	CA-C	5.99	1.57	1.52
1	A	468	ILE	CA-CB	5.96	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	482	ASN	CA-C	-5.96	1.45	1.53
1	B	476	HIS	C-O	5.95	1.31	1.23
1	A	154	ALA	CA-CB	5.93	1.64	1.53
1	A	162	ILE	CA-CB	5.93	1.62	1.54
1	B	143	LEU	CA-CB	5.93	1.62	1.53
1	B	194	MSE	SE-CE	5.93	2.13	1.95
1	B	329	ARG	C-O	5.92	1.30	1.24
1	B	191	ASP	CA-C	5.92	1.61	1.53
1	B	82	VAL	CA-CB	5.92	1.61	1.54
1	B	129	LEU	CA-C	-5.92	1.44	1.52
1	B	82	VAL	C-O	5.88	1.31	1.24
1	B	73	VAL	CA-CB	5.86	1.61	1.54
1	A	321	ALA	C-O	-5.86	1.16	1.23
1	A	540	ALA	N-CA	5.85	1.53	1.46
1	B	156	VAL	C-O	-5.84	1.17	1.24
1	B	63	THR	C-O	5.82	1.28	1.24
1	A	422	ARG	CA-CB	5.82	1.62	1.53
1	A	53	ILE	CA-C	-5.82	1.47	1.53
1	B	154	ALA	CA-CB	5.79	1.65	1.54
1	A	396	SER	CA-C	-5.75	1.45	1.52
1	B	283	GLY	CA-C	5.74	1.59	1.51
1	A	537	GLY	C-O	5.74	1.30	1.23
1	A	200	GLN	CA-C	5.73	1.60	1.52
1	A	82	VAL	N-CA	5.73	1.51	1.46
1	B	530	PHE	CA-C	5.72	1.59	1.52
1	A	167	MSE	CA-C	5.72	1.61	1.52
1	A	538	ASN	CA-CB	5.72	1.62	1.53
1	B	350	ILE	N-CA	5.72	1.53	1.46
1	B	137	PRO	CA-C	5.71	1.60	1.52
1	B	171	HIS	N-CA	5.70	1.53	1.46
1	B	41	ALA	CA-C	5.67	1.59	1.53
1	B	77	VAL	CA-CB	5.66	1.61	1.54
1	A	199	HIS	CA-C	-5.66	1.45	1.52
1	A	335	MSE	SE-CE	-5.66	1.78	1.95
1	B	266	ARG	CA-C	5.65	1.58	1.52
1	B	361	THR	C-O	-5.62	1.17	1.23
1	A	47	TYR	N-CA	5.62	1.53	1.46
1	A	67	PHE	C-O	-5.62	1.17	1.24
1	A	404	VAL	CA-CB	5.62	1.60	1.55
1	B	464	ALA	CA-C	5.61	1.60	1.52
1	A	334	ASN	CA-CB	5.59	1.62	1.53
1	B	90	LEU	C-O	5.59	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	539	VAL	CA-CB	5.58	1.60	1.54
1	B	560	THR	C-O	5.58	1.30	1.24
1	A	133	LEU	N-CA	5.57	1.52	1.46
1	A	39	SER	CA-CB	5.57	1.61	1.53
1	A	414	VAL	CA-CB	5.56	1.62	1.54
1	A	22	ARG	CZ-NH2	5.55	1.40	1.33
1	B	419	ILE	CA-CB	5.55	1.62	1.54
1	A	378	VAL	C-O	-5.54	1.18	1.24
1	A	389	TYR	C-O	-5.54	1.18	1.24
1	B	272	ALA	N-CA	5.53	1.53	1.46
1	B	84	ILE	C-O	5.53	1.30	1.24
1	A	462	PHE	CA-C	5.52	1.60	1.52
1	A	176	LYS	CA-C	-5.51	1.45	1.52
1	B	260	ILE	CA-C	-5.51	1.45	1.52
1	B	486	ASP	CA-C	5.51	1.60	1.52
1	A	176	LYS	N-CA	5.48	1.52	1.46
1	B	73	VAL	C-O	5.46	1.30	1.24
1	B	448	PRO	C-O	-5.46	1.18	1.24
1	A	400	LEU	C-O	5.44	1.30	1.24
1	A	325	ASN	N-CA	5.43	1.52	1.46
1	B	555	ILE	CA-C	5.42	1.58	1.52
1	B	273	ARG	N-CA	5.40	1.52	1.46
1	B	451	GLY	N-CA	5.39	1.49	1.44
1	B	312	THR	CA-CB	5.38	1.62	1.54
1	A	182	LEU	N-CA	5.36	1.52	1.46
1	A	524	ASP	N-CA	5.35	1.52	1.46
1	A	178	THR	CA-C	-5.35	1.46	1.52
1	B	95	ARG	CA-CB	5.35	1.59	1.53
1	A	363	LYS	N-CA	5.34	1.52	1.46
1	A	292	GLN	CA-C	5.33	1.59	1.52
1	A	382	THR	CA-CB	5.33	1.63	1.53
1	B	150	ASN	C-O	5.33	1.30	1.23
1	A	277	LEU	N-CA	5.33	1.52	1.45
1	B	400	LEU	C-O	5.33	1.30	1.24
1	A	369	LYS	N-CA	5.32	1.52	1.46
1	A	27	ALA	N-CA	5.31	1.52	1.46
1	B	458	ASN	N-CA	5.31	1.52	1.46
1	B	140	ASP	CA-C	5.30	1.59	1.52
1	B	204	ASP	C-O	-5.30	1.17	1.24
1	B	350	ILE	CA-CB	-5.30	1.47	1.54
1	B	460	ALA	CA-CB	5.30	1.61	1.53
1	B	85	ASP	N-CA	5.29	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	450	TYR	N-CA	-5.28	1.38	1.46
1	A	495	PRO	C-O	5.28	1.30	1.24
1	B	36	GLU	C-O	-5.27	1.17	1.24
1	A	447	ALA	CA-C	5.26	1.57	1.52
1	B	359	GLY	N-CA	5.26	1.50	1.44
1	B	263	ILE	CA-CB	5.25	1.60	1.54
1	B	258	LEU	N-CA	5.24	1.51	1.46
1	B	400	LEU	N-CA	5.24	1.52	1.46
1	B	82	VAL	N-CA	5.23	1.52	1.46
1	B	349	ALA	CA-C	-5.22	1.46	1.52
1	A	408	ILE	CA-CB	5.22	1.59	1.53
1	B	39	SER	CA-CB	5.22	1.61	1.53
1	B	123	PRO	CA-CB	5.22	1.60	1.53
1	B	536	ARG	CA-C	5.22	1.59	1.52
1	B	186	VAL	CA-CB	5.19	1.59	1.54
1	B	303	ASP	C-O	5.18	1.30	1.24
1	B	257	ASP	N-CA	5.18	1.52	1.46
1	B	560	THR	CA-C	5.17	1.59	1.52
1	A	295	ASP	C-O	-5.16	1.18	1.24
1	B	22	ARG	C-O	-5.15	1.17	1.24
1	A	327	GLN	N-CA	5.15	1.52	1.46
1	A	315	ALA	C-O	5.14	1.29	1.23
1	B	425	VAL	CA-CB	5.13	1.60	1.54
1	B	150	ASN	CA-CB	5.13	1.61	1.53
1	B	12	GLY	N-CA	5.12	1.52	1.45
1	B	335	MSE	SE-CE	-5.12	1.80	1.95
1	B	16	ALA	CA-C	5.12	1.59	1.52
1	A	41	ALA	C-O	5.11	1.29	1.23
1	A	422	ARG	N-CA	5.11	1.52	1.46
1	B	155	THR	CA-CB	5.10	1.61	1.53
1	A	265	VAL	CA-CB	5.10	1.63	1.55
1	A	331	ALA	C-O	-5.10	1.18	1.24
1	B	410	GLY	C-O	-5.08	1.18	1.24
1	A	230	ALA	CA-C	5.08	1.59	1.52
1	B	133	LEU	C-O	5.07	1.29	1.23
1	A	292	GLN	CB-CG	-5.06	1.37	1.52
1	B	105	SER	C-O	5.06	1.30	1.23
1	B	178	THR	CA-CB	5.06	1.63	1.53
1	B	287	VAL	C-O	5.05	1.28	1.24
1	A	27	ALA	C-O	-5.05	1.17	1.23
1	A	302	GLY	CA-C	5.05	1.57	1.52
1	B	253	LEU	N-CA	5.05	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	ASP	C-O	-5.04	1.17	1.24
1	A	49	ILE	CA-CB	5.03	1.61	1.54
1	A	509	ILE	C-O	-5.02	1.18	1.24
1	B	151	VAL	N-CA	5.02	1.52	1.46
1	A	240	ILE	CA-CB	5.02	1.61	1.54
1	A	429	ALA	N-CA	5.02	1.52	1.46
1	B	359	GLY	CA-C	5.01	1.56	1.52

