



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 1DDI / pdb_00001ddi
Title : CRYSTAL STRUCTURE OF SIR-FP60
Authors : Gruez, A.; Pignol, D.; Zeghouf, M.; Coves, J.; Fontecave, M.; Ferrer, J.L.;
Fontecilla-Camps, J.C.
Deposited on : 1999-11-10
Resolution : 2.51 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

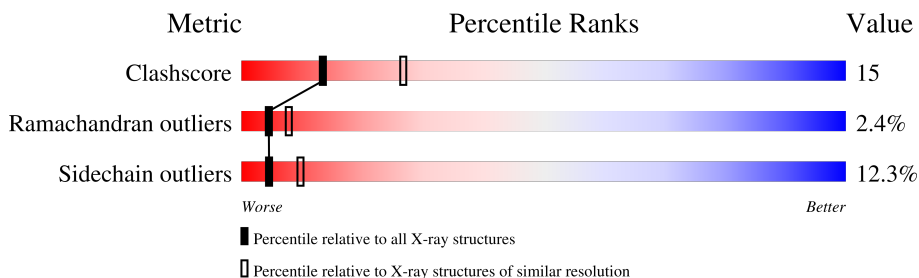
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	

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	FAD	A	600	X	-	-	-
3	NAP	A	601	X	X	-	-

2 Entry composition [i](#)

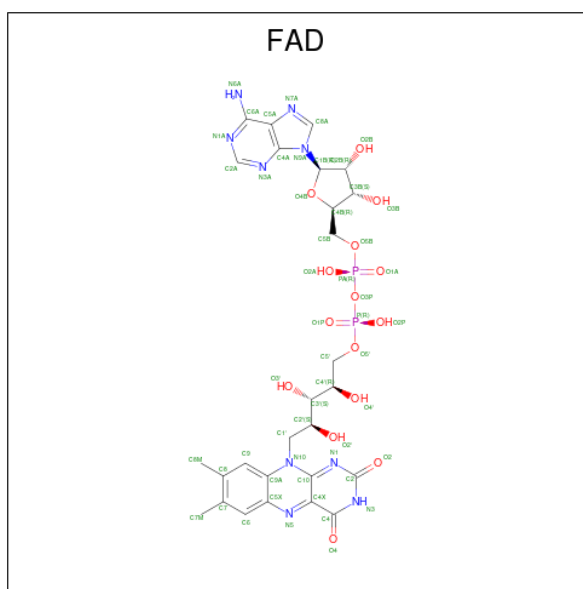
There are 4 unique types of molecules in this entry. The entry contains 3247 atoms, of which 1 is hydrogen and 0 are deuteriums.

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 SULFITE REDUCTASE [NADPH] FLAVOPROTEIN ALPHA-COMPONENT.

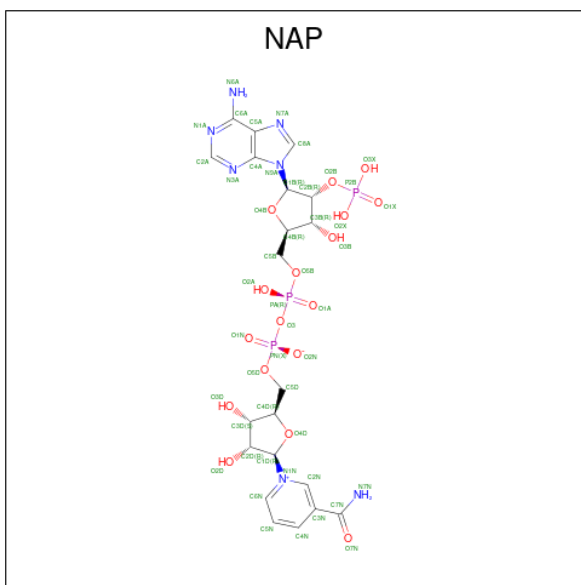
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2896	1842	506	543	5			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			27	10	1	5	9	2		

- Molecule 4 is water.

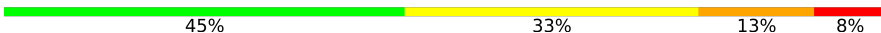
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	271	Total O 271 271	0	0

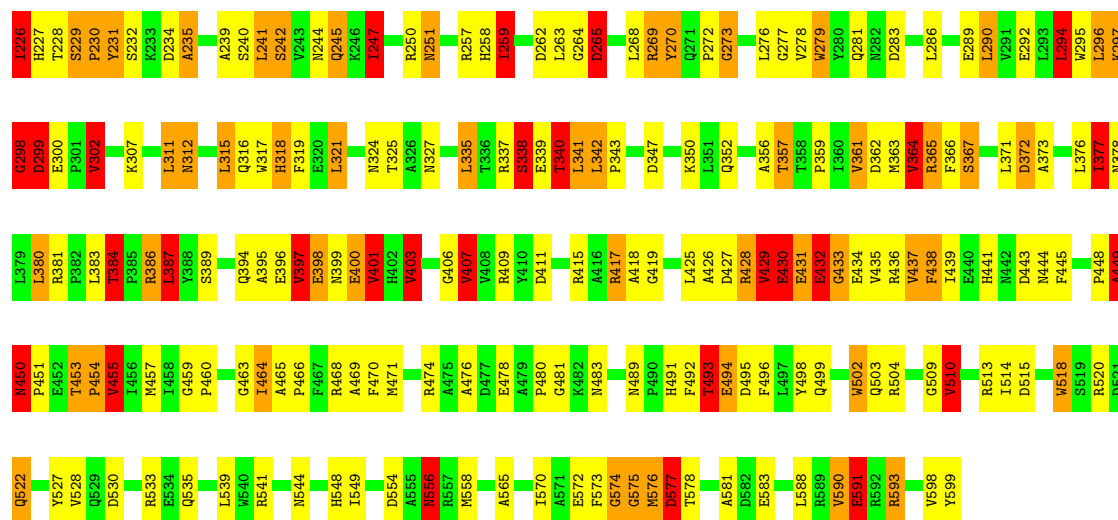
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: SULFITE REDUCTASE [NADPH] FLAVOPROTEIN ALPHA-COMPONENT

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.61 Å 98.61 Å 123.94 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.51	Depositor
% Data completeness (in resolution range)	98.4 (20.00-2.51)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3247	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.33	17/2963 (0.6%)	3.02	290/4045 (7.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	21

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	VAL	C-O	17.80	1.41	1.23
1	A	398	GLU	N-CA	17.75	1.69	1.46
1	A	397	VAL	CA-C	-10.59	1.43	1.52
1	A	235	ALA	C-O	10.13	1.28	1.23
1	A	269	ARG	CD-NE	9.72	1.59	1.46
1	A	433	GLY	N-CA	9.55	1.55	1.45
1	A	265	ASP	CA-CB	9.27	1.69	1.53
1	A	230	PRO	C-N	-8.23	1.22	1.33
1	A	235	ALA	N-CA	8.20	1.53	1.46
1	A	432	GLU	C-N	7.08	1.41	1.32
1	A	432	GLU	N-CA	6.96	1.55	1.46
1	A	269	ARG	CZ-NH1	6.35	1.41	1.32
1	A	433	GLY	CA-C	6.30	1.58	1.51
1	A	575	GLY	N-CA	6.26	1.54	1.45
1	A	403	VAL	N-CA	5.76	1.52	1.46
1	A	574	GLY	N-CA	5.49	1.51	1.45
1	A	335	LEU	N-CA	-5.44	1.39	1.46

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	54.66	168.40	119.20
1	A	432	GLU	CA-C-O	-29.21	78.73	120.51
1	A	269	ARG	NE-CZ-NH1	-25.63	95.87	121.50
1	A	429	VAL	O-C-N	-25.48	90.72	122.57
1	A	397	VAL	O-C-N	-22.91	100.82	122.12
1	A	397	VAL	CA-C-O	-21.50	104.69	121.68
1	A	230	PRO	O-C-N	-21.36	93.81	122.64
1	A	449	ALA	CA-C-O	-19.44	99.77	120.96
1	A	269	ARG	NH1-CZ-NH2	-18.13	95.73	119.30
1	A	234	ASP	O-C-N	-17.90	102.44	122.85
1	A	397	VAL	N-CA-CB	-17.58	92.03	112.07
1	A	247	ILE	CA-CB-CG2	17.27	139.85	110.50
1	A	449	ALA	O-C-N	-16.04	103.81	123.06
1	A	433	GLY	O-C-N	-15.49	97.50	122.91
1	A	590	VAL	CA-C-O	-14.98	103.76	121.28
1	A	504	ARG	CD-NE-CZ	14.28	144.39	124.40
1	A	297	LYS	N-CA-CB	14.20	134.48	110.49
1	A	265	ASP	CA-CB-CG	-13.88	98.72	112.60
1	A	429	VAL	CA-C-O	13.86	138.11	120.78
1	A	357	THR	N-CA-CB	-13.79	92.77	110.98
1	A	433	GLY	N-CA-C	13.22	128.43	111.37
1	A	340	THR	N-CA-CB	-13.01	90.81	110.33
1	A	250	ARG	NE-CZ-NH2	12.93	130.84	119.20
1	A	541	ARG	CD-NE-CZ	11.54	140.55	124.40
1	A	228	THR	N-CA-C	11.51	124.92	111.11
1	A	257	ARG	NE-CZ-NH2	11.17	129.25	119.20
1	A	437	VAL	N-CA-CB	-10.92	92.15	112.36
1	A	533	ARG	NE-CZ-NH2	-10.87	109.42	119.20
1	A	234	ASP	CA-C-O	-10.77	109.11	121.81
1	A	401	VAL	CB-CA-C	-10.62	94.80	110.62
1	A	432	GLU	N-CA-CB	-10.54	92.67	110.49
1	A	250	ARG	NE-CZ-NH1	-10.24	111.26	121.50
1	A	339	GLU	CA-C-O	10.15	131.65	119.97
1	A	599	TYR	CA-C-O	-10.06	103.70	120.80
1	A	384	THR	N-CA-CB	-10.00	93.20	111.19
1	A	434	GLU	CB-CG-CD	9.98	129.57	112.60
1	A	378	ASN	CA-C-O	9.94	131.08	120.55
1	A	493	THR	N-CA-CB	-9.86	94.99	110.46
1	A	251	ASN	CA-C-O	-9.84	107.61	119.32
1	A	397	VAL	CA-C-N	-9.77	102.88	121.54
1	A	397	VAL	C-N-CA	-9.77	102.88	121.54
1	A	444	ASN	CA-CB-CG	-9.39	103.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	GLY	CA-C-O	-9.19	104.57	120.57
1	A	265	ASP	N-CA-CB	-9.19	95.43	110.40
1	A	577	ASP	CA-C-O	8.96	133.33	120.51
1	A	533	ARG	NH1-CZ-NH2	8.95	130.93	119.30
1	A	431	GLU	N-CA-C	-8.90	99.46	110.41
1	A	298	GLY	CA-C-O	-8.88	105.13	120.57
1	A	312	ASN	OD1-CG-ND2	8.77	131.37	122.60
1	A	321	LEU	CA-C-O	8.62	128.38	118.90
1	A	427	ASP	CA-CB-CG	8.58	121.18	112.60
1	A	492	PHE	O-C-N	-8.55	113.06	122.12
1	A	231	TYR	N-CA-CB	8.51	124.87	110.49
1	A	265	ASP	CB-CA-C	-8.45	92.32	109.99
1	A	296	LEU	CA-C-O	-8.41	110.27	121.46
1	A	574	GLY	O-C-N	-8.40	115.28	122.92
1	A	247	ILE	N-CA-CB	-8.32	101.53	112.26
1	A	247	ILE	CA-CB-CG1	-8.29	96.31	110.40
1	A	265	ASP	N-CA-C	8.29	123.16	112.89
1	A	430	GLU	CB-CA-C	8.24	124.79	109.71
1	A	257	ARG	NE-CZ-NH1	-8.23	113.27	121.50
1	A	441	HIS	CA-CB-CG	-8.19	105.61	113.80
1	A	430	GLU	CA-C-O	8.17	129.19	120.36
1	A	436	ARG	NE-CZ-NH2	8.17	126.56	119.20
1	A	577	ASP	CA-C-N	8.12	137.05	121.54
1	A	577	ASP	C-N-CA	8.12	137.05	121.54
1	A	455	VAL	CA-C-O	8.07	130.11	120.67
1	A	434	GLU	N-CA-C	8.05	122.56	109.76
1	A	590	VAL	O-C-N	-8.05	114.14	122.75
1	A	366	PHE	CA-C-O	-8.02	110.75	119.97
1	A	556	ASN	N-CA-C	7.93	119.56	111.07
1	A	409	ARG	NE-CZ-NH1	7.89	129.39	121.50
1	A	251	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	A	468	ARG	CA-C-O	-7.80	112.15	120.42
1	A	411	ASP	CA-CB-CG	-7.72	104.88	112.60
1	A	302	VAL	N-CA-CB	-7.71	96.19	112.00
1	A	298	GLY	O-C-N	-7.71	112.68	122.70
1	A	581	ALA	CA-C-N	7.70	130.45	120.44
1	A	581	ALA	C-N-CA	7.70	130.45	120.44
1	A	498	TYR	CA-C-O	7.65	129.75	120.57
1	A	235	ALA	CA-C-N	7.64	127.80	120.31
1	A	235	ALA	C-N-CA	7.64	127.80	120.31
1	A	556	ASN	CA-CB-CG	-7.50	105.10	112.60
1	A	492	PHE	CA-C-O	7.47	128.70	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	ASP	CA-C-O	-7.46	109.84	120.51
1	A	245	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	A	535	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	A	565	ALA	CA-C-O	-7.44	112.66	120.55
1	A	361	VAL	O-C-N	-7.34	114.60	121.94
1	A	295	TRP	O-C-N	-7.34	112.58	122.41
1	A	434	GLU	CB-CA-C	-7.34	97.88	109.84
1	A	432	GLU	CB-CA-C	7.31	124.97	110.42
1	A	428	ARG	NE-CZ-NH2	7.28	125.75	119.20
1	A	415	ARG	NE-CZ-NH2	7.24	125.72	119.20
1	A	347	ASP	CA-C-N	7.23	130.84	120.79
1	A	347	ASP	C-N-CA	7.23	130.84	120.79
1	A	450	ASN	N-CA-CB	7.22	123.21	110.37
1	A	556	ASN	OD1-CG-ND2	7.21	129.81	122.60
1	A	411	ASP	CB-CG-OD1	-7.13	102.01	118.40
1	A	448	PRO	CA-C-O	-7.07	113.66	121.23
1	A	433	GLY	CA-C-N	7.05	131.58	121.50
1	A	433	GLY	C-N-CA	7.05	131.58	121.50
1	A	509	GLY	CA-C-N	-7.05	109.92	121.34
1	A	509	GLY	C-N-CA	-7.05	109.92	121.34
1	A	324	ASN	CA-CB-CG	-7.02	105.58	112.60
1	A	297	LYS	CA-C-N	7.02	135.17	121.41
1	A	297	LYS	C-N-CA	7.02	135.17	121.41
1	A	401	VAL	CG1-CB-CG2	7.01	126.22	110.80
1	A	377	ILE	CA-CB-CG1	-6.98	98.53	110.40
1	A	476	ALA	CA-C-O	-6.98	113.16	120.55
1	A	378	ASN	O-C-N	-6.97	114.73	122.12
1	A	428	ARG	NE-CZ-NH1	-6.96	114.54	121.50
1	A	574	GLY	CA-C-O	-6.95	114.03	122.03
1	A	399	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	A	264	GLY	CA-C-N	6.91	133.23	121.14
1	A	264	GLY	C-N-CA	6.91	133.23	121.14
1	A	419	GLY	CA-C-O	-6.85	115.38	121.41
1	A	491	HIS	N-CA-C	6.82	119.53	108.41
1	A	549	ILE	CA-C-O	6.82	127.55	120.39
1	A	384	THR	CB-CA-C	6.79	120.11	108.91
1	A	325	THR	CA-C-N	6.78	129.70	120.54
1	A	325	THR	C-N-CA	6.78	129.70	120.54
1	A	401	VAL	N-CA-CB	6.77	123.17	111.39
1	A	418	ALA	CA-C-N	6.72	126.38	119.92
1	A	418	ALA	C-N-CA	6.72	126.38	119.92
1	A	378	ASN	CA-CB-CG	-6.70	105.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ASN	N-CA-C	-6.70	102.17	111.81
1	A	530	ASP	CA-CB-CG	-6.69	105.91	112.60
1	A	315	LEU	CA-C-O	6.63	127.45	120.42
1	A	478	GLU	CA-CB-CG	6.60	127.30	114.10
1	A	398	GLU	CB-CA-C	6.59	123.53	110.42
1	A	591	GLU	N-CA-CB	6.54	121.55	110.49
1	A	533	ARG	CG-CD-NE	-6.48	97.74	112.00
1	A	319	PHE	CA-CB-CG	-6.46	107.34	113.80
1	A	503	GLN	CB-CG-CD	6.45	123.56	112.60
1	A	276	LEU	CA-C-N	6.42	127.79	121.62
1	A	276	LEU	C-N-CA	6.42	127.79	121.62
1	A	340	THR	CA-C-O	-6.41	112.10	119.60
1	A	439	ILE	CA-C-O	-6.41	113.40	120.84
1	A	380	LEU	N-CA-CB	-6.40	100.22	110.46
1	A	340	THR	CB-CA-C	6.36	122.46	109.67
1	A	366	PHE	CA-C-N	-6.35	115.47	123.15
1	A	366	PHE	C-N-CA	-6.35	115.47	123.15
1	A	430	GLU	O-C-N	-6.31	115.79	123.30
1	A	574	GLY	N-CA-C	-6.28	100.58	112.27
1	A	397	VAL	CG1-CB-CG2	6.26	124.58	110.80
1	A	327	ASN	CA-CB-CG	-6.25	106.35	112.60
1	A	365	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	A	428	ARG	CD-NE-CZ	6.23	133.13	124.40
1	A	270	TYR	CA-C-O	-6.21	114.80	121.38
1	A	483	ASN	OD1-CG-ND2	6.19	128.79	122.60
1	A	244	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	443	ASP	CA-CB-CG	-6.18	106.42	112.60
1	A	241	LEU	O-C-N	-6.17	115.43	123.02
1	A	593	ARG	CD-NE-CZ	6.17	133.04	124.40
1	A	281	GLN	CB-CG-CD	-6.16	102.13	112.60
1	A	387	LEU	O-C-N	-6.16	116.31	123.27
1	A	363	MET	CA-C-O	-6.16	114.02	120.55
1	A	247	ILE	CB-CA-C	6.13	118.81	111.20
1	A	283	ASP	CA-C-O	6.13	125.52	119.51
1	A	478	GLU	CB-CA-C	-6.12	101.83	111.51
1	A	298	GLY	N-CA-C	-6.11	98.70	113.18
1	A	409	ARG	NE-CZ-NH2	-6.08	113.73	119.20
1	A	231	TYR	CB-CA-C	-6.06	98.36	110.42
1	A	244	ASN	O-C-N	-6.06	114.82	123.06
1	A	403	VAL	CA-CB-CG1	6.06	120.70	110.40
1	A	470	PHE	CA-C-O	6.03	126.81	120.42
1	A	294	LEU	O-C-N	-6.02	114.81	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ASP	CA-C-N	5.99	128.30	120.28
1	A	362	ASP	C-N-CA	5.99	128.30	120.28
1	A	377	ILE	N-CA-CB	-5.98	99.94	110.77
1	A	590	VAL	N-CA-C	-5.98	100.96	109.51
1	A	226	ILE	CA-CB-CG2	5.97	120.64	110.50
1	A	432	GLU	CA-C-N	5.97	132.47	121.67
1	A	432	GLU	C-N-CA	5.97	132.47	121.67
1	A	302	VAL	CB-CA-C	5.96	121.22	110.48
1	A	494	GLU	O-C-N	5.96	130.51	122.59
1	A	230	PRO	N-CA-C	-5.93	100.25	112.47
1	A	312	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	450	ASN	CA-C-O	5.92	128.28	120.16
1	A	481	GLY	O-C-N	-5.92	115.00	122.70
1	A	434	GLU	N-CA-CB	5.90	119.10	109.95
1	A	364	VAL	N-CA-CB	5.86	121.38	110.77
1	A	372	ASP	O-C-N	-5.84	115.91	122.75
1	A	338	SER	CB-CA-C	-5.80	101.64	109.71
1	A	400	GLU	CA-C-O	-5.75	114.40	121.06
1	A	297	LYS	CA-C-O	-5.73	112.32	120.51
1	A	364	VAL	CA-CB-CG2	5.72	120.13	110.40
1	A	279	TRP	O-C-N	-5.68	116.16	122.86
1	A	268	LEU	CA-C-O	-5.66	114.46	120.92
1	A	386	ARG	CD-NE-CZ	5.64	132.30	124.40
1	A	242	SER	CA-CB-OG	-5.63	99.84	111.10
1	A	235	ALA	N-CA-C	5.61	124.02	112.40
1	A	483	ASN	CA-C-N	-5.61	114.10	122.74
1	A	483	ASN	C-N-CA	-5.61	114.10	122.74
1	A	389	SER	O-C-N	-5.60	116.13	122.97
1	A	503	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	318	HIS	CA-CB-CG	-5.59	108.21	113.80
1	A	377	ILE	CA-CB-CG2	5.58	119.99	110.50
1	A	470	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	239	ALA	CA-C-N	-5.58	113.09	122.29
1	A	239	ALA	C-N-CA	-5.58	113.09	122.29
1	A	357	THR	CA-CB-CG2	5.57	119.97	110.50
1	A	407	VAL	CB-CA-C	5.56	117.69	110.96
1	A	359	PRO	CB-CA-C	-5.55	103.68	110.95
1	A	495	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	292	GLU	N-CA-C	5.54	117.32	111.28
1	A	431	GLU	O-C-N	-5.54	115.89	122.65
1	A	296	LEU	N-CA-CB	-5.54	100.62	110.14
1	A	578	THR	N-CA-C	5.53	122.58	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	THR	CA-C-N	5.53	125.45	119.76
1	A	453	THR	C-N-CA	5.53	125.45	119.76
1	A	307	LYS	CA-C-N	5.49	130.07	122.77
1	A	307	LYS	C-N-CA	5.49	130.07	122.77
1	A	352	GLN	CA-C-O	5.48	126.23	120.42
1	A	515	ASP	CA-CB-CG	-5.47	107.13	112.60
1	A	572	GLU	N-CA-C	5.47	116.92	111.07
1	A	514	ILE	CA-C-O	-5.46	114.47	120.43
1	A	259	ILE	O-C-N	-5.46	117.30	122.98
1	A	396	GLU	CA-CB-CG	5.46	125.02	114.10
1	A	395	ALA	O-C-N	-5.46	115.84	122.22
1	A	426	ALA	CA-C-N	-5.46	113.73	122.08
1	A	426	ALA	C-N-CA	-5.46	113.73	122.08
1	A	518	TRP	CA-C-N	5.44	128.58	120.31
1	A	518	TRP	C-N-CA	5.44	128.58	120.31
1	A	444	ASN	O-C-N	-5.43	115.42	122.37
1	A	279	TRP	N-CA-C	-5.43	102.85	110.50
1	A	258	HIS	CA-C-O	-5.42	114.35	120.43
1	A	465	ALA	CA-C-N	5.42	125.09	119.56
1	A	465	ALA	C-N-CA	5.42	125.09	119.56
1	A	468	ARG	CD-NE-CZ	5.40	131.96	124.40
1	A	235	ALA	CA-C-O	5.40	124.19	120.47
1	A	459	GLY	O-C-N	-5.38	116.39	121.77
1	A	231	TYR	CA-C-O	5.36	128.17	120.51
1	A	324	ASN	CA-C-O	-5.33	114.96	121.36
1	A	381	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	350	LYS	O-C-N	5.33	128.22	122.15
1	A	407	VAL	N-CA-CB	5.32	117.06	111.00
1	A	544	ASN	OD1-CG-ND2	5.32	127.92	122.60
1	A	362	ASP	N-CA-C	5.31	117.98	111.82
1	A	341	LEU	CA-C-N	5.31	126.72	120.09
1	A	341	LEU	C-N-CA	5.31	126.72	120.09
1	A	262	ASP	O-C-N	5.29	129.23	123.04
1	A	363	MET	N-CA-C	-5.29	105.52	111.28
1	A	403	VAL	N-CA-CB	-5.27	101.61	111.62
1	A	572	GLU	CA-C-O	-5.27	115.29	120.82
1	A	598	VAL	CA-C-O	-5.26	114.37	121.32
1	A	365	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	A	436	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	395	ALA	N-CA-C	-5.24	105.69	111.71
1	A	232	SER	CA-CB-OG	-5.22	100.65	111.10
1	A	406	GLY	O-C-N	-5.22	115.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	VAL	CA-CB-CG1	5.21	119.26	110.40
1	A	417	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	A	398	GLU	N-CA-CB	-5.21	101.69	110.49
1	A	227	HIS	CA-C-N	5.21	127.57	120.54
1	A	227	HIS	C-N-CA	5.21	127.57	120.54
1	A	494	GLU	CB-CA-C	-5.21	100.06	110.42
1	A	583	GLU	N-CA-C	-5.20	105.61	111.28
1	A	273	GLY	N-CA-C	-5.20	107.71	113.79
1	A	575	GLY	N-CA-C	-5.20	100.86	113.18
1	A	438	PHE	CA-C-O	-5.18	115.91	121.45
1	A	381	ARG	CB-CG-CD	5.18	123.21	111.30
1	A	570	ILE	CA-C-N	5.17	127.48	120.65
1	A	570	ILE	C-N-CA	5.17	127.48	120.65
1	A	397	VAL	CB-CA-C	5.17	120.04	112.03
1	A	426	ALA	N-CA-CB	5.16	118.25	110.30
1	A	296	LEU	O-C-N	-5.15	115.63	122.59
1	A	429	VAL	CB-CA-C	5.15	119.74	111.29
1	A	240	SER	N-CA-C	5.14	117.20	109.23
1	A	321	LEU	N-CA-CB	-5.13	103.80	110.88
1	A	510	VAL	CA-CB-CG2	5.13	119.13	110.40
1	A	502	TRP	N-CA-CB	5.13	117.66	110.12
1	A	384	THR	OG1-CB-CG2	5.09	119.47	109.30
1	A	419	GLY	N-CA-C	-5.09	105.41	111.36
1	A	463	GLY	O-C-N	-5.09	116.09	122.70
1	A	478	GLU	CA-C-O	-5.09	114.50	120.81
1	A	466	PRO	N-CA-C	-5.08	107.23	113.84
1	A	435	VAL	CA-C-N	5.07	129.14	122.30
1	A	435	VAL	C-N-CA	5.07	129.14	122.30
1	A	316	GLN	CA-C-O	-5.05	114.63	120.24
1	A	513	ARG	CD-NE-CZ	5.04	131.46	124.40
1	A	319	PHE	CA-C-N	5.04	129.02	121.72
1	A	319	PHE	C-N-CA	5.04	129.02	121.72
1	A	226	ILE	O-C-N	-5.03	114.95	123.00
1	A	425	LEU	CA-C-O	5.02	125.75	120.42
1	A	481	GLY	CA-C-O	5.02	129.30	120.57
1	A	453	THR	CA-C-O	5.01	124.81	119.80
1	A	520	ARG	CA-C-N	-5.01	112.84	121.66
1	A	520	ARG	C-N-CA	-5.01	112.84	121.66

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	ILE	Mainchain
1	A	251	ASN	Mainchain
1	A	259	ILE	Mainchain
1	A	265	ASP	Mainchain
1	A	289	GLU	Mainchain
1	A	296	LEU	Peptide
1	A	338	SER	Mainchain
1	A	356	ALA	Mainchain
1	A	364	VAL	Mainchain
1	A	372	ASP	Mainchain
1	A	377	ILE	Mainchain
1	A	387	LEU	Mainchain
1	A	407	VAL	Mainchain
1	A	429	VAL	Mainchain,Peptide
1	A	430	GLU	Peptide
1	A	432	GLU	Mainchain,Peptide
1	A	449	ALA	Mainchain
1	A	454	PRO	Mainchain
1	A	575	GLY	Mainchain

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	2896	0	2766	80	1
2	A	53	0	29	1	0
3	A	26	1	5	7	0
4	A	271	0	0	14	2
All	All	3246	1	2800	85	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (85) 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:398:GLU:N	1:A:398:GLU:CA	1.69	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:601:NAP:O3	3:A:601:NAP:O2A	1.58	1.18
1:A:397:VAL:O	1:A:398:GLU:CA	1.94	1.15
1:A:397:VAL:C	1:A:398:GLU:CA	2.34	0.99
1:A:397:VAL:O	1:A:398:GLU:HA	1.61	0.97
1:A:449:ALA:O	1:A:450:ASN:CB	2.19	0.85
3:A:601:NAP:H52A	3:A:601:NAP:N3A	1.92	0.84
1:A:428:ARG:O	1:A:430:GLU:N	2.12	0.82
1:A:398:GLU:N	1:A:398:GLU:CB	2.47	0.77
1:A:338:SER:HB3	1:A:341:LEU:H	1.53	0.74
1:A:297:LYS:O	1:A:300:GLU:OE1	2.07	0.72
1:A:398:GLU:N	1:A:398:GLU:C	2.46	0.72
1:A:230:PRO:O	1:A:231:TYR:CB	2.37	0.70
1:A:298:GLY:O	1:A:300:GLU:N	2.23	0.70
1:A:338:SER:OG	1:A:367:SER:HB3	1.95	0.67
3:A:601:NAP:N3A	3:A:601:NAP:C5B	2.58	0.65
1:A:433:GLY:N	4:A:971:HOH:O	2.30	0.65
1:A:231:TYR:HA	1:A:235:ALA:O	1.97	0.64
1:A:365:ARG:HD3	4:A:903:HOH:O	1.95	0.64
1:A:590:VAL:O	1:A:591:GLU:CB	2.44	0.63
1:A:433:GLY:CA	4:A:971:HOH:O	2.46	0.63
1:A:431:GLU:O	1:A:433:GLY:HA3	1.98	0.62
1:A:302:VAL:HG21	1:A:377:ILE:HD12	1.83	0.61
1:A:335:LEU:HD23	1:A:371:LEU:HD11	1.86	0.58
1:A:433:GLY:HA2	4:A:971:HOH:O	2.04	0.57
1:A:290:LEU:HD22	1:A:294:LEU:HD22	1.88	0.56
1:A:397:VAL:HG13	1:A:400:GLU:HB2	1.91	0.53
1:A:451:PRO:O	1:A:480:PRO:HD2	2.09	0.52
1:A:493:THR:HG23	1:A:494:GLU:OE1	2.09	0.52
1:A:342:LEU:N	1:A:343:PRO:CD	2.74	0.51
1:A:230:PRO:O	1:A:231:TYR:HB2	2.08	0.51
1:A:272:PRO:HB3	1:A:469:ALA:HB1	1.93	0.51
1:A:428:ARG:O	1:A:429:VAL:C	2.54	0.50
1:A:548:HIS:CD2	1:A:593:ARG:HG2	2.46	0.50
1:A:460:PRO:HG2	1:A:558:MET:HG3	1.94	0.50
1:A:471:MET:HE3	1:A:510:VAL:CG2	2.42	0.50
1:A:384:THR:HG22	1:A:386:ARG:NH2	2.27	0.49
1:A:298:GLY:HA3	1:A:312:ASN:ND2	2.26	0.49
1:A:298:GLY:O	1:A:299:ASP:CB	2.59	0.49
1:A:522:GLN:HG3	4:A:611:HOH:O	2.12	0.49
1:A:298:GLY:O	1:A:299:ASP:C	2.52	0.48
1:A:337:ARG:O	1:A:338:SER:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:HG13	1:A:474:ARG:NH1	2.28	0.48
1:A:361:VAL:HG11	1:A:417:ARG:CZ	2.44	0.48
1:A:493:THR:CG2	1:A:494:GLU:OE1	2.62	0.48
1:A:263:LEU:HD21	1:A:401:VAL:HG22	1.95	0.47
1:A:277:GLY:HA2	1:A:387:LEU:HD12	1.96	0.47
1:A:340:THR:CG2	4:A:853:HOH:O	2.62	0.47
3:A:601:NAP:PA	4:A:786:HOH:O	2.71	0.47
1:A:269:ARG:HH11	1:A:269:ARG:HD3	0.90	0.47
1:A:311:LEU:HG	1:A:373:ALA:HB1	1.96	0.46
1:A:493:THR:HB	4:A:639:HOH:O	2.14	0.46
1:A:245:GLN:HG3	1:A:247:ILE:HD12	1.95	0.46
1:A:554:ASP:OD1	1:A:556:ASN:HB2	2.14	0.46
1:A:297:LYS:C	1:A:298:GLY:O	2.57	0.46
1:A:317:TRP:HB2	1:A:318:HIS:CD2	2.50	0.46
1:A:340:THR:HG23	4:A:853:HOH:O	2.17	0.45
1:A:259:ILE:HB	1:A:403:VAL:HG12	1.99	0.45
1:A:270:TYR:CZ	1:A:394:GLN:HG3	2.51	0.45
1:A:493:THR:HG22	1:A:494:GLU:HG2	1.98	0.45
1:A:278:VAL:HG12	1:A:279:TRP:O	2.16	0.45
1:A:455:VAL:HG23	1:A:457:MET:HG3	1.99	0.45
1:A:464:ILE:HD11	1:A:502:TRP:CZ2	2.52	0.45
1:A:489:ASN:O	1:A:518:TRP:HA	2.17	0.45
1:A:527:TYR:CD2	3:A:601:NAP:H52A	2.52	0.45
1:A:528:VAL:HG22	3:A:601:NAP:H2A	1.99	0.45
2:A:600:FAD:N9A	2:A:600:FAD:O3B	2.50	0.44
1:A:429:VAL:HA	4:A:695:HOH:O	2.18	0.44
1:A:273:GLY:HA3	1:A:445:PHE:O	2.18	0.43
1:A:342:LEU:N	1:A:343:PRO:HD2	2.32	0.43
1:A:384:THR:HB	4:A:745:HOH:O	2.18	0.43
1:A:453:THR:HA	1:A:454:PRO:HD3	1.81	0.43
1:A:241:LEU:CD1	1:A:259:ILE:HG23	2.48	0.43
1:A:527:TYR:HD2	3:A:601:NAP:H52A	1.83	0.43
1:A:471:MET:HE3	1:A:510:VAL:HG23	2.01	0.42
1:A:365:ARG:NH1	4:A:903:HOH:O	2.53	0.41
1:A:338:SER:O	1:A:342:LEU:HB2	2.20	0.41
1:A:576:MET:O	1:A:577:ASP:C	2.61	0.41
1:A:496:PHE:CE1	1:A:499:GLN:HG3	2.56	0.41
1:A:493:THR:HG21	4:A:901:HOH:O	2.21	0.41
1:A:277:GLY:HA3	1:A:438:PHE:CZ	2.56	0.41
1:A:573:PHE:C	1:A:574:GLY:O	2.64	0.40
1:A:241:LEU:HD11	1:A:259:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:NH2	4:A:746:HOH:O	2.54	0.40
1:A:335:LEU:CD2	1:A:371:LEU:HD11	2.50	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:N	4:A:974:HOH:O[4_565]	1.87	0.33
4:A:957:HOH:O	4:A:973:HOH:O[3_564]	2.02	0.18

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	372/374 (100%)	341 (92%)	22 (6%)	9 (2%)	4 8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	VAL
1	A	432	GLU
1	A	450	ASN
1	A	299	ASP
1	A	577	ASP
1	A	591	GLU
1	A	229	SER
1	A	298	GLY
1	A	576	MET

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	292/316 (92%)	256 (88%)	36 (12%)	4 10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	ILE
1	A	242	SER
1	A	247	ILE
1	A	265	ASP
1	A	286	LEU
1	A	290	LEU
1	A	294	LEU
1	A	302	VAL
1	A	311	LEU
1	A	315	LEU
1	A	321	LEU
1	A	338	SER
1	A	340	THR
1	A	342	LEU
1	A	357	THR
1	A	364	VAL
1	A	367	SER
1	A	376	LEU
1	A	377	ILE
1	A	380	LEU
1	A	383	LEU
1	A	384	THR
1	A	387	LEU
1	A	397	VAL
1	A	401	VAL
1	A	403	VAL
1	A	407	VAL
1	A	437	VAL
1	A	455	VAL
1	A	464	ILE

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Mol	Chain	Res	Type
1	A	493	THR
1	A	510	VAL
1	A	522	GLN
1	A	539	LEU
1	A	556	ASN
1	A	588	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	A	312	ASN
1	A	318	HIS
1	A	352	GLN
1	A	378	ASN
1	A	548	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	600	-	58,58,58	2.17	15 (25%)	85,89,89	2.36	23 (27%)
3	NAP	A	601	-	27,27,52	13.02	10 (37%)	35,40,80	11.54	28 (80%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	-	2/2/9/9	3/34/50/50	0/6/6/6
3	NAP	A	601	-	1/1/4/12	9/20/20/67	0/2/2/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NAP	PA-O1A	49.71	3.05	1.50
3	A	601	NAP	PA-O3	43.43	3.16	1.54
2	A	600	FAD	P-O3P	-10.24	1.48	1.59
3	A	601	NAP	P2B-O2B	-9.46	1.43	1.59
3	A	601	NAP	O5B-C5B	7.14	1.73	1.44
2	A	600	FAD	PA-O3P	4.37	1.64	1.59
3	A	601	NAP	PA-O5B	-4.34	1.46	1.60
2	A	600	FAD	PA-O2A	-4.00	1.36	1.55
2	A	600	FAD	O5'-C5'	3.86	1.59	1.44
3	A	601	NAP	P2B-O2X	-3.26	1.42	1.54
3	A	601	NAP	P2B-O3X	-3.22	1.42	1.54
2	A	600	FAD	O4B-C1B	3.13	1.49	1.42
3	A	601	NAP	C1B-N9A	3.04	1.50	1.46
2	A	600	FAD	P-O1P	-3.00	1.40	1.50
3	A	601	NAP	PA-O2A	2.99	1.65	1.54
2	A	600	FAD	PA-O5B	-2.87	1.48	1.59
2	A	600	FAD	C1'-C2'	2.76	1.56	1.52
3	A	601	NAP	P2B-O1X	-2.68	1.42	1.50
2	A	600	FAD	C6-C7	-2.68	1.36	1.39
2	A	600	FAD	C4A-N9A	2.62	1.43	1.37
2	A	600	FAD	C2B-C3B	2.31	1.59	1.53
2	A	600	FAD	C5A-C6A	2.30	1.47	1.41
2	A	600	FAD	O2-C2	-2.28	1.19	1.24
2	A	600	FAD	P-O5'	-2.16	1.50	1.59
2	A	600	FAD	O4'-C4'	2.07	1.47	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAP	O3B-C3B-C4B	-29.15	42.96	109.14
3	A	601	NAP	O3-PA-O1A	-28.02	1.67	110.83
3	A	601	NAP	O2A-PA-O1A	-25.57	11.21	110.83
3	A	601	NAP	O3-PA-O2A	-25.46	12.33	107.80
3	A	601	NAP	O3B-C3B-C2B	19.05	150.36	109.98
3	A	601	NAP	O2B-C2B-C1B	18.28	143.41	106.92
3	A	601	NAP	O2X-P2B-O1X	-10.99	68.02	110.83
2	A	600	FAD	C2B-C1B-N9A	10.58	139.60	113.30
3	A	601	NAP	O3X-P2B-O2X	9.77	144.44	107.80
3	A	601	NAP	C5A-C4A-N9A	-9.23	96.52	105.98
3	A	601	NAP	N9A-C8A-N7A	-9.15	105.69	114.16
3	A	601	NAP	C4A-N9A-C8A	8.95	112.18	105.75
3	A	601	NAP	O3-PA-O5B	-8.82	83.67	106.67
3	A	601	NAP	O2A-PA-O5B	-8.26	85.13	106.67
3	A	601	NAP	O2X-P2B-O2B	-8.21	73.84	105.85
3	A	601	NAP	N3A-C4A-N9A	8.01	136.78	126.87
3	A	601	NAP	O5B-PA-O1A	-7.94	84.97	106.44
3	A	601	NAP	O2B-P2B-O1X	7.02	134.36	109.33
3	A	601	NAP	PA-O5B-C5B	6.37	135.53	118.21
2	A	600	FAD	PA-O5B-C5B	6.13	156.50	121.35
2	A	600	FAD	C2B-C3B-C4B	-6.05	90.92	102.61
2	A	600	FAD	O2B-C2B-C1B	5.27	128.26	110.10
3	A	601	NAP	C1B-N9A-C8A	-5.00	118.63	126.63
3	A	601	NAP	N3A-C2A-N1A	4.59	135.52	128.58
2	A	600	FAD	C5B-C4B-C3B	4.50	131.42	115.21
2	A	600	FAD	O4B-C1B-N9A	-4.47	99.50	108.09
2	A	600	FAD	O3'-C3'-C4'	4.17	118.42	108.93
2	A	600	FAD	C3B-C2B-C1B	-3.78	94.31	101.46
2	A	600	FAD	O3B-C3B-C4B	3.58	121.36	111.08
3	A	601	NAP	C6A-C5A-N7A	-3.56	125.22	132.09
3	A	601	NAP	C4A-C5A-N7A	3.50	114.59	110.58
2	A	600	FAD	O3B-C3B-C2B	-3.47	100.69	111.82
3	A	601	NAP	O3X-P2B-O2B	3.39	119.05	105.85
2	A	600	FAD	O4B-C4B-C5B	3.28	119.85	109.33
2	A	600	FAD	C4A-N9A-C8A	-3.25	102.33	105.74
2	A	600	FAD	O3'-C3'-C2'	3.20	116.21	108.93
2	A	600	FAD	N3A-C2A-N1A	-3.09	123.90	128.58
3	A	601	NAP	N6A-C6A-N1A	3.06	125.19	118.38
2	A	600	FAD	C4X-C10-N10	2.99	120.76	116.48
3	A	601	NAP	P2B-O2B-C2B	-2.95	115.62	123.54
3	A	601	NAP	C4B-C3B-C2B	2.94	119.05	112.12
2	A	600	FAD	O4B-C1B-C2B	-2.94	100.32	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	C4-N3-C2	-2.48	121.23	125.64
2	A	600	FAD	C5A-C4A-N3A	-2.45	123.34	126.72
3	A	601	NAP	C1B-N9A-C4A	2.37	129.16	126.41
2	A	600	FAD	C4A-C5A-N7A	-2.34	107.91	110.58
2	A	600	FAD	C4X-C10-N1	-2.34	118.86	124.59
2	A	600	FAD	C4B-O4B-C1B	-2.32	104.35	109.47
2	A	600	FAD	C5A-N7A-C8A	2.23	106.95	103.45
3	A	601	NAP	C6A-C5A-C4A	2.18	120.16	117.18
2	A	600	FAD	C4-C4X-C10	2.01	120.37	116.93

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	600	FAD	C2B
2	A	600	FAD	C3B
3	A	601	NAP	C2B

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAP	C3B-C4B-C5B-O5B
3	A	601	NAP	C1B-C2B-C3B-C4B
3	A	601	NAP	N9A-C1B-C2B-C3B
2	A	600	FAD	C3B-C4B-C5B-O5B
3	A	601	NAP	C2B-C3B-C4B-C5B
3	A	601	NAP	O3B-C3B-C4B-C5B
2	A	600	FAD	O4B-C4B-C5B-O5B
3	A	601	NAP	C1B-C2B-C3B-O3B
2	A	600	FAD	C5B-O5B-PA-O1A
3	A	601	NAP	C2B-C1B-N9A-C8A
3	A	601	NAP	C2B-O2B-P2B-O1X
3	A	601	NAP	O2B-C2B-C3B-C4B

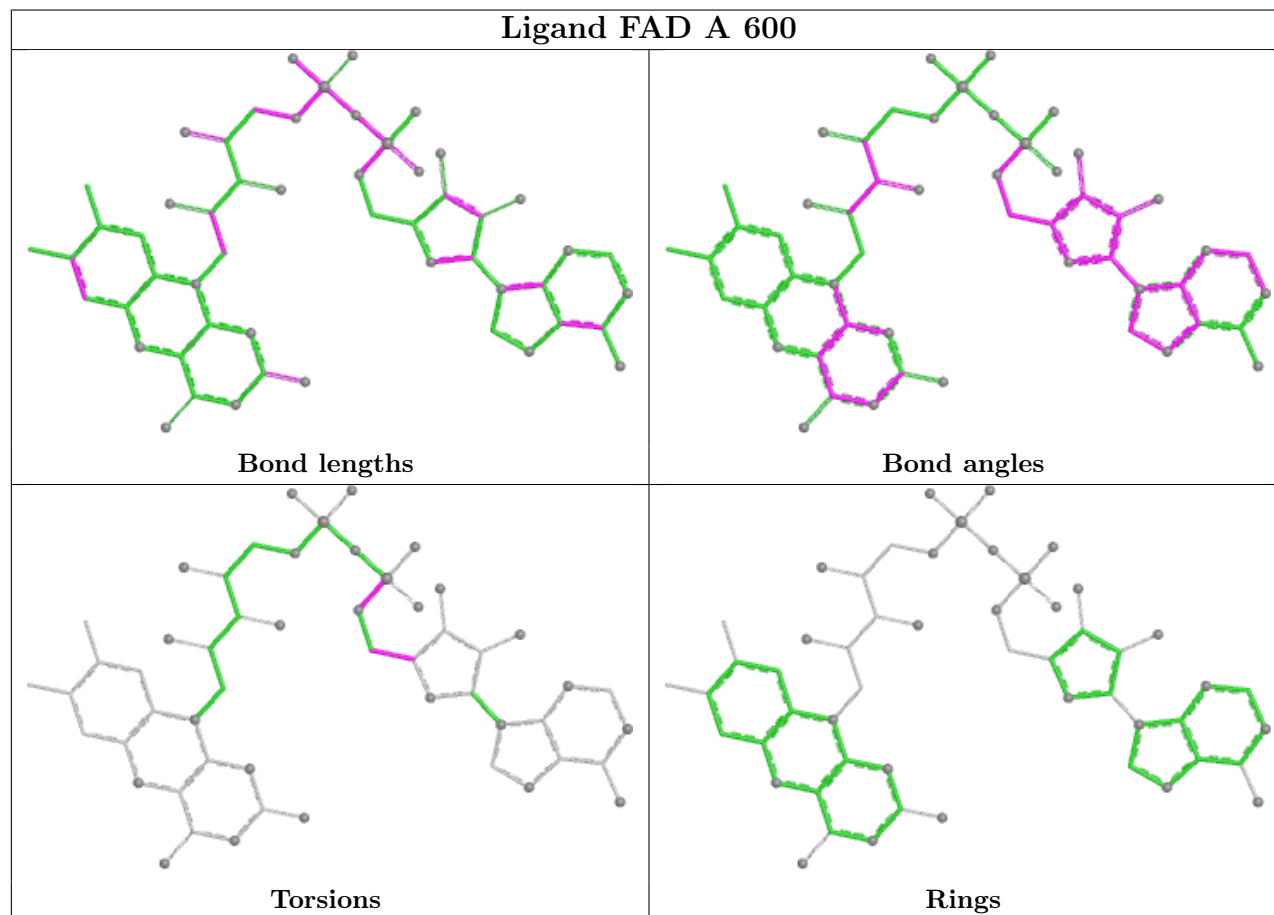
There are no ring outliers.

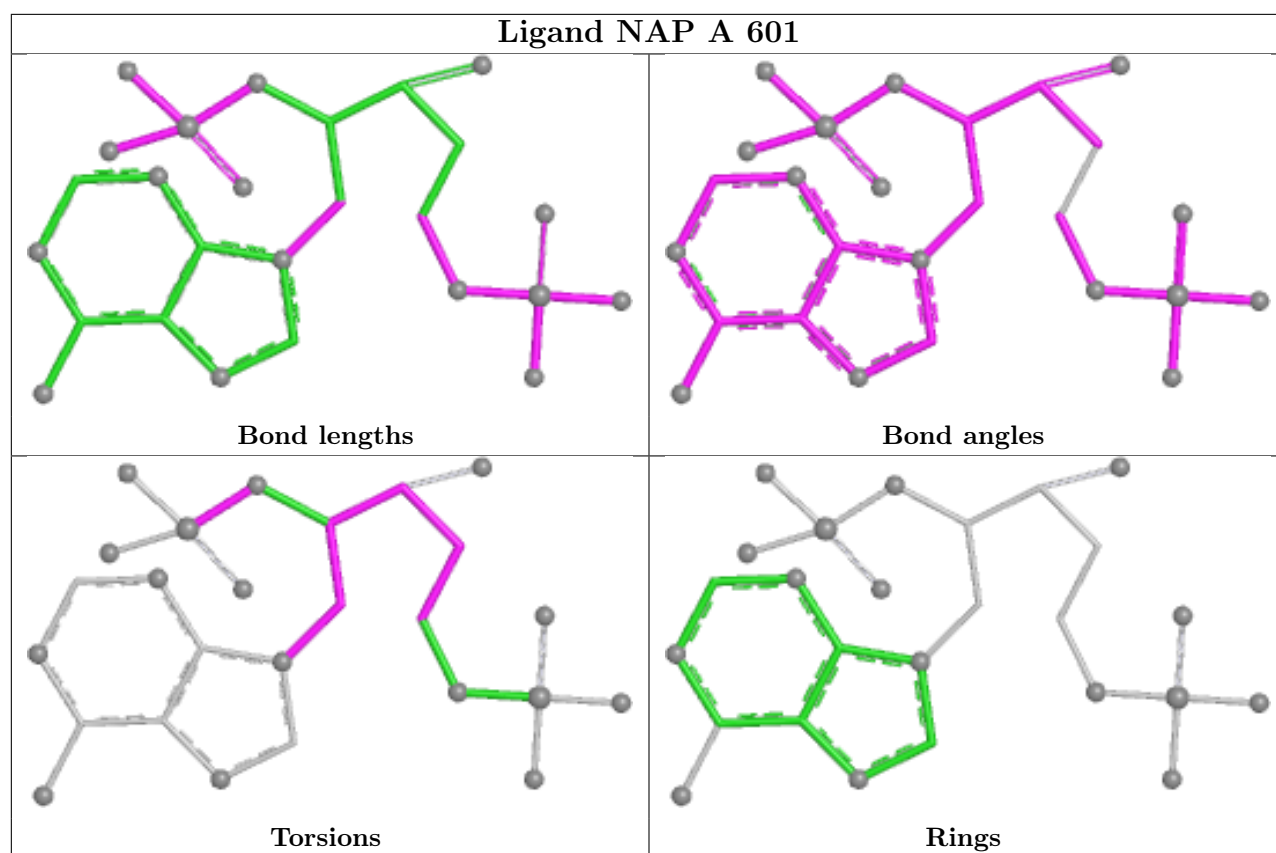
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	1	0
3	A	601	NAP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.