



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:57 PM GMT

PDB ID : 1DDI
Title : CRYSTAL STRUCTURE OF SIR-FP60
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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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

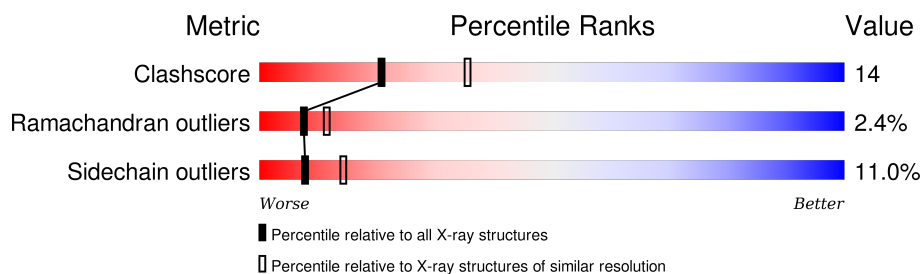
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

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	-	-	-

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 (three-letter code: 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 (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 4 is water.

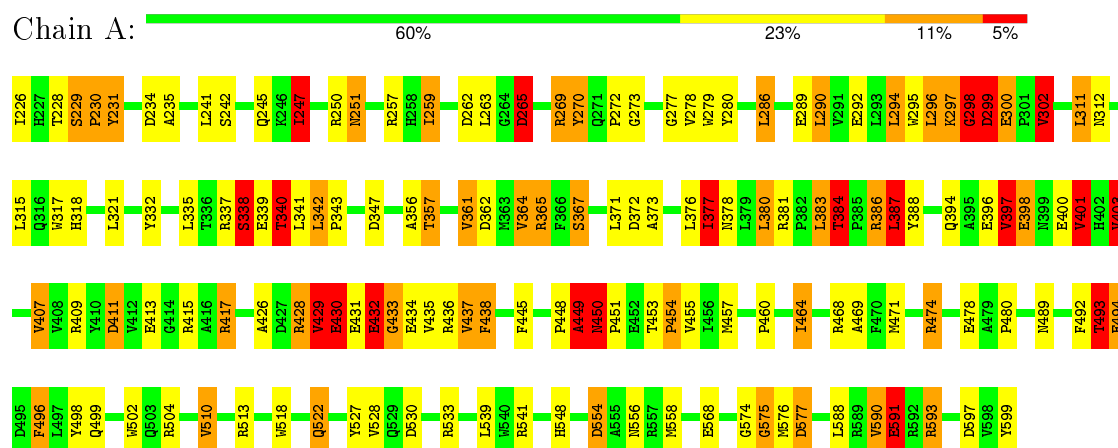
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	271	Total	O	0	0
			271	271		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.61Å 98.61Å 123.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.51	Depositor
% Data completeness (in resolution range)	0.1 (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: NAP, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	8/2963 (0.3%)	3.00	151/4045 (3.7%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	GLU	N-CA	11.37	1.69	1.46
1	A	397	VAL	C-O	9.63	1.41	1.23
1	A	269	ARG	CD-NE	7.88	1.59	1.46
1	A	265	ASP	CA-CB	6.85	1.69	1.53
1	A	269	ARG	CZ-NH1	6.61	1.41	1.33
1	A	433	GLY	N-CA	6.57	1.55	1.46
1	A	575	GLY	N-CA	5.60	1.54	1.46
1	A	230	PRO	C-N	-5.17	1.22	1.34

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	96.19	168.40	120.30
1	A	269	ARG	NE-CZ-NH1	-48.86	95.87	120.30
1	A	533	ARG	NE-CZ-NH2	-21.76	109.42	120.30
1	A	269	ARG	NH1-CZ-NH2	-21.52	95.73	119.40
1	A	250	ARG	NE-CZ-NH2	21.08	130.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	VAL	O-C-N	-19.98	90.72	122.70
1	A	432	GLU	CA-C-O	-19.70	78.73	120.10
1	A	409	ARG	NE-CZ-NH1	18.18	129.39	120.30
1	A	411	ASP	CB-CG-OD1	-18.10	102.01	118.30
1	A	250	ARG	NE-CZ-NH1	-18.08	111.26	120.30
1	A	230	PRO	O-C-N	-18.06	93.81	122.70
1	A	257	ARG	NE-CZ-NH2	17.90	129.25	120.30
1	A	449	ALA	CA-C-N	17.43	155.55	117.20
1	A	397	VAL	CA-C-N	16.94	154.46	117.20
1	A	433	GLY	O-C-N	-15.75	97.50	122.70
1	A	504	ARG	CD-NE-CZ	14.85	144.39	123.60
1	A	247	ILE	CA-CB-CG2	14.48	139.85	110.90
1	A	257	ARG	NE-CZ-NH1	-14.05	113.27	120.30
1	A	234	ASP	CA-C-N	14.02	148.04	117.20
1	A	397	VAL	O-C-N	-13.68	100.82	122.70
1	A	297	LYS	N-CA-CB	13.27	134.48	110.60
1	A	409	ARG	NE-CZ-NH2	-13.14	113.73	120.30
1	A	417	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	A	234	ASP	O-C-N	-12.66	102.44	122.70
1	A	436	ARG	NE-CZ-NH2	12.51	126.56	120.30
1	A	541	ARG	CD-NE-CZ	12.11	140.55	123.60
1	A	449	ALA	O-C-N	-11.81	103.81	122.70
1	A	388	TYR	CB-CG-CD2	11.74	128.04	121.00
1	A	428	ARG	NE-CZ-NH1	-11.51	114.54	120.30
1	A	432	GLU	CA-C-N	11.37	138.94	116.20
1	A	298	GLY	CA-C-N	11.28	142.02	117.20
1	A	590	VAL	CA-C-N	11.24	141.94	117.20
1	A	411	ASP	CB-CG-OD2	11.04	128.23	118.30
1	A	428	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	A	415	ARG	NE-CZ-NH2	10.83	125.72	120.30
1	A	533	ARG	NH1-CZ-NH2	10.48	130.93	119.40
1	A	230	PRO	CA-C-N	10.42	140.13	117.20
1	A	340	THR	N-CA-CB	-10.26	90.81	110.30
1	A	417	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	A	365	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	A	468	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	A	432	GLU	N-CA-CB	-9.96	92.67	110.60
1	A	449	ALA	CA-C-O	-9.68	99.77	120.10
1	A	401	VAL	CG1-CB-CG2	9.58	126.22	110.90
1	A	388	TYR	CB-CG-CD1	-9.30	115.42	121.00
1	A	433	GLY	CA-C-N	9.23	137.50	117.20
1	A	357	THR	N-CA-CB	-9.22	92.77	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ASP	CB-CA-C	-9.04	92.32	110.40
1	A	384	THR	N-CA-CB	-9.00	93.20	110.30
1	A	265	ASP	CB-CG-OD1	-8.93	110.27	118.30
1	A	575	GLY	CA-C-O	-8.90	104.57	120.60
1	A	397	VAL	N-CA-CB	-8.85	92.03	111.50
1	A	437	VAL	N-CA-CB	-8.79	92.15	111.50
1	A	401	VAL	CB-CA-C	-8.74	94.80	111.40
1	A	298	GLY	CA-C-O	-8.60	105.13	120.60
1	A	429	VAL	CA-C-O	8.57	138.11	120.10
1	A	397	VAL	CG1-CB-CG2	8.55	124.58	110.90
1	A	498	TYR	CB-CG-CD2	-8.50	115.90	121.00
1	A	530	ASP	CB-CG-OD2	8.45	125.91	118.30
1	A	265	ASP	N-CA-CB	-8.43	95.43	110.60
1	A	436	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	A	493	THR	N-CA-CB	-8.06	94.99	110.30
1	A	332	TYR	CB-CG-CD2	-7.99	116.21	121.00
1	A	231	TYR	N-CA-CB	7.93	124.87	110.60
1	A	599	TYR	CA-C-O	-7.81	103.70	120.10
1	A	590	VAL	CA-C-O	-7.78	103.76	120.10
1	A	247	ILE	CA-CB-CG1	-7.73	96.31	111.00
1	A	297	LYS	CA-C-N	7.62	131.45	116.20
1	A	397	VAL	C-N-CA	-7.53	102.88	121.70
1	A	381	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	332	TYR	CB-CG-CD1	7.39	125.43	121.00
1	A	397	VAL	CA-C-O	-7.34	104.69	120.10
1	A	432	GLU	CB-CA-C	7.28	124.97	110.40
1	A	365	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	430	GLU	CB-CA-C	7.19	124.79	110.40
1	A	574	GLY	CA-C-N	7.14	130.48	116.20
1	A	296	LEU	CA-C-N	7.12	132.86	117.20
1	A	383	LEU	CA-CB-CG	7.10	131.63	115.30
1	A	383	LEU	CB-CG-CD1	7.02	122.94	111.00
1	A	450	ASN	N-CA-CB	7.01	123.21	110.60
1	A	302	VAL	N-CA-CB	-6.96	96.19	111.50
1	A	428	ARG	CD-NE-CZ	6.80	133.13	123.60
1	A	593	ARG	CD-NE-CZ	6.74	133.04	123.60
1	A	533	ARG	CG-CD-NE	-6.69	97.74	111.80
1	A	265	ASP	CA-CB-CG	-6.67	98.72	113.40
1	A	262	ASP	CB-CG-OD1	6.64	124.27	118.30
1	A	231	TYR	CB-CG-CD1	-6.61	117.04	121.00
1	A	398	GLU	CB-CA-C	6.57	123.53	110.40
1	A	377	ILE	CA-CB-CG1	-6.56	98.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	403	VAL	CA-CB-CG1	6.54	120.70	110.90
1	A	347	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	575	GLY	CA-C-N	6.42	131.31	117.20
1	A	295	TRP	O-C-N	-6.33	112.58	122.70
1	A	478	GLU	CA-CB-CG	6.32	127.30	113.40
1	A	577	ASP	CA-C-O	6.30	133.33	120.10
1	A	298	GLY	O-C-N	-6.26	112.68	122.70
1	A	434	GLU	CB-CA-C	-6.26	97.88	110.40
1	A	386	ARG	CD-NE-CZ	6.21	132.30	123.60
1	A	494	GLU	OE1-CD-OE2	-6.21	115.84	123.30
1	A	364	VAL	CA-CB-CG2	6.15	120.13	110.90
1	A	577	ASP	C-N-CA	6.14	137.05	121.70
1	A	433	GLY	N-CA-C	6.13	128.43	113.10
1	A	297	LYS	C-N-CA	6.13	135.17	122.30
1	A	591	GLU	N-CA-CB	6.08	121.55	110.60
1	A	492	PHE	O-C-N	-6.02	113.06	122.70
1	A	231	TYR	CB-CA-C	-6.02	98.36	110.40
1	A	231	TYR	CA-C-N	-6.01	103.98	117.20
1	A	468	ARG	CD-NE-CZ	5.97	131.96	123.60
1	A	251	ASN	CA-C-O	-5.95	107.61	120.10
1	A	280	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	A	568	GLU	OE1-CD-OE2	-5.83	116.30	123.30
1	A	426	ALA	N-CA-CB	5.82	118.25	110.10
1	A	299	ASP	CA-C-N	5.78	129.91	117.20
1	A	298	GLY	N-CA-C	-5.76	98.70	113.10
1	A	530	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	A	474	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	554	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	434	GLU	CB-CG-CD	5.69	129.57	114.20
1	A	295	TRP	CA-C-N	5.64	129.60	117.20
1	A	513	ARG	CD-NE-CZ	5.62	131.46	123.60
1	A	437	VAL	CA-CB-CG1	5.58	119.26	110.90
1	A	300	GLU	OE1-CD-OE2	-5.56	116.62	123.30
1	A	438	PHE	CB-CG-CD1	-5.55	116.92	120.80
1	A	437	VAL	CG1-CB-CG2	5.51	119.71	110.90
1	A	339	GLU	CA-C-O	5.50	131.65	120.10
1	A	286	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	435	VAL	CG1-CB-CG2	-5.49	102.12	110.90
1	A	510	VAL	CA-CB-CG2	5.48	119.13	110.90
1	A	415	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	A	413	GLU	OE1-CD-OE2	-5.42	116.80	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	THR	CA-CB-CG2	5.40	119.97	112.40
1	A	590	VAL	O-C-N	-5.35	114.14	122.70
1	A	597	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	401	VAL	N-CA-CB	5.31	123.17	111.50
1	A	396	GLU	CA-CB-CG	5.28	125.02	113.40
1	A	231	TYR	CD1-CE1-CZ	-5.26	115.06	119.80
1	A	381	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	A	234	ASP	CA-C-O	-5.24	109.11	120.10
1	A	378	ASN	CA-C-O	5.23	131.08	120.10
1	A	409	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	270	TYR	CB-CG-CD1	5.17	124.10	121.00
1	A	494	GLU	CB-CA-C	-5.17	100.06	110.40
1	A	302	VAL	CB-CA-C	5.17	121.22	111.40
1	A	228	THR	N-CA-C	5.16	124.92	111.00
1	A	292	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	A	380	LEU	N-CA-CB	-5.09	100.22	110.40
1	A	361	VAL	O-C-N	-5.07	114.60	122.70
1	A	362	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	362	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	A	574	GLY	N-CA-C	-5.01	100.58	113.10

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

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Mol	Chain	Res	Type	Group
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	78	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	83	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 14.

All (83) 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:CA	1:A:398:GLU:N	1.69	1.55
3:A:601:NAP:O2A	3:A:601:NAP:O3	1.58	1.18
1:A:397:VAL:O	1:A:398:GLU:CA	1.94	1.15
1:A:397:VAL:O	1:A:398:GLU:HA	1.61	0.97
1:A:397:VAL:C	1:A:398:GLU:CA	2.34	0.94
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:CB	1:A:398:GLU:N	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: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:398:GLU:C	1:A:398:GLU:N	2.46	0.68
1:A:338:SER:OG	1:A:367:SER:HB3	1.95	0.67
3:A:601:NAP:C5B	3:A:601:NAP:N3A	2.58	0.65
1:A:433:GLY:N	4:A:971:HOH:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:493:THR:HB	4:A:639:HOH:O	2.14	0.46
1:A:311:LEU:HG	1:A:373:ALA:HB1	1.96	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:317:TRP:HB2	1:A:318:HIS:CD2	2.50	0.46
1:A:428:ARG:O	1:A:429:VAL:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:HG22	3:A:601:NAP:H2A	1.99	0.45
1:A:527:TYR:CD2	3:A:601:NAP:H52A	2.52	0.45
1:A:489:ASN:O	1:A:518:TRP:HA	2.17	0.45
1:A:464:ILE:HD11	1:A:502:TRP:CZ2	2.52	0.45
2:A:600:FAD:O3B	2:A:600:FAD:N9A	2.50	0.44
1:A:429:VAL:HA	4:A:695:HOH:O	2.18	0.44
1:A:471:MET:HE1	1:A:510:VAL:HG23	1.98	0.44
1:A:298:GLY:O	1:A:299:ASP:C	2.52	0.44
1:A:342:LEU:N	1:A:343:PRO:HD2	2.32	0.43
1:A:273:GLY:HA3	1:A:445:PHE:O	2.18	0.43
1:A:448:PRO:C	1:A:449:ALA:O	2.56	0.43
1:A:337:ARG:O	1:A:338:SER:C	2.56	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:297:LYS:C	1:A:298:GLY:O	2.57	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: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:241:LEU:HD11	1:A:259:ILE:HG23	2.02	0.40
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	372/374 (100%)	341 (92%)	22 (6%)	9 (2%)	7 11

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%)	260 (89%)	32 (11%)	8 14

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
1	A	338	SER
1	A	340	THR
1	A	342	LEU
1	A	357	THR
1	A	367	SER
1	A	376	LEU
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	411	ASP
1	A	437	VAL
1	A	464	ILE
1	A	493	THR
1	A	496	PHE
1	A	522	GLN
1	A	539	LEU
1	A	588	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	ASN
1	A	318	HIS
1	A	352	GLN
1	A	548	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	48,58,58	1.86	7 (14%)	54,89,89	3.28	14 (25%)
3	NAP	A	601	-	24,27,52	13.47	10 (41%)	23,40,80	15.33	20 (86%)

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	0/30/50/50	0/6/6/6
3	NAP	A	601	-	1/1/4/12	0/18/20/67	0/2/2/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NAP	P2B-O2B	-5.62	1.43	1.60
2	A	600	FAD	C10-N10	-5.11	1.33	1.39
2	A	600	FAD	PA-O2A	-4.25	1.36	1.54
3	A	601	NAP	PA-O5B	-4.08	1.46	1.60
3	A	601	NAP	P2B-O2X	-3.34	1.42	1.54
3	A	601	NAP	P2B-O3X	-3.30	1.42	1.54
2	A	600	FAD	P-O1P	-2.95	1.40	1.51
3	A	601	NAP	P2B-O1X	-2.74	1.42	1.51
2	A	600	FAD	PA-O5B	-2.37	1.48	1.59
3	A	601	NAP	C1B-N9A	2.05	1.50	1.48
2	A	600	FAD	C2B-C3B	2.28	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NAP	PA-O2A	3.11	1.65	1.54
2	A	600	FAD	O5'-C5'	3.53	1.59	1.44
2	A	600	FAD	O4B-C1B	6.35	1.49	1.41
3	A	601	NAP	O5B-C5B	6.72	1.73	1.44
3	A	601	NAP	PA-O3	44.95	3.16	1.54
3	A	601	NAP	PA-O1A	46.79	3.05	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAP	O3-PA-O1A	-33.83	1.67	110.58
3	A	601	NAP	O2A-PA-O1A	-30.87	11.21	110.58
3	A	601	NAP	O3B-C3B-C4B	-29.84	42.96	109.35
3	A	601	NAP	O3-PA-O2A	-24.96	12.33	107.38
3	A	601	NAP	C5B-C4B-C3B	-13.78	90.48	113.54
3	A	601	NAP	O2X-P2B-O1X	-13.22	68.02	110.58
3	A	601	NAP	O5B-C5B-C4B	-13.15	57.33	109.03
3	A	601	NAP	O5B-PA-O1A	-8.71	84.97	107.14
3	A	601	NAP	O3-PA-O5B	-7.95	83.67	106.56
3	A	601	NAP	C1B-C2B-C3B	-7.68	98.00	110.61
3	A	601	NAP	O2A-PA-O5B	-7.44	85.13	106.56
2	A	600	FAD	N3A-C2A-N1A	-6.53	123.90	128.89
2	A	600	FAD	C2B-C3B-C4B	-5.69	90.92	102.61
2	A	600	FAD	C4X-C4-N3	-5.54	116.01	123.59
2	A	600	FAD	C4B-O4B-C1B	-4.88	104.35	109.72
2	A	600	FAD	O4B-C1B-N9A	-4.11	99.50	108.10
3	A	601	NAP	C1B-N9A-C8A	-3.45	118.63	125.70
2	A	600	FAD	O3B-C3B-C2B	-3.42	100.69	111.83
2	A	600	FAD	N6A-C6A-N1A	-2.26	114.36	119.20
3	A	601	NAP	N6A-C6A-N1A	2.79	125.19	119.20
2	A	600	FAD	O4B-C4B-C5B	2.94	119.85	109.32
2	A	600	FAD	O3'-C3'-C2'	2.96	116.21	108.75
3	A	601	NAP	C4B-C3B-C2B	3.41	119.05	111.75
2	A	600	FAD	O3B-C3B-C4B	3.44	121.36	111.05
2	A	600	FAD	O3'-C3'-C4'	3.84	118.42	108.75
2	A	600	FAD	C5B-C4B-C3B	4.08	131.42	115.21
3	A	601	NAP	C4A-C5A-N7A	5.55	114.59	109.48
2	A	600	FAD	C4-N3-C2	6.92	121.23	115.25
3	A	601	NAP	N3A-C2A-N1A	8.66	135.52	128.89
3	A	601	NAP	O3X-P2B-O2X	9.73	144.44	107.38
3	A	601	NAP	O2B-P2B-O1X	10.91	134.36	107.11
2	A	600	FAD	C2B-C1B-N9A	16.56	139.60	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAP	O2B-C2B-C1B	17.41	143.41	106.76
3	A	601	NAP	O3B-C3B-C2B	18.48	150.36	109.92

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

There are no torsion outliers.

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.