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	511	VAL	CB-CA-C	-9.99	96.68	112.16
1	A	304	ALA	N-CA-C	8.75	123.05	112.38
1	A	292	GLN	CB-CA-C	8.51	123.57	109.53
1	B	98	ASP	CB-CA-C	-8.33	95.53	109.03
1	A	174	GLY	N-CA-C	-7.99	103.98	115.64
1	A	517	ARG	N-CA-C	-7.56	103.13	112.88
1	B	119	VAL	CA-C-N	-7.56	112.60	120.38
1	B	119	VAL	C-N-CA	-7.56	112.60	120.38
1	B	107	ASP	N-CA-C	-7.47	102.07	112.45
1	A	136	ILE	CA-C-N	-7.24	111.32	119.28
1	A	136	ILE	C-N-CA	-7.24	111.32	119.28
1	B	498	LEU	CA-C-N	7.18	130.22	120.38
1	B	498	LEU	C-N-CA	7.18	130.22	120.38
1	B	147	GLN	N-CA-C	6.97	118.77	111.03
1	A	246	LEU	CA-C-N	-6.94	113.15	122.72
1	A	246	LEU	C-N-CA	-6.94	113.15	122.72
1	A	535	LEU	N-CA-C	6.83	119.73	111.40
1	A	122	ILE	CA-C-N	-6.68	112.88	119.76
1	A	122	ILE	C-N-CA	-6.68	112.88	119.76
1	B	20	ALA	N-CA-C	-6.64	104.13	111.36
1	B	88	ALA	N-CA-C	6.63	120.97	113.01
1	B	403	PRO	CA-C-N	-6.52	116.33	122.66
1	B	403	PRO	C-N-CA	-6.52	116.33	122.66
1	A	479	GLN	N-CA-C	-6.39	106.45	114.56
1	A	195	ALA	N-CA-C	6.38	120.63	112.34
1	A	20	ALA	N-CA-C	-6.36	104.44	111.82
1	A	399	LEU	CA-C-N	6.33	131.46	122.72
1	A	399	LEU	C-N-CA	6.33	131.46	122.72
1	A	138	ASP	N-CA-C	-6.33	104.38	111.28
1	B	272	ALA	N-CA-C	6.33	118.17	111.28
1	A	147	GLN	CA-C-O	6.29	127.08	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ALA	N-CA-C	6.27	119.08	110.24
1	B	343	GLN	N-CA-C	6.21	120.12	111.56
1	A	448	PRO	N-CA-C	6.17	118.23	110.70
1	B	134	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	A	541	TYR	N-CA-C	5.97	117.45	111.07
1	A	82	VAL	N-CA-C	-5.94	107.47	113.47
1	A	453	ALA	N-CA-C	5.93	118.51	111.33
1	B	422	ARG	N-CA-C	5.91	117.72	111.28
1	A	23	LEU	N-CA-C	5.89	118.65	111.82
1	B	195	ALA	N-CA-C	5.87	119.54	112.38
1	B	119	VAL	CA-C-O	5.81	122.38	119.12
1	B	251	GLY	N-CA-C	5.79	123.06	115.47
1	A	416	LYS	CD-CE-NZ	-5.77	93.43	111.90
1	B	303	ASP	CB-CG-OD1	-5.75	105.17	118.40
1	A	390	PRO	N-CA-C	5.74	120.22	111.15
1	B	69	ALA	N-CA-C	5.74	118.03	111.02
1	B	547	ASN	N-CA-C	5.73	119.25	112.72
1	A	224	THR	N-CA-C	-5.68	106.34	113.72
1	A	27	ALA	N-CA-C	5.64	118.41	110.23
1	A	67	PHE	N-CA-C	5.61	118.12	111.33
1	A	454	LYS	CD-CE-NZ	5.61	129.84	111.90
1	A	19	ARG	N-CA-C	5.60	118.10	111.33
1	B	521	LEU	CA-C-N	-5.58	113.97	119.99
1	B	521	LEU	C-N-CA	-5.58	113.97	119.99
1	A	166	MSE	N-CA-C	5.54	117.76	111.11
1	B	325	ASN	N-CA-C	-5.54	105.16	111.14
1	A	227	ALA	N-CA-C	-5.54	103.08	110.55
1	B	161	PHE	N-CA-C	5.53	118.02	111.33
1	A	65	GLU	N-CA-C	-5.52	105.27	112.23
1	B	338	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	A	152	GLU	N-CA-C	-5.51	107.57	114.56
1	B	541	TYR	N-CA-C	5.50	117.71	111.11
1	A	119	VAL	CB-CA-C	-5.43	104.89	110.71
1	B	475	ILE	N-CA-C	-5.43	100.49	108.85
1	B	535	LEU	CD1-CG-CD2	-5.40	98.93	110.80
1	B	167	MSE	N-CA-C	5.39	117.58	111.11
1	B	302	GLY	CA-C-N	5.38	128.03	120.28
1	B	302	GLY	C-N-CA	5.38	128.03	120.28
1	A	171	HIS	N-CA-C	-5.38	105.50	111.36
1	A	482	ASN	CB-CA-C	-5.36	103.76	111.70
1	B	543	GLN	N-CA-C	5.36	117.12	111.28
1	B	539	VAL	N-CA-C	-5.35	105.28	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	GLN	CA-C-O	5.30	124.60	118.55
1	A	86	ARG	N-CA-C	5.26	117.10	111.36
1	A	426	MSE	CA-C-N	-5.26	113.23	120.28
1	A	426	MSE	C-N-CA	-5.26	113.23	120.28
1	B	357	ALA	N-CA-C	-5.25	101.32	109.72
1	A	34	ARG	CB-CG-CD	5.21	123.29	111.30
1	B	103	GLN	N-CA-C	5.21	118.56	110.17
1	B	479	GLN	N-CA-C	-5.21	107.95	114.56
1	A	466	ASN	CA-C-O	-5.20	115.34	120.90
1	B	452	SER	N-CA-C	-5.20	101.17	109.07
1	B	22	ARG	N-CA-C	-5.18	105.81	111.82
1	A	26	THR	N-CA-C	5.16	117.81	111.82
1	A	338	ARG	N-CA-C	5.11	118.78	112.54
1	A	119	VAL	N-CA-C	5.11	112.92	107.76
1	B	436	VAL	N-CA-CB	5.10	117.48	110.54
1	B	218	VAL	CA-C-N	-5.08	115.84	123.00
1	B	218	VAL	C-N-CA	-5.08	115.84	123.00
1	B	305	VAL	N-CA-C	5.06	115.19	108.11
1	B	58	ALA	N-CA-C	5.04	118.53	112.38
1	A	446	TYR	N-CA-C	5.04	116.99	108.02
1	B	209	LEU	CB-CA-C	-5.01	102.07	110.19
1	A	382	THR	CB-CA-C	5.01	118.76	109.70

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	4301	0	4303	123	1
1	B	4294	0	4300	139	1
2	A	1	0	0	1	0
2	B	1	0	0	2	0
3	A	53	0	31	6	0
3	B	53	0	31	3	0
4	A	48	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	48	0	32	4	0
5	A	264	0	0	4	0
5	B	281	0	0	12	0
All	All	9344	0	8729	255	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 15.

