Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:57 PM GMT

PDB ID	:	1DDG
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	:	2.01 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

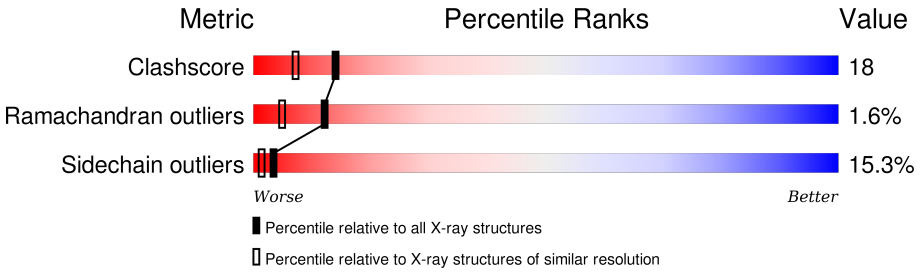
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 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 <=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	56% 32% 10%
1	B	374	67% 25% 7%

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
3	FAD	A	600	X	-	-	-
3	FAD	B	601	X	-	-	-

2 Entry composition

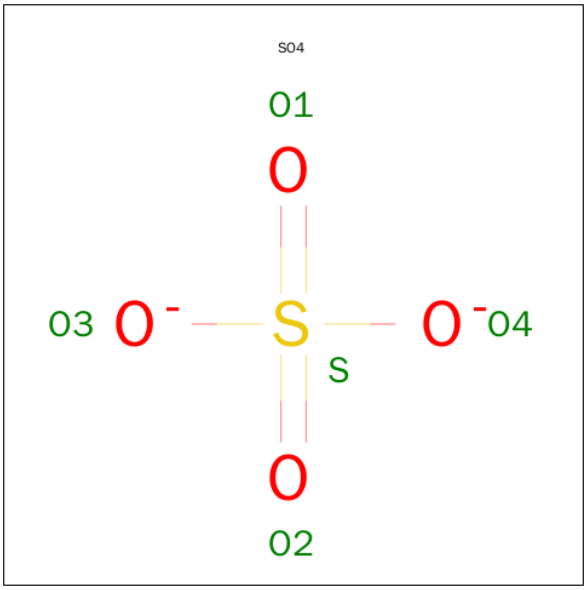
There are 4 unique types of molecules in this entry. The entry contains 6697 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SULFITE REDUCTASE (NADPH) FLAVOPROTEIN ALPHA-COMPONENT.

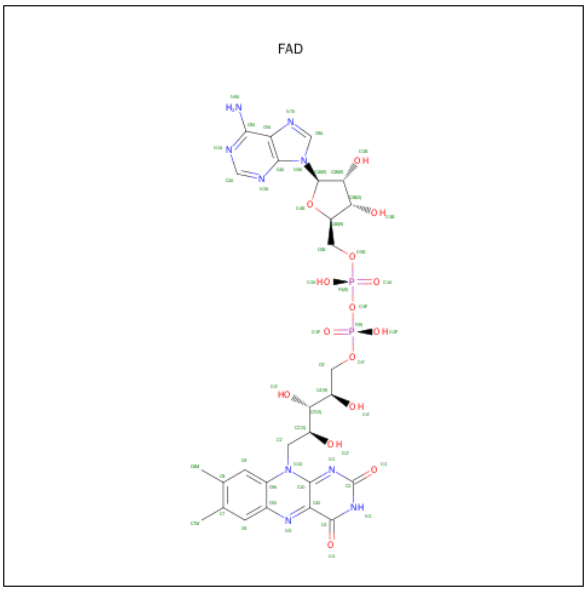
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	4	0
			3028	1915	532	575	6			
1	B	374	Total	C	N	O	S	0	3	0
			3010	1906	523	575	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	271	Total	O	0	0
			271	271		
4	B	277	Total	O	0	0
			277	277		