All (255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:MSE:HE3	1:A:339:GLU:HA	1.17	1.14
1:A:475:ILE:HG23	1:A:552:ARG:HD3	1.31	1.11
1:A:474:PRO:HB3	1:A:555:ILE:HD11	1.34	1.10
1:B:243:HIS:CE1	1:B:255:GLU:HG3	1.93	1.03
1:B:243:HIS:HE1	1:B:255:GLU:HG3	1.24	1.01
1:A:421:LYS:HD2	1:B:424:ASP:OD2	1.59	1.01
1:A:290:MSE:CE	1:A:339:GLU:HA	1.90	1.01
1:A:474:PRO:CB	1:A:555:ILE:HD11	1.91	0.99
1:B:318:VAL:HG22	1:B:318:VAL:O	1.63	0.98
1:A:290:MSE:HE3	1:A:339:GLU:CA	1.97	0.94
1:A:518:MSE:HE2	1:A:549:TYR:HE1	1.31	0.94
1:B:67:PHE:CD1	1:B:73:VAL:HG11	2.02	0.93
1:B:482:ASN:O	1:B:483:LEU:HB2	1.67	0.92
1:B:288:ASN:HD21	1:B:292:GLN:HE21	1.18	0.92
1:A:13:GLY:O	1:A:31:MSE:HE1	1.73	0.88
1:A:43:CYS:HG	4:A:901:COA:HS1	0.88	0.88
1:A:475:ILE:HG23	1:A:552:ARG:CD	2.04	0.86
1:A:475:ILE:CG2	1:A:552:ARG:HD3	2.06	0.86
1:B:518:MSE:HE1	1:B:547:ASN:HB2	1.59	0.85
1:B:250:ASN:ND2	1:B:252:GLU:OE1	2.09	0.85
1:A:454:LYS:HE3	1:B:325:ASN:HB3	1.60	0.83
1:A:6:ILE:HG21	1:A:31:MSE:HE2	1.60	0.83
1:B:223:GLN:HE21	1:B:224:THR:N	1.75	0.83
1:A:518:MSE:HE1	1:A:547:ASN:HB2	1.62	0.82
1:A:518:MSE:CE	1:A:549:TYR:CE1	2.63	0.81
1:B:127:ASN:OD1	1:B:130:THR:HG23	1.81	0.81
1:B:211:LEU:O	1:B:213:THR:HG22	1.81	0.80
1:A:518:MSE:HE2	1:A:549:TYR:CE1	2.15	0.80
1:B:318:VAL:O	1:B:318:VAL:CG2	2.30	0.80
1:A:290:MSE:HE1	1:A:339:GLU:HG2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:MSE:HE3	1:A:544:LEU:HD23	1.63	0.79
1:B:531:CYS:SG	2:B:575:CL:CL	2.78	0.79
1:B:500:ASN:HB3	5:B:803:HOH:O	1.82	0.78
1:B:346:GLN:HE21	1:B:430:GLN:HE21	1.31	0.75
1:B:127:ASN:CG	1:B:130:THR:HG23	2.11	0.75
1:A:168:GLU:HG2	5:A:922:HOH:O	1.86	0.74
1:A:518:MSE:CE	1:A:549:TYR:HE1	2.00	0.74
1:A:288:ASN:HD21	1:A:292:GLN:HE21	1.34	0.73
1:A:290:MSE:CE	1:A:339:GLU:HG2	2.18	0.73
1:B:518:MSE:HE3	1:B:544:LEU:HD23	1.71	0.73
1:B:402:ASP:OD2	5:B:624:HOH:O	2.07	0.73
1:A:1:MSE:HG3	1:A:1:MSE:O	1.90	0.72
1:B:67:PHE:HD1	1:B:73:VAL:HG11	1.50	0.71
1:A:211:LEU:CD1	1:A:211:LEU:N	2.54	0.70
1:B:295:ASP:OD2	5:B:765:HOH:O	2.10	0.70
1:B:10:VAL:HG12	1:B:11:ALA:N	2.07	0.70
1:A:13:GLY:O	1:A:31:MSE:CE	2.40	0.69
1:A:223:GLN:HE21	1:A:225:HIS:H	1.39	0.69
1:A:531:CYS:SG	2:A:575:CL:CL	2.88	0.68
1:B:178:THR:HG22	1:B:180:LEU:CD1	2.24	0.68
1:A:494:ASN:OD1	5:A:672:HOH:O	2.11	0.67
1:B:488:LEU:HD21	1:B:507:VAL:HG11	1.77	0.67
1:B:210:ARG:HB3	1:B:213:THR:HG21	1.76	0.67
1:B:483:LEU:HA	1:B:487:GLN:OE1	1.96	0.66
1:B:86:ARG:HD2	1:B:295:ASP:OD1	1.96	0.66
1:A:518:MSE:HE3	1:A:549:TYR:CE1	2.31	0.66
1:B:210:ARG:O	1:B:213:THR:HG23	1.96	0.66
1:B:273:ARG:HG2	1:B:279:ILE:HD13	1.78	0.66
1:B:250:ASN:OD1	1:B:252:GLU:HG3	1.95	0.66
1:B:130:THR:HB	1:B:259:LEU:HB3	1.78	0.65
1:A:17:ALA:HB2	1:A:31:MSE:HE3	1.77	0.65
1:A:211:LEU:N	1:A:211:LEU:HD12	2.11	0.65
1:B:518:MSE:HE1	1:B:547:ASN:CB	2.27	0.65
1:A:475:ILE:HG12	1:A:552:ARG:HB3	1.79	0.64
1:B:10:VAL:HG12	1:B:11:ALA:H	1.60	0.64
1:A:475:ILE:CG2	1:A:552:ARG:CD	2.71	0.64
1:A:290:MSE:HE1	1:A:339:GLU:CG	2.27	0.63
1:B:43:CYS:HG	4:B:901:COA:HS1	1.44	0.63
1:A:436:VAL:HG21	1:A:468:ILE:HD12	1.81	0.63
1:B:94:ARG:NH1	5:B:737:HOH:O	2.26	0.63
1:A:43:CYS:HG	4:A:901:COA:C2P	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLN:HE21	1:B:224:THR:H	1.44	0.63
1:A:17:ALA:HB2	1:A:31:MSE:CE	2.29	0.62
1:B:110:LEU:HB2	1:B:335:MSE:HE1	1.82	0.62
1:A:425:VAL:HG13	1:B:428:VAL:HG21	1.82	0.62
1:A:209:LEU:HD22	1:A:211:LEU:HD11	1.81	0.61
1:B:518:MSE:HE2	1:B:549:TYR:CE1	2.35	0.61
1:B:127:ASN:HD21	1:B:130:THR:CG2	2.13	0.61
1:B:223:GLN:HE21	1:B:225:HIS:H	1.48	0.61
1:B:38:VAL:O	1:B:39:SER:HB2	1.99	0.61
1:B:120:PRO:HB2	1:B:122:ILE:HG13	1.82	0.61
1:A:243:HIS:HE1	1:A:255:GLU:OE2	1.84	0.61
1:B:67:PHE:CD1	1:B:73:VAL:CG1	2.83	0.60
1:B:517:ARG:O	1:B:520:GLU:HG3	2.00	0.60
1:B:290:MSE:O	1:B:291:MSE:HB2	2.01	0.60
1:B:56:ARG:HD2	5:B:659:HOH:O	2.01	0.60
1:B:490:LEU:HD12	1:B:507:VAL:O	2.01	0.60
1:A:186:VAL:O	1:A:187:MSE:O	2.19	0.60
1:A:474:PRO:CB	1:A:555:ILE:CD1	2.76	0.59
1:A:475:ILE:HD12	1:A:554:LEU:HA	1.85	0.59
1:B:127:ASN:HD21	1:B:130:THR:HG21	1.66	0.59
1:B:518:MSE:HE2	1:B:549:TYR:HE1	1.68	0.59
1:B:131:HIS:HE1	1:B:145:THR:OG1	1.86	0.58
1:A:209:LEU:HD22	1:A:211:LEU:CD1	2.33	0.58
1:B:223:GLN:NE2	1:B:224:THR:N	2.50	0.58
1:B:223:GLN:NE2	1:B:224:THR:H	2.01	0.57
1:B:43:CYS:SG	4:B:901:COA:S1P	2.95	0.57
1:B:67:PHE:HD1	1:B:73:VAL:CG1	2.15	0.57
1:B:55:GLN:HG2	5:B:878:HOH:O	2.04	0.57
1:B:127:ASN:ND2	1:B:130:THR:HG23	2.20	0.57
1:A:1:MSE:CE	1:A:28:GLU:HB2	2.35	0.57
1:B:500:ASN:C	1:B:500:ASN:HD22	2.12	0.57
1:A:13:GLY:C	1:A:31:MSE:HE1	2.29	0.56
1:B:127:ASN:ND2	1:B:130:THR:CG2	2.68	0.56
1:A:85:ASP:HB3	5:A:733:HOH:O	2.05	0.56
1:A:535:LEU:C	1:A:535:LEU:HD23	2.30	0.56
1:A:436:VAL:HG21	1:A:468:ILE:CD1	2.35	0.56
1:B:94:ARG:CZ	5:B:674:HOH:O	2.52	0.56
1:A:193:GLU:OE2	1:A:379:TYR:OH	2.22	0.56
1:A:25:GLU:OE2	1:B:543:GLN:HG2	2.07	0.55
1:A:1:MSE:HE1	1:A:28:GLU:HB2	1.89	0.55
1:A:475:ILE:O	1:A:554:LEU:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:HG11	3:B:900:FAD:O2A	2.07	0.55
1:B:223:GLN:NE2	1:B:225:HIS:H	2.05	0.55
1:B:211:LEU:O	1:B:213:THR:CG2	2.54	0.54
1:A:300:ALA:O	1:A:301:VAL:HG12	2.06	0.54
1:B:184:ASP:OD2	1:B:192:ARG:HD3	2.08	0.54
1:A:518:MSE:HE1	1:A:547:ASN:CB	2.36	0.54
1:A:428:VAL:HG21	1:B:425:VAL:HG13	1.90	0.53
1:B:120:PRO:HG3	1:B:261:MSE:HE2	1.90	0.53
1:A:378:VAL:HG12	1:A:399:LEU:HB3	1.90	0.53
1:A:474:PRO:HB2	1:A:555:ILE:HD11	1.84	0.53
1:A:110:LEU:HB2	1:A:335:MSE:HE1	1.90	0.53
1:B:500:ASN:C	1:B:500:ASN:ND2	2.66	0.53
1:A:301:VAL:HB	1:A:327:GLN:HB3	1.91	0.53
1:A:300:ALA:C	1:A:301:VAL:CG1	2.81	0.53
1:B:127:ASN:OD1	1:B:130:THR:CG2	2.55	0.53
1:B:243:HIS:CE1	1:B:255:GLU:CG	2.81	0.53
1:B:67:PHE:HB3	1:B:73:VAL:HG13	1.91	0.52
1:B:437:GLU:C	1:B:437:GLU:CD	2.77	0.52
1:B:459:GLN:O	1:B:463:VAL:HG23	2.10	0.52
1:A:290:MSE:CE	1:A:339:GLU:CG	2.84	0.51
1:A:385:HIS:O	1:A:386:ALA:C	2.53	0.51
1:B:273:ARG:HG2	1:B:279:ILE:CD1	2.39	0.51
1:B:178:THR:HG22	1:B:180:LEU:HD11	1.92	0.51
1:A:43:CYS:SG	4:A:901:COA:S1P	2.74	0.51
1:A:187:MSE:HG3	1:A:189:PRO:HD2	1.93	0.51
1:A:474:PRO:HB2	1:A:555:ILE:CD1	2.41	0.51
1:A:227:ALA:N	1:A:238:GLN:OE1	2.35	0.51
1:B:300:ALA:C	1:B:301:VAL:HG13	2.35	0.51
1:B:90:LEU:HG	1:B:103:GLN:HG2	1.93	0.50
1:A:10:VAL:HG12	1:A:11:ALA:N	2.26	0.50
1:A:6:ILE:CG2	1:A:31:MSE:HE2	2.38	0.50
1:A:34:ARG:HD3	3:A:900:FAD:O2B	2.12	0.50
1:A:420:ASP:OD2	1:B:421:LYS:NZ	2.41	0.50
1:B:309:ASP:OD2	1:B:363:LYS:NZ	2.39	0.50
1:A:209:LEU:CD2	1:A:211:LEU:HD11	2.42	0.50
1:B:243:HIS:HD2	5:B:753:HOH:O	1.94	0.49
1:B:127:ASN:HB2	1:B:128:PRO:HD2	1.93	0.49
1:A:503:LEU:HD12	1:A:530:PHE:CE2	2.47	0.49
1:B:300:ALA:C	1:B:301:VAL:CG1	2.86	0.49
1:A:112:SER:N	1:A:113:PRO:CD	2.75	0.49
1:A:33:GLU:OE2	1:A:34:ARG:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LEU:N	1:B:498:LEU:HD23	2.28	0.49
1:A:436:VAL:HG23	1:A:437[B]:GLU:H	1.77	0.49
1:B:250:ASN:CG	1:B:252:GLU:HG3	2.36	0.49
1:A:518:MSE:HE3	1:A:549:TYR:CD1	2.48	0.48
1:A:400:LEU:N	1:A:400:LEU:HD12	2.27	0.48
1:B:424:ASP:O	1:B:428:VAL:HG23	2.14	0.48
1:A:108:THR:HG21	1:A:335:MSE:HG2	1.95	0.48
1:B:215:LEU:CD1	1:B:246:LEU:HB3	2.43	0.48
1:B:376:GLU:HG3	1:B:377:LYS:N	2.26	0.48
1:A:13:GLY:C	1:A:31:MSE:CE	2.87	0.48
1:A:108:THR:HG22	1:A:335:MSE:HE2	1.95	0.48
1:B:88:ALA:HB1	1:B:90:LEU:HD22	1.96	0.47
1:A:541:TYR:C	1:A:541:TYR:CD2	2.91	0.47
1:A:112:SER:N	1:A:113:PRO:HD3	2.29	0.47
1:A:10:VAL:HG23	3:A:900:FAD:H4B	1.97	0.47
1:A:81:VAL:HG22	1:A:93:VAL:HG22	1.95	0.47
1:B:437:GLU:HB3	5:B:714:HOH:O	2.15	0.47
1:B:291:MSE:HE3	1:B:301:VAL:HG12	1.97	0.47
1:A:34:ARG:CD	3:A:900:FAD:O2B	2.63	0.46
1:A:377:LYS:HG3	1:A:398:LYS:HE3	1.97	0.46
1:A:535:LEU:HD23	1:A:536:ARG:N	2.30	0.46
1:A:221:GLN:HE22	1:A:245:SER:HB2	1.81	0.46
1:B:290:MSE:HE3	1:B:292:GLN:NE2	2.29	0.46
1:B:300:ALA:O	1:B:301:VAL:CG1	2.63	0.46
1:A:475:ILE:HD12	1:A:554:LEU:CA	2.45	0.46
1:B:34:ARG:HD3	3:B:900:FAD:O2B	2.15	0.46
1:B:465:SER:O	1:B:469:LYS:HD3	2.15	0.46
1:A:164:LEU:HD12	1:A:187:MSE:HE2	1.98	0.46
1:B:182:LEU:O	1:B:212:GLY:HA2	2.16	0.46
1:A:86:ARG:HD2	1:A:295:ASP:OD1	2.16	0.46
1:B:225:HIS:NE2	1:B:233:GLU:OE2	2.43	0.46
1:A:214:ALA:HB3	1:A:249:SER:HB3	1.98	0.45
1:A:424:ASP:OD2	1:B:421:LYS:HD2	2.16	0.45
1:A:125:VAL:HG13	1:A:126:ASP:N	2.31	0.45
1:B:305:VAL:HG23	1:B:305:VAL:O	2.15	0.45
1:B:500:ASN:HD22	1:B:501:GLY:N	2.14	0.45
1:A:475:ILE:HD12	1:A:475:ILE:O	2.17	0.45
1:B:179:LEU:C	1:B:180:LEU:HD12	2.41	0.45
1:A:300:ALA:C	1:A:301:VAL:HG13	2.41	0.45
1:B:188:THR:N	1:B:189:PRO:CD	2.80	0.45
1:A:186:VAL:O	1:A:187:MSE:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:MSE:CE	1:A:549:TYR:CD1	3.00	0.44
1:A:114:GLY:HA2	1:A:303:ASP:HB2	1.99	0.44
1:A:475:ILE:CG1	1:A:552:ARG:HB3	2.46	0.44
1:B:300:ALA:O	1:B:301:VAL:HG12	2.17	0.44
1:B:10:VAL:CG1	1:B:11:ALA:H	2.22	0.44
1:B:243:HIS:HE1	1:B:255:GLU:CG	2.11	0.44
1:B:485:GLU:O	1:B:525:LYS:HE3	2.18	0.44
1:A:33:GLU:OE2	3:A:900:FAD:H1B	2.18	0.44
1:B:106:TYR:CD2	1:B:106:TYR:C	2.95	0.44
1:B:176:LYS:HG2	5:B:1025:HOH:O	2.17	0.44
1:B:96:LEU:O	1:B:97:LEU:C	2.61	0.44
1:B:10:VAL:O	1:B:14:ALA:HB3	2.17	0.44
1:A:191:ASP:OD2	1:A:398:LYS:NZ	2.50	0.43
1:A:300:ALA:O	1:A:301:VAL:CG1	2.66	0.43
1:B:33:GLU:OE2	1:B:34:ARG:N	2.51	0.43
1:B:50:SER:OG	1:B:52:GLU:OE1	2.19	0.43
1:A:190:VAL:HG11	1:A:358:VAL:CG1	2.49	0.43
1:B:38:VAL:O	1:B:39:SER:CB	2.67	0.43
1:B:497:GLU:C	1:B:499:GLN:N	2.75	0.43
1:B:115:ALA:HB2	1:B:303:ASP:HB3	1.99	0.43
1:B:67:PHE:HB3	1:B:73:VAL:CG1	2.49	0.43
1:B:280:GLY:HA3	1:B:306:GLU:OE1	2.19	0.43
1:B:307:GLU:CD	1:B:327:GLN:HE22	2.27	0.43
1:B:385:HIS:HB3	1:B:450:TYR:O	2.18	0.43
1:A:288:ASN:HD21	1:A:292:GLN:NE2	2.08	0.43
1:B:301:VAL:HB	1:B:327:GLN:HB3	2.01	0.42
1:A:10:VAL:HG11	3:A:900:FAD:O2A	2.19	0.42
1:B:378:VAL:HG11	1:B:463:VAL:HB	2.01	0.42
1:A:131:HIS:CE1	1:A:141:ARG:HG2	2.54	0.42
1:B:187:MSE:C	1:B:189:PRO:HD2	2.44	0.42
1:B:223:GLN:HE21	1:B:223:GLN:C	2.27	0.42
1:B:454:LYS:HB2	1:B:454:LYS:HE3	1.64	0.42
1:A:221:GLN:NE2	1:A:245:SER:HB2	2.35	0.42
1:B:201:ALA:CB	1:B:356:LEU:HD22	2.50	0.42
1:B:11:ALA:HB2	4:B:901:COA:H31	2.02	0.42
1:B:180:LEU:CD1	1:B:180:LEU:N	2.83	0.42
1:A:49:ILE:HG12	1:A:143:LEU:HD13	2.01	0.41
1:A:423:ILE:HD13	1:A:423:ILE:HA	1.83	0.41
1:B:10:VAL:HG23	3:B:900:FAD:H4B	2.02	0.41
1:B:529:ILE:HD11	1:B:544:LEU:HD12	2.02	0.41
1:A:188:THR:N	1:A:189:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLU:OE2	5:B:991:HOH:O	2.21	0.41
1:B:321:ALA:HB1	4:B:901:COA:H21	2.02	0.41
1:A:194:MSE:HE3	1:A:414:VAL:HG23	2.02	0.41
1:A:329:ARG:HD2	5:A:698:HOH:O	2.20	0.41
1:B:418:GLY:N	5:B:721:HOH:O	2.42	0.41
1:B:533:VAL:HG22	2:B:575:CL:CL	2.58	0.41
1:B:114:GLY:HA2	1:B:303:ASP:HB2	2.03	0.41
1:B:181:GLU:OE2	1:B:183:ALA:N	2.49	0.41
1:B:346:GLN:HG2	1:B:430:GLN:NE2	2.35	0.41
1:A:303:ASP:OD2	3:A:900:FAD:H5'1	2.21	0.41
1:A:240:ILE:HD13	1:A:240:ILE:HG21	1.69	0.40
1:A:333:ASP:OD2	1:A:340:GLU:OE1	2.39	0.40
1:A:434:MSE:HE1	1:A:442:LEU:HD21	2.02	0.40
1:B:269:THR:O	1:B:273:ARG:HG3	2.21	0.40
1:B:561:TYR:CD2	1:B:561:TYR:C	2.98	0.40
1:B:178:THR:HA	1:B:208:ASP:O	2.21	0.40
1:A:34:ARG:HG2	1:A:35:GLY:N	2.36	0.40
1:A:45:LEU:HB2	1:A:46:PRO:HD3	2.03	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]	2.15	0.05

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	564/574 (98%)	537 (95%)	24 (4%)	3 (0%)	24 21
1	B	563/574 (98%)	535 (95%)	24 (4%)	4 (1%)	18 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1127/1148 (98%)	1072 (95%)	48 (4%)	7 (1%)	21	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	MSE
1	B	10	VAL
1	B	482	ASN
1	A	10	VAL
1	A	294	SER
1	B	97	LEU
1	B	483	LEU

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	450/443 (102%)	417 (93%)	33 (7%)	13	9
1	B	449/443 (101%)	401 (89%)	48 (11%)	6	4
All	All	899/886 (102%)	818 (91%)	81 (9%)	9	6

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	34	ARG
1	A	42	ASN
1	A	90	LEU
1	A	97	LEU
1	A	129	LEU
1	A	132	SER
1	A	143	LEU
1	A	192	ARG
1	A	209	LEU
1	A	211	LEU

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Mol	Chain	Res	Type
1	A	238	GLN
1	A	241	LYS
1	A	253	LEU
1	A	254	LEU
1	A	259	LEU
1	A	266	ARG
1	A	281	GLU
1	A	282	LEU
1	A	292	GLN
1	A	301	VAL
1	A	356	LEU
1	A	363	LYS
1	A	377	LYS
1	A	378	VAL
1	A	382	THR
1	A	475	ILE
1	A	483	LEU
1	A	485	GLU
1	A	490	LEU
1	A	504	GLU
1	A	523	LYS
1	A	524	ASP
1	B	34	ARG
1	B	42	ASN
1	B	52	GLU
1	B	55	GLN
1	B	67	PHE
1	B	90	LEU
1	B	97	LEU
1	B	98	ASP
1	B	101	GLU
1	B	103	GLN
1	B	130	THR
1	B	136	ILE
1	B	144	GLN
1	B	176	LYS
1	B	180	LEU
1	B	182	LEU
1	B	209	LEU
1	B	213	THR
1	B	221	GLN
1	B	228	SER

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Mol	Chain	Res	Type
1	B	229	ASP
1	B	238	GLN
1	B	241	LYS
1	B	246	LEU
1	B	253	LEU
1	B	254	LEU
1	B	255	GLU
1	B	267	PRO
1	B	271	LEU
1	B	281	GLU
1	B	292	GLN
1	B	318	VAL
1	B	343	GLN
1	B	356	LEU
1	B	380	VAL
1	B	407	THR
1	B	436	VAL
1	B	437	GLU
1	B	445	SER
1	B	482	ASN
1	B	483	LEU
1	B	498	LEU
1	B	500	ASN
1	B	507	VAL
1	B	511	VAL
1	B	545	VAL
1	B	560	THR
1	B	565	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	221	GLN
1	A	223	GLN
1	A	243	HIS
1	A	292	GLN
1	A	343	GLN
1	A	385	HIS
1	A	441	HIS
1	A	500	ASN
1	A	546	ASN

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Mol	Chain	Res	Type
1	A	547	ASN
1	B	62	GLN
1	B	131	HIS
1	B	144	GLN
1	B	171	HIS
1	B	172	HIS
1	B	200	GLN
1	B	205	GLN
1	B	221	GLN
1	B	223	GLN
1	B	243	HIS
1	B	292	GLN
1	B	343	GLN
1	B	370	GLN
1	B	430	GLN
1	B	500	ASN
1	B	547	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
3	FAD	B	900	-	58,58,58	1.43	11 (18%)	85,89,89	1.97	24 (28%)
4	COA	B	901	-	47,50,50	1.54	9 (19%)	69,75,75	2.12	23 (33%)
3	FAD	A	900	-	58,58,58	1.46	11 (18%)	85,89,89	1.80	20 (23%)
4	COA	A	901	-	47,50,50	1.61	10 (21%)	69,75,75	1.99	14 (20%)

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
3	FAD	B	900	-	-	0/34/50/50	0/6/6/6
4	COA	B	901	-	-	5/48/64/64	0/3/3/3
3	FAD	A	900	-	-	0/34/50/50	0/6/6/6
4	COA	A	901	-	-	4/48/64/64	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	COA	O9P-C9P	6.19	1.35	1.23
4	B	901	COA	O9P-C9P	5.36	1.33	1.23
4	B	901	COA	C2A-N1A	4.34	1.41	1.33
3	A	900	FAD	C2A-N1A	4.10	1.41	1.33
3	B	900	FAD	C10-N1	3.73	1.40	1.33
4	A	901	COA	C8A-N9A	3.05	1.42	1.37
4	A	901	COA	C5A-N7A	-3.00	1.33	1.39
3	B	900	FAD	P-O3P	2.89	1.62	1.59
3	A	900	FAD	C4X-N5	2.86	1.36	1.30
3	A	900	FAD	C2A-N3A	2.86	1.39	1.33
3	B	900	FAD	C2A-N1A	2.84	1.39	1.33
4	B	901	COA	C2A-N3A	2.81	1.38	1.33
3	B	900	FAD	C6-C5X	2.78	1.44	1.40
3	A	900	FAD	O4B-C4B	-2.78	1.38	1.45
3	B	900	FAD	C5X-N5	2.72	1.44	1.39
4	B	901	COA	C8A-N7A	2.64	1.36	1.31
3	B	900	FAD	C4A-N3A	2.62	1.39	1.34
3	A	900	FAD	C5'-C4'	2.62	1.55	1.51
4	B	901	COA	CCP-CBP	2.60	1.56	1.52
3	B	900	FAD	C6-C7	2.54	1.43	1.39
3	A	900	FAD	C4'-C3'	2.50	1.57	1.53
4	B	901	COA	C6A-N1A	2.43	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C4-N3	-2.42	1.34	1.38
3	A	900	FAD	C10-N1	2.40	1.38	1.33
3	B	900	FAD	O2'-C2'	-2.37	1.38	1.43
4	A	901	COA	C2A-N1A	2.37	1.38	1.33
3	B	900	FAD	C5A-N7A	-2.36	1.34	1.39
4	B	901	COA	C5A-N7A	-2.27	1.34	1.39
4	A	901	COA	P1A-O2A	-2.24	1.45	1.55
4	A	901	COA	P3B-O9A	-2.22	1.46	1.54
3	A	900	FAD	C4X-C10	-2.21	1.37	1.44
4	B	901	COA	C8A-N9A	2.19	1.41	1.37
3	A	900	FAD	C9A-C5X	-2.14	1.37	1.41
3	B	900	FAD	C1'-C2'	2.10	1.55	1.52
4	B	901	COA	C4A-N3A	2.09	1.38	1.34
3	B	900	FAD	O4B-C1B	2.08	1.46	1.42
4	A	901	COA	O3B-C3B	-2.06	1.37	1.44
4	A	901	COA	OAP-CAP	-2.05	1.38	1.42
4	A	901	COA	P1A-O3A	-2.04	1.57	1.59
3	A	900	FAD	C6-C5X	2.03	1.43	1.40
4	A	901	COA	C8A-N7A	2.01	1.35	1.31

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	COA	N3A-C2A-N1A	-7.06	117.90	128.58
4	A	901	COA	N3A-C2A-N1A	-5.98	119.53	128.58
3	B	900	FAD	N3A-C2A-N1A	-5.83	119.76	128.58
4	B	901	COA	N9A-C8A-N7A	-5.57	106.03	113.94
3	B	900	FAD	N9A-C8A-N7A	-5.41	106.26	113.94
4	A	901	COA	N9A-C8A-N7A	-5.16	106.61	113.94
3	A	900	FAD	N3A-C2A-N1A	-4.99	121.03	128.58
3	A	900	FAD	N9A-C8A-N7A	-4.85	107.06	113.94
4	A	901	COA	CEP-CBP-CDP	-4.59	100.05	109.20
3	B	900	FAD	C4A-N9A-C8A	4.28	110.23	105.74
4	B	901	COA	C5A-N7A-C8A	4.17	110.01	103.45
4	B	901	COA	C2A-N3A-C4A	4.11	121.87	111.83
4	A	901	COA	C5A-N7A-C8A	3.99	109.72	103.45
3	A	900	FAD	C5A-C4A-N3A	-3.98	121.23	126.72
4	B	901	COA	C7P-C6P-C5P	-3.91	105.88	112.39
3	A	900	FAD	C5A-N7A-C8A	3.89	109.57	103.45
4	A	901	COA	CDP-CBP-CAP	3.84	115.31	108.77
3	A	900	FAD	O4'-C4'-C3'	-3.83	100.29	109.25
3	B	900	FAD	O3B-C3B-C4B	3.82	122.06	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	900	FAD	C5A-N7A-C8A	3.79	109.41	103.45
4	A	901	COA	O3A-P1A-O1A	-3.79	99.29	110.70
4	B	901	COA	C5A-C4A-N3A	-3.70	121.62	126.72
4	B	901	COA	O2A-P1A-O3A	3.62	117.06	107.27
4	A	901	COA	C2A-N3A-C4A	3.55	120.50	111.83
4	A	901	COA	O5A-P2A-O3A	3.52	116.78	107.27
3	B	900	FAD	O2B-C2B-C1B	3.49	122.14	110.10
4	A	901	COA	C5A-C4A-N3A	-3.39	122.05	126.72
3	A	900	FAD	C4A-N9A-C8A	3.35	109.25	105.74
3	B	900	FAD	C8M-C8-C9	-3.22	113.91	119.57
3	B	900	FAD	C9-C9A-N10	-3.21	117.54	121.85
3	A	900	FAD	C10-C4X-N5	-3.17	118.34	124.81
4	A	901	COA	C7P-C6P-C5P	-3.15	107.14	112.39
3	B	900	FAD	C4X-C10-N10	3.13	120.96	116.48
4	B	901	COA	CAP-C9P-N8P	3.13	122.41	116.48
3	A	900	FAD	O2A-PA-O3P	3.12	115.70	107.27
3	B	900	FAD	C5A-C4A-N3A	-3.10	122.44	126.72
3	B	900	FAD	C9A-C5X-N5	-3.08	119.19	122.45
4	B	901	COA	C4A-N9A-C8A	3.08	108.97	105.74
4	B	901	COA	CEP-CBP-CDP	-3.06	103.11	109.20
3	A	900	FAD	N3A-C4A-N9A	3.05	132.36	127.17
4	A	901	COA	O2A-P1A-O3A	3.00	115.38	107.27
3	B	900	FAD	N3A-C4A-N9A	2.99	132.25	127.17
4	A	901	COA	CDP-CBP-CCP	2.98	113.14	108.22
4	B	901	COA	N3A-C4A-N9A	2.97	132.22	127.17
3	B	900	FAD	O4B-C4B-C5B	-2.93	99.96	109.33
4	B	901	COA	O5A-P2A-O3A	2.92	115.17	107.27
3	A	900	FAD	C4-N3-C2	-2.91	120.47	125.64
3	B	900	FAD	C4B-O4B-C1B	-2.91	103.05	109.47
3	A	900	FAD	C4X-C10-N10	2.83	120.53	116.48
3	A	900	FAD	C2A-N3A-C4A	2.77	118.60	111.83
4	B	901	COA	OAP-CAP-CBP	-2.77	103.77	110.18
3	A	900	FAD	C4-C4X-C10	2.74	121.63	116.93
3	B	900	FAD	C2A-N3A-C4A	2.71	118.46	111.83
3	A	900	FAD	C4X-C10-N1	-2.67	118.04	124.59
4	B	901	COA	O9P-C9P-CAP	-2.67	113.44	120.89
3	A	900	FAD	C6A-C5A-C4A	2.65	120.79	117.18
4	A	901	COA	CAP-C9P-N8P	2.57	121.36	116.48
3	A	900	FAD	O4'-C4'-C5'	-2.57	104.33	109.99
4	B	901	COA	CDP-CBP-CCP	2.56	112.44	108.22
3	A	900	FAD	C9A-C5X-N5	-2.54	119.76	122.45
4	B	901	COA	C4A-N9A-C1B	-2.51	120.77	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	C4A-C5A-N7A	-2.49	107.73	110.58
3	B	900	FAD	C2B-C1B-N9A	2.46	119.42	113.30
3	B	900	FAD	O4B-C4B-C3B	2.45	110.01	105.15
4	B	901	COA	O3A-P2A-O4A	-2.39	103.52	110.70
4	B	901	COA	P3B-O3B-C3B	-2.39	117.06	123.43
3	A	900	FAD	C4X-C4-N3	2.38	119.31	113.25
3	A	900	FAD	C2B-C3B-C4B	2.34	107.13	102.61
4	B	901	COA	C5A-C6A-N6A	-2.34	117.50	123.29
4	A	901	COA	C2B-C3B-C4B	2.27	107.21	103.24
4	B	901	COA	O2B-C2B-C1B	2.23	117.80	110.10
3	B	900	FAD	C2A-N1A-C6A	2.23	122.40	118.73
3	B	900	FAD	C10-C4X-N5	-2.21	120.30	124.81
3	B	900	FAD	C5'-C4'-C3'	-2.20	108.06	112.22
3	B	900	FAD	O3P-PA-O1A	-2.20	104.07	110.70
4	B	901	COA	C2P-C3P-N4P	2.19	117.28	112.31
4	B	901	COA	O8A-P3B-O3B	2.15	114.22	105.85
3	B	900	FAD	C4X-C4-N3	2.13	118.67	113.25
3	B	900	FAD	O2'-C2'-C1'	-2.12	101.48	110.20
3	B	900	FAD	C10-N1-C2	2.11	121.41	116.85
4	B	901	COA	O4B-C1B-N9A	2.03	111.99	108.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	901	COA	C6P-C5P-N4P-C3P
4	A	901	COA	P2A-O3A-P1A-O5B
4	B	901	COA	P2A-O3A-P1A-O5B
4	A	901	COA	CDP-CBP-CCP-O6A
4	B	901	COA	O5P-C5P-N4P-C3P
4	B	901	COA	P1A-O3A-P2A-O4A
4	B	901	COA	S1P-C2P-C3P-N4P
4	A	901	COA	P1A-O3A-P2A-O4A
4	A	901	COA	P1A-O3A-P2A-O5A

There are no ring outliers.

4 monomers are involved in 16 short contacts:

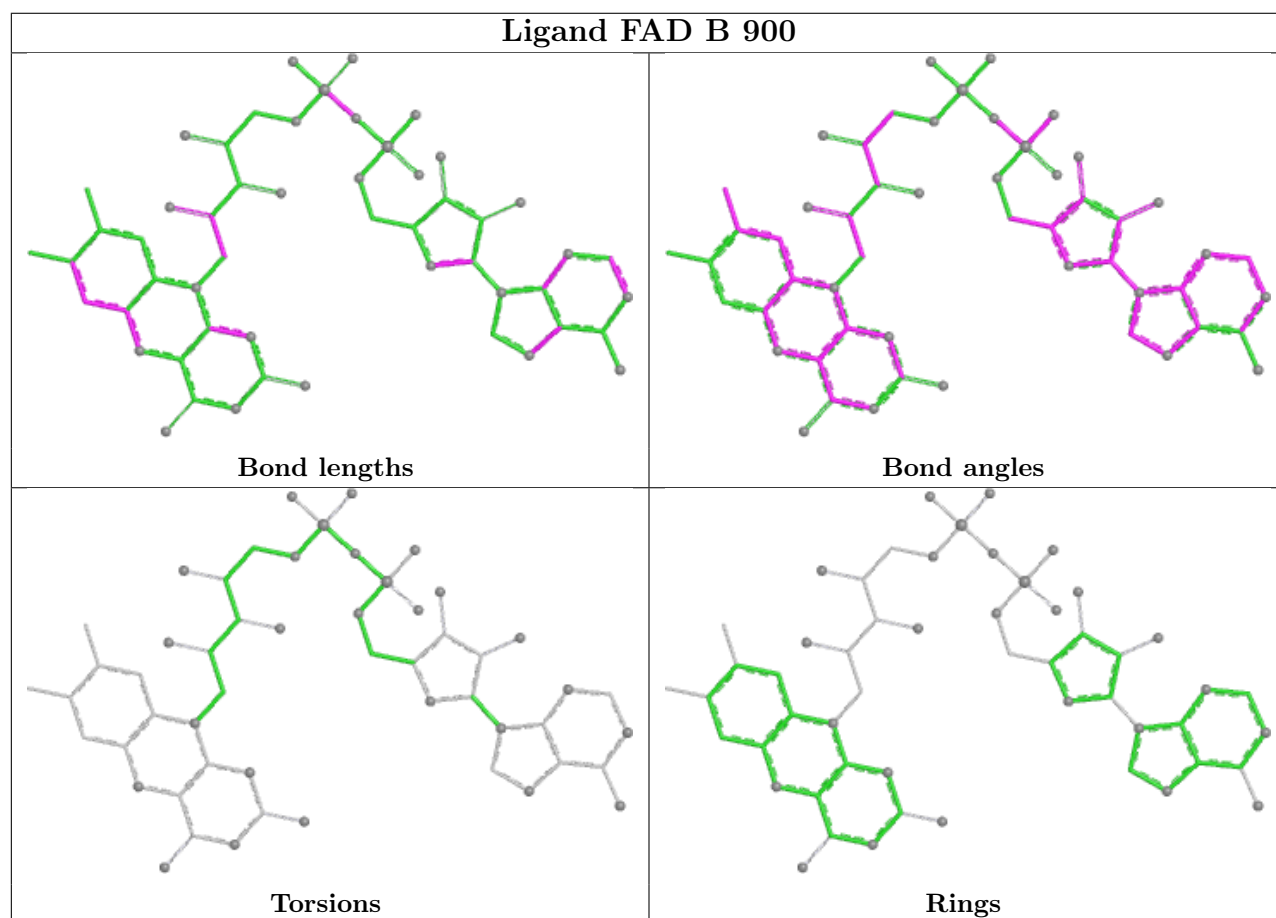
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	900	FAD	3	0
4	B	901	COA	4	0

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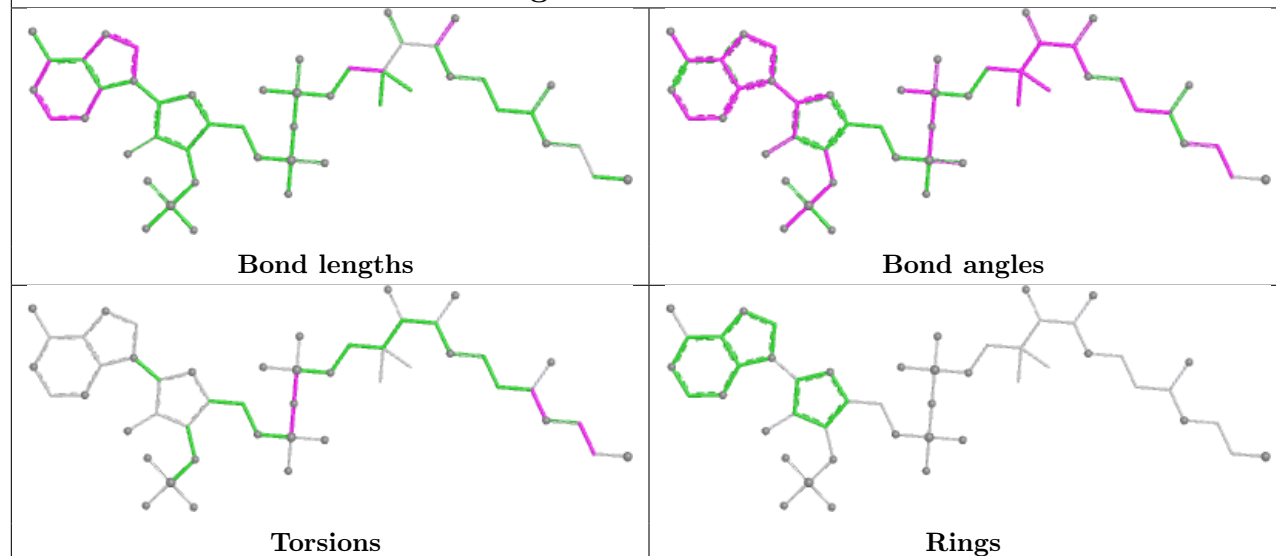
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	6	0
4	A	901	COA	3	0

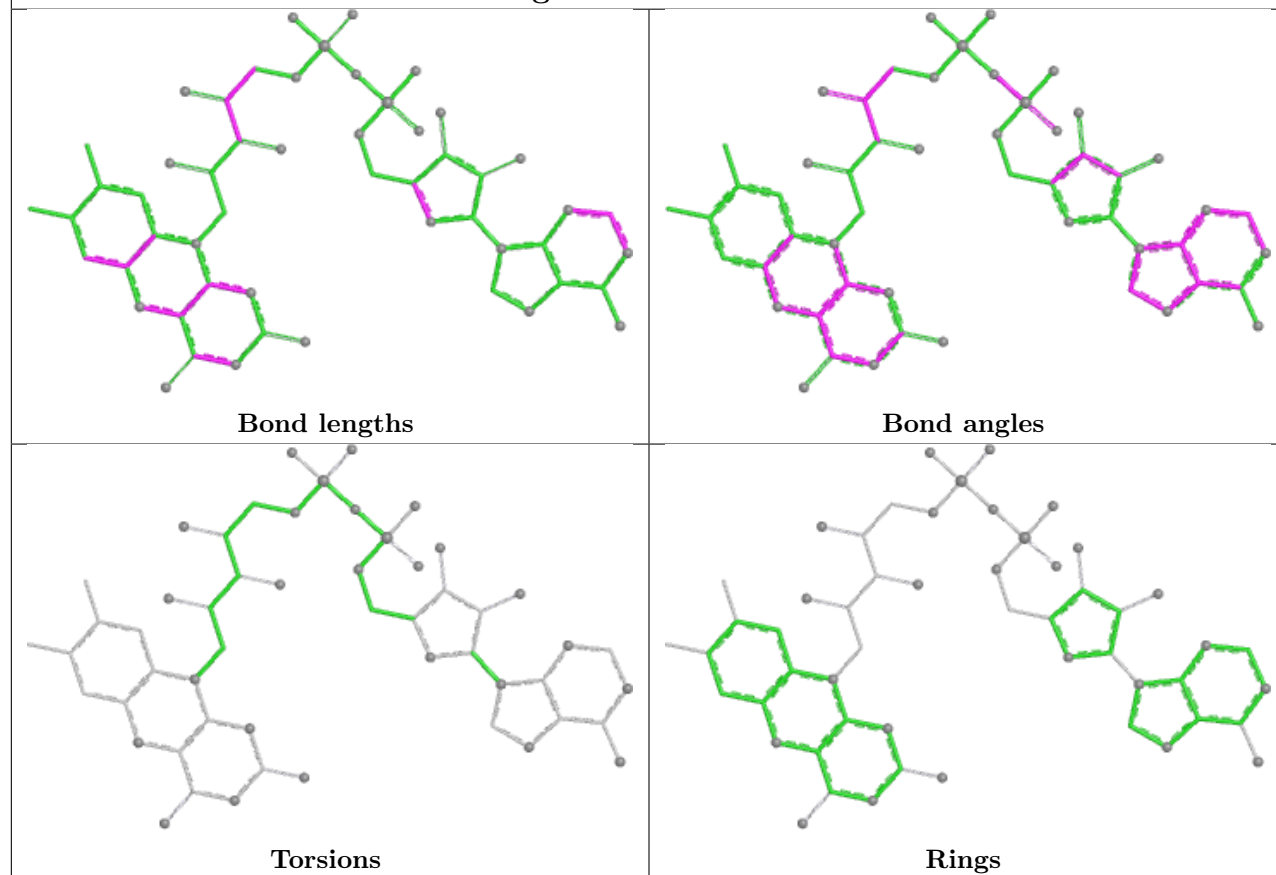
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

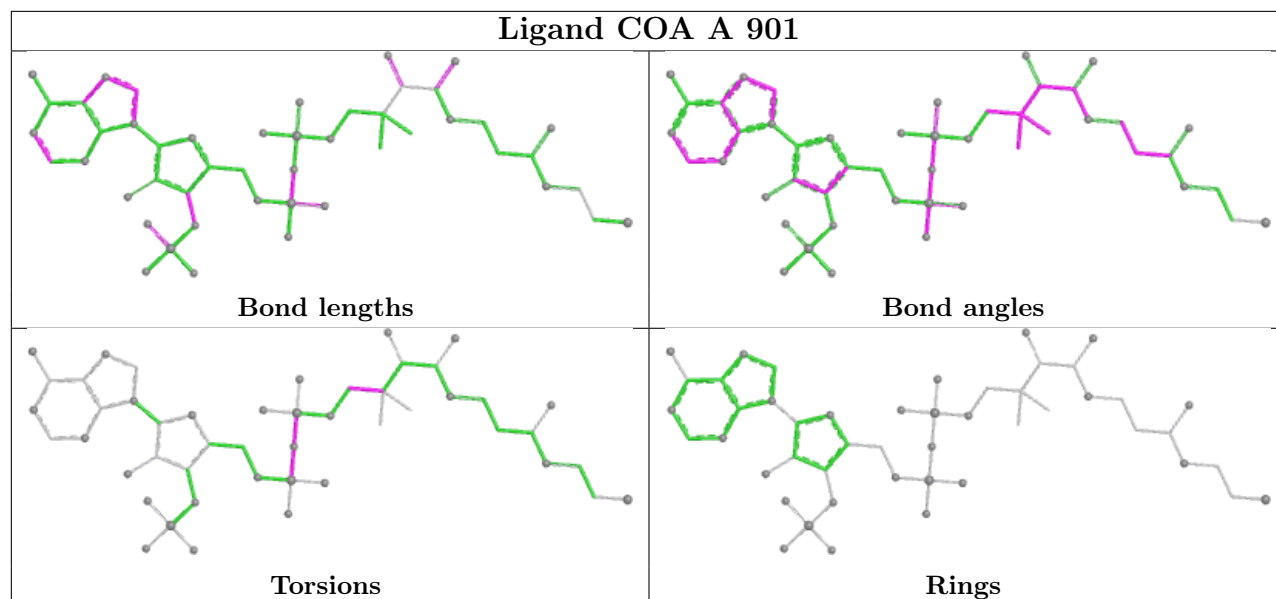


Ligand COA B 901



Ligand FAD A 900





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	549/574 (95%)	-0.19	13 (2%) 59 59	24, 36, 54, 73	1 (0%)
1	B	549/574 (95%)	-0.21	15 (2%) 56 55	27, 36, 52, 66	0
All	All	1098/1148 (95%)	-0.20	28 (2%) 57 56	24, 36, 53, 73	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	LEU	5.3
1	A	475	ILE	4.9
1	B	342	TYR	4.8
1	A	565	SER	4.2
1	A	10	VAL	4.2
1	B	301	VAL	4.0
1	A	93	VAL	3.9
1	B	507	VAL	3.6
1	B	213	THR	3.3
1	A	75	VAL	3.3
1	A	301	VAL	3.3
1	A	486	ASP	3.2
1	B	38	VAL	3.0
1	B	56	ARG	3.0
1	B	10	VAL	2.9
1	A	436	VAL	2.7
1	A	303	ASP	2.7
1	B	231	ALA	2.7
1	B	318	VAL	2.6
1	B	101	GLU	2.5
1	A	420	ASP	2.4
1	B	447	ALA	2.4
1	B	450	TYR	2.3
1	B	483	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	52	GLU	2.2
1	A	461	ALA	2.1
1	A	386	ALA	2.1
1	A	230	ALA	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](#)

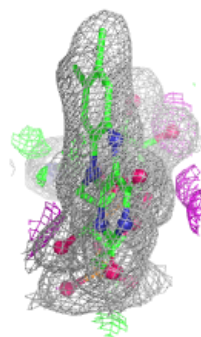
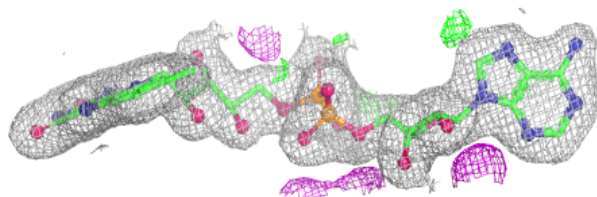
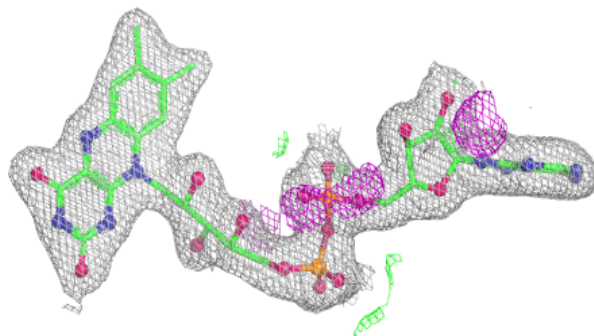
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CL	A	575	1/1	0.97	0.07	57,57,57,57	0
2	CL	B	575	1/1	0.98	0.08	53,53,53,53	0
3	FAD	A	900	53/53	0.98	0.05	27,33,39,42	0
3	FAD	B	900	53/53	0.98	0.05	24,32,36,37	0
4	COA	B	901	48/48	0.98	0.05	24,35,42,55	0
4	COA	A	901	48/48	0.99	0.05	29,34,39,54	0

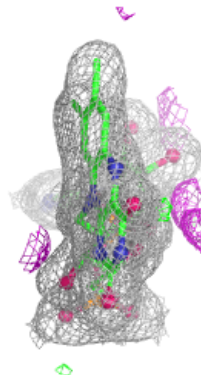
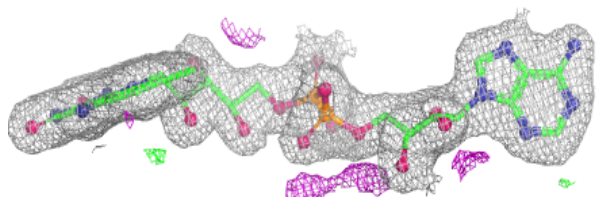
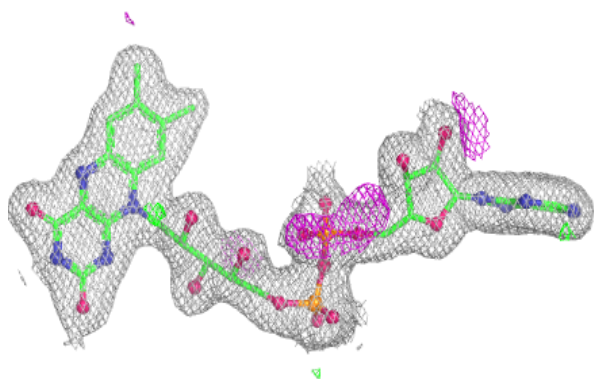
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

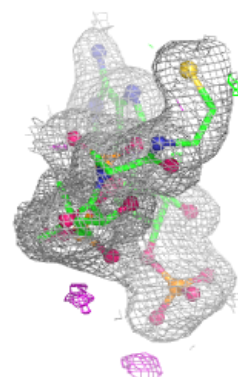
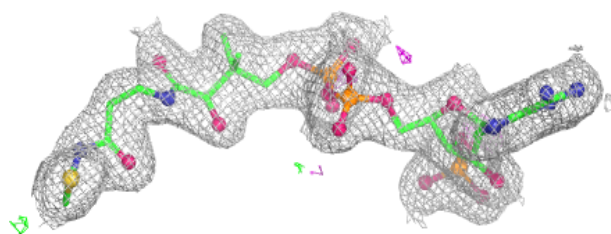
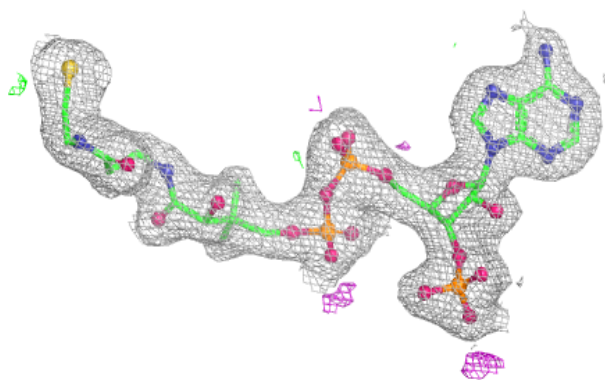
**Electron density around FAD B 900:**

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

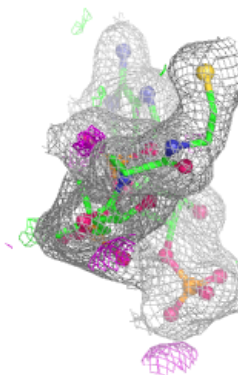
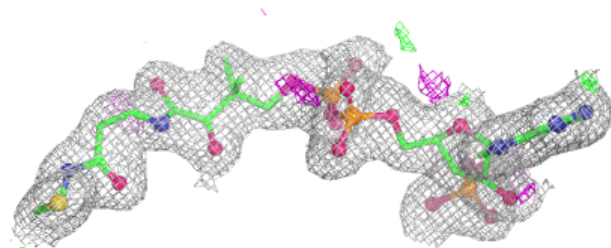
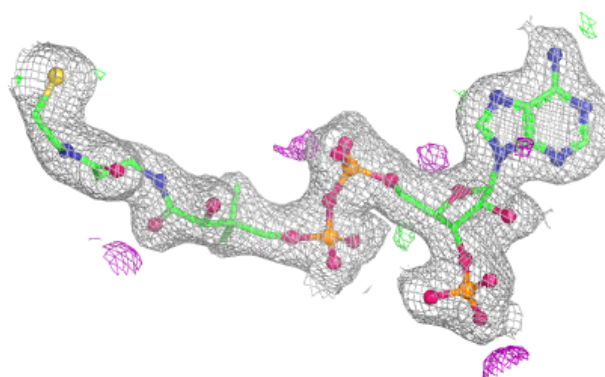


Electron density around COA B 901:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.