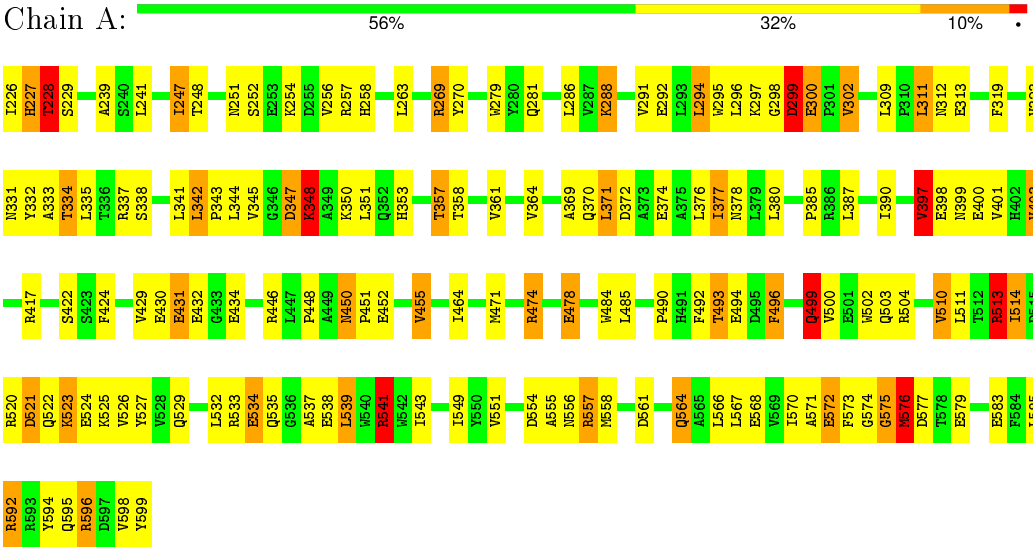
3 Residue-property plots (i)

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.

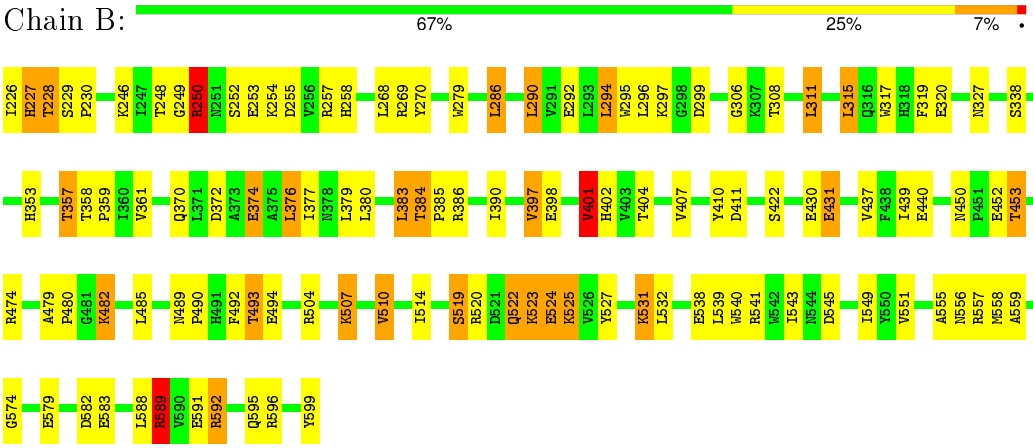
• Molecule 1: SULFITE REDUCTASE (NADPH) FLAVOPROTEIN ALPHA-COMPONENT

Chain A:



• Molecule 1: SULFITE REDUCTASE (NADPH) FLAVOPROTEIN ALPHA-COMPONENT

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	34.84Å 82.54Å 105.36Å 79.71° 83.05° 89.90°	Depositor
Resolution (Å)	10.00 – 2.01	Depositor
% Data completeness (in resolution range)	91.0 (10.00-2.01)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.206 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6697	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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: SO4, 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	0.38	1/3095 (0.0%)	1.16	19/4206 (0.5%)
1	B	0.51	1/3077 (0.0%)	1.06	15/4185 (0.4%)
All	All	0.45	2/6172 (0.0%)	1.11	34/8391 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	599	TYR	C-OXT	20.34	1.62	1.23
1	A	599	TYR	C-OXT	6.34	1.35	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	398	GLU	C-N-CA	10.46	147.85	121.70
1	B	383	LEU	CA-CB-CG	10.15	138.64	115.30
1	A	541	ARG	CD-NE-CZ	10.07	137.70	123.60
1	A	397	VAL	O-C-N	-9.99	106.72	122.70
1	A	269	ARG	CD-NE-CZ	9.87	137.41	123.60
1	A	269	ARG	NE-CZ-NH1	9.45	125.02	120.30
1	B	397	VAL	O-C-N	-8.99	108.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	397	VAL	CA-C-N	8.96	136.92	117.20
1	A	397	VAL	C-N-CA	-8.55	100.33	121.70
1	B	397	VAL	C-N-CA	-8.22	101.14	121.70
1	B	589	ARG	CD-NE-CZ	7.50	134.10	123.60
1	B	397	VAL	CA-C-N	6.94	132.47	117.20
1	B	401	VAL	CB-CA-C	-6.87	98.34	111.40
1	B	431	GLU	C-N-CA	-6.77	104.78	121.70
1	A	446	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	513	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	249	GLY	C-N-CA	5.95	136.58	121.70
1	B	269	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	417	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	417	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	347	ASP	C-N-CA	5.60	135.69	121.70
1	A	499	GLN	CA-CB-CG	5.52	125.54	113.40
1	B	592	ARG	CD-NE-CZ	5.48	131.28	123.60
1	B	589	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	269	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	403	VAL	CB-CA-C	5.32	121.50	111.40
1	A	474	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	575	GLY	C-N-CA	5.20	134.71	121.70
1	B	474	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	257	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	492	PHE	CB-CG-CD2	5.07	124.35	120.80
1	B	401	VAL	N-CA-CB	5.05	122.61	111.50
1	A	492	PHE	CB-CG-CD2	5.04	124.33	120.80
1	A	372	ASP	CA-CB-CG	5.03	124.46	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	PRO	Peptide
1	B	430	GLU	Peptide

5.2 Too-close contacts (i)

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	3028	0	2957	129	0
1	B	3010	0	2935	92	0
2	B	5	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	30	1	0
4	A	271	0	0	21	0
4	B	277	0	0	17	0
All	All	6697	0	5953	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (222) 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:571:ALA:HB1	1:A:576:MET:HG2	1.55	0.87
1:A:302:VAL:HG11	1:A:377:ILE:HD13	1.62	0.81
1:A:347:ASP:HB3	1:A:350:LYS:HD3	1.63	0.79
1:A:361:VAL:HB	4:A:764:HOH:O	1.83	0.78
1:A:344:LEU:HD22	1:A:350:LYS:HB3	1.66	0.77
1:A:490:PRO:HA	1:A:519:SER:HB3	1.67	0.77
1:B:453:THR:HG21	4:B:649:HOH:O	1.84	0.77
1:B:357:THR:HG21	4:B:821:HOH:O	1.84	0.77
1:A:592:ARG:HB2	1:A:592:ARG:HH11	1.49	0.75
1:B:520:ARG:HE	1:B:523:LYS:NZ	1.86	0.74
1:A:566:LEU:O	1:A:570:ILE:HD12	1.87	0.74
1:B:308:THR:HB	4:B:800:HOH:O	1.86	0.74
1:A:344:LEU:O	1:A:347:ASP:HB2	1.89	0.72
1:A:338:SER:OG	1:A:341:LEU:HB2	1.89	0.72
1:B:374:GLU:OE2	4:B:706:HOH:O	2.08	0.72
1:A:299:ASP:O	1:A:311:LEU:HB2	1.90	0.71
1:A:471:MET:HE2	1:A:511:LEU:HD13	1.71	0.71
1:B:227:HIS:O	1:B:228:THR:O	2.09	0.71
1:B:357:THR:HG22	1:B:358:THR:OG1	1.90	0.70
1:A:226:ILE:O	1:A:227:HIS:HB2	1.90	0.70
1:A:543:ILE:HD12	1:A:549:ILE:HD11	1.74	0.70
1:A:500:VAL:O	1:A:504:ARG:HG3	1.92	0.69
1:A:500:VAL:HG23	4:A:703:HOH:O	1.92	0.69
1:B:589:ARG:HD2	4:B:864:HOH:O	1.92	0.68
1:A:485:LEU:HB3	1:A:514:ILE:HG23	1.76	0.68
1:A:592:ARG:NH1	1:A:592:ARG:HB2	2.09	0.67
1:A:551:VAL:HB	1:A:596:ARG:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:HD11	1:A:401[B]:VAL:HG22	1.76	0.67
1:B:531:LYS:HZ2	1:B:531:LYS:HA	1.60	0.66
1:B:404:THR:HA	4:B:866:HOH:O	1.94	0.66
1:B:504:ARG:HA	1:B:507:LYS:HE2	1.77	0.66
1:A:514:ILE:HG21	4:A:865:HOH:O	1.96	0.66
1:B:290:LEU:HD22	1:B:294:LEU:HD22	1.76	0.66
1:A:227:HIS:O	1:A:228:THR:HB	1.96	0.66
1:B:520:ARG:HE	1:B:523:LYS:HZ1	1.43	0.66
1:B:226:ILE:HG23	1:B:227:HIS:N	2.11	0.66
1:A:331:ASN:O	1:A:335:LEU:HB2	1.96	0.66
1:B:286:LEU:HD22	1:B:361[A]:VAL:HG21	1.78	0.65
1:A:490:PRO:HB3	1:A:520:ARG:HD2	1.77	0.65
1:A:286:LEU:HD11	1:A:361:VAL:HG21	1.78	0.64
1:A:312:ASN:HB3	4:A:642:HOH:O	1.98	0.63
1:B:404:THR:HG23	4:B:866:HOH:O	1.99	0.63
1:A:270:TYR:CE2	1:A:401[B]:VAL:HG13	2.34	0.62
1:A:353:HIS:O	1:A:357:THR:HB	1.99	0.62
1:A:228:THR:HA	4:A:786:HOH:O	2.00	0.62
1:A:357:THR:HG22	1:A:358:THR:OG1	1.99	0.61
1:B:551:VAL:HB	1:B:596:ARG:HG2	1.83	0.61
1:A:281:GLN:HG2	1:A:424:PHE:CE1	2.36	0.61
1:B:523:LYS:HA	4:B:852:HOH:O	2.01	0.61
1:B:297:LYS:HG3	1:B:299:ASP:OD1	2.02	0.60
1:B:411:ASP:HB2	4:B:868:HOH:O	2.01	0.60
1:A:397:VAL:HG13	1:A:400:GLU:HB2	1.84	0.60
1:A:543:ILE:CD1	1:A:549:ILE:HD11	2.32	0.59
1:B:254:LYS:NZ	1:B:489:ASN:HD21	2.02	0.57
1:B:268:LEU:HD21	1:B:439:ILE:HD11	1.87	0.57
1:A:557[A]:ARG:HG3	1:A:558:MET:N	2.20	0.57
1:A:576:MET:O	1:A:577:ASP:HB3	2.06	0.56
1:A:571:ALA:HA	1:A:576:MET:HA	1.87	0.56
1:B:450:ASN:O	1:B:453:THR:HG23	2.06	0.55
1:B:258:HIS:HA	4:B:866:HOH:O	2.06	0.55
1:A:523:LYS:HD2	1:A:523:LYS:H	1.71	0.55
1:A:573:PHE:HB3	4:A:826:HOH:O	2.07	0.55
1:B:353:HIS:O	1:B:357:THR:HB	2.06	0.54
1:B:296:LEU:HD13	1:B:311:LEU:HD11	1.89	0.54
1:B:524:GLU:HG2	1:B:524:GLU:O	2.06	0.54
1:B:522:GLN:O	1:B:523:LYS:HB2	2.06	0.54
1:A:254:LYS:HD2	4:A:802:HOH:O	2.08	0.54
1:A:568:GLU:O	1:A:572:GLU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LYS:CE	1:B:482:LYS:H	2.20	0.53
1:B:227:HIS:CE1	1:B:228:THR:HG22	2.43	0.53
1:A:485:LEU:O	1:A:514:ILE:HA	2.08	0.53
1:B:306:GLY:HA2	4:B:763:HOH:O	2.09	0.53
1:A:513:ARG:CZ	1:A:538:GLU:HG2	2.39	0.53
1:A:537:ALA:HB2	1:A:573:PHE:CE2	2.42	0.53
1:A:516:LEU:HG	1:A:518:TRP:CZ2	2.44	0.52
1:A:490:PRO:HA	1:A:519:SER:CB	2.39	0.52
1:A:522:GLN:NE2	1:A:526:VAL:HG23	2.24	0.52
1:B:227:HIS:HE1	4:B:745:HOH:O	1.92	0.52
1:B:532:LEU:HD22	1:B:539:LEU:HD21	1.92	0.51
1:A:478:GLU:OE1	1:A:478:GLU:HA	2.10	0.51
1:A:374:GLU:HG2	4:A:704:HOH:O	2.11	0.51
1:B:525:LYS:HB2	1:B:527:TYR:CE2	2.45	0.51
1:A:351:LEU:HG	4:A:664:HOH:O	2.10	0.51
1:A:534:GLU:OE1	1:A:535:GLN:HG2	2.11	0.51
1:A:493:THR:HB	4:A:753:HOH:O	2.10	0.51
1:A:555:ALA:HB2	1:A:598:VAL:HB	1.94	0.50
1:B:460:PRO:HG2	1:B:558:MET:HG3	1.92	0.50
1:A:343:PRO:O	1:A:347:ASP:OD2	2.29	0.50
1:A:298:GLY:O	1:A:312:ASN:OD1	2.30	0.50
1:A:575:GLY:O	1:A:576:MET:O	2.29	0.49
1:A:294:LEU:O	1:A:295:TRP:HB2	2.10	0.49
1:B:374:GLU:CA	1:B:374:GLU:OE1	2.60	0.49
1:A:286:LEU:CD1	1:A:361:VAL:HG21	2.43	0.49
1:B:531:LYS:HZ2	1:B:531:LYS:CA	2.25	0.49
1:B:540:TRP:CE2	1:B:574:GLY:HA2	2.47	0.49
1:A:514:ILE:HG12	4:A:865:HOH:O	2.12	0.49
1:A:279:TRP:CH2	1:A:385:PRO:HD3	2.47	0.49
1:A:592:ARG:HD2	4:A:628:HOH:O	2.12	0.49
1:A:333:ALA:HA	1:A:338:SER:OG	2.12	0.49
1:B:374:GLU:HA	1:B:374:GLU:OE1	2.12	0.48
1:B:268:LEU:HD21	1:B:439:ILE:CG1	2.44	0.48
1:A:587:GLU:HG3	1:A:588:LEU:N	2.27	0.48
1:B:359:PRO:HG3	1:B:410:TYR:OH	2.14	0.48
1:A:431:GLU:HA	1:A:431:GLU:OE1	2.13	0.48
1:A:431:GLU:N	4:A:784:HOH:O	2.47	0.47
1:B:493:THR:HG23	1:B:494:GLU:OE2	2.15	0.47
1:B:338:SER:OG	1:B:341:LEU:HB2	2.14	0.47
1:A:309:LEU:HD13	1:A:313:GLU:HG2	1.96	0.47
1:B:250:ARG:HG2	4:B:861:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD13	1:A:311:LEU:HD11	1.95	0.47
1:B:227:HIS:ND1	1:B:228:THR:HG22	2.29	0.47
1:A:302:VAL:CG1	1:A:377:ILE:HD13	2.41	0.47
1:A:335:LEU:HD23	1:A:371:LEU:HD11	1.97	0.47
1:A:371:LEU:HA	1:A:371:LEU:HD12	1.75	0.47
1:A:241:LEU:HD23	1:A:429:VAL:HB	1.96	0.47
1:A:485:LEU:O	1:A:514:ILE:HG22	2.15	0.47
1:A:288:LYS:NZ	1:A:292:GLU:OE1	2.46	0.47
1:B:384:THR:HG22	1:B:386:ARG:NH1	2.30	0.46
1:A:397:VAL:CG1	1:A:400:GLU:HB2	2.45	0.46
1:A:574:GLY:N	4:A:826:HOH:O	2.48	0.46
1:B:286:LEU:CD2	1:B:361[A]:VAL:HG21	2.45	0.46
1:A:247:ILE:HD13	1:A:258:HIS:HB3	1.98	0.46
1:A:347:ASP:HB3	1:A:350:LYS:CD	2.40	0.46
1:B:290:LEU:HG	1:B:361[A]:VAL:HG22	1.98	0.46
1:B:252:SER:HB2	1:B:494:GLU:HB3	1.98	0.46
1:A:338:SER:O	1:A:342:LEU:HD22	2.15	0.46
1:A:228:THR:HG22	4:A:829:HOH:O	2.16	0.46
1:A:270:TYR:CE1	1:A:390:ILE:HG21	2.51	0.46
1:A:592:ARG:HG3	1:A:595:GLN:NE2	2.30	0.46
1:B:591:GLU:O	1:B:592:ARG:HB2	2.16	0.46
1:A:450:ASN:HA	1:A:451:PRO:HD2	1.65	0.46
1:A:579:GLU:O	1:A:583:GLU:HG3	2.14	0.46
1:A:471:MET:CE	1:A:511:LEU:HD13	2.45	0.46
1:B:507:LYS:HE2	1:B:507:LYS:HB3	1.60	0.45
1:A:533:ARG:NH2	4:A:788:HOH:O	2.50	0.45
1:B:450:ASN:HB3	1:B:453:THR:CG2	2.47	0.45
1:A:564:GLN:NE2	1:A:568:GLU:OE2	2.50	0.45
1:A:319:PHE:CE2	1:A:377:ILE:HG12	2.51	0.45
1:B:290:LEU:HD22	1:B:294:LEU:CD2	2.46	0.45
1:A:407:VAL:HA	1:A:422:SER:HB2	1.99	0.45
1:A:592:ARG:NH1	4:A:619:HOH:O	2.50	0.45
1:A:471:MET:HG3	1:A:502:TRP:HZ3	1.81	0.45
1:A:342:LEU:HD12	1:A:345:VAL:HG21	1.98	0.45
1:B:538:GLU:OE2	1:B:541:ARG:NH1	2.50	0.45
1:A:537:ALA:O	1:A:541:ARG:NH1	2.50	0.44
1:A:348:LYS:N	4:A:664:HOH:O	2.49	0.44
1:A:269:ARG:NH1	4:A:794:HOH:O	2.49	0.44
1:A:525:LYS:HB3	1:A:527:TYR:CE2	2.52	0.44
1:B:523:LYS:HD2	1:B:523:LYS:HA	1.57	0.44
1:B:228:THR:HG23	1:B:230:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LYS:HE2	1:B:482:LYS:HB2	1.65	0.44
1:A:455:VAL:HG13	1:A:474:ARG:NH1	2.32	0.44
1:B:450:ASN:HB3	1:B:453:THR:HG22	2.00	0.44
1:A:288:LYS:HE3	4:A:685:HOH:O	2.18	0.44
1:A:471:MET:HE3	1:A:510:VAL:HG22	1.99	0.44
1:B:297:LYS:HE3	1:B:299:ASP:OD1	2.18	0.44
1:B:254:LYS:HZ1	1:B:489:ASN:HD21	1.64	0.44
1:B:270:TYR:CE2	1:B:390:ILE:HG21	2.52	0.44
1:B:595:GLN:NE2	4:B:676:HOH:O	2.50	0.44
1:A:323:VAL:HG22	3:A:600:FAD:H51A	2.00	0.44
1:B:407[B]:VAL:HA	1:B:422:SER:HB2	1.99	0.44
1:B:370:GLN:H	1:B:370:GLN:CD	2.21	0.44
1:A:263:LEU:HD21	1:A:401[B]:VAL:CG2	2.48	0.43
1:B:579:GLU:O	1:B:582:ASP:HB2	2.18	0.43
1:A:228:THR:HG23	1:A:229:SER:N	2.33	0.43
1:A:288:LYS:HG2	1:A:288:LYS:O	2.14	0.43
1:A:302:VAL:HG11	1:A:377:ILE:CD1	2.42	0.43
1:A:554:ASP:O	1:A:558:MET:HB3	2.19	0.43
1:B:543:ILE:CD1	1:B:549:ILE:HD11	2.48	0.43
1:A:572:GLU:HB3	1:A:573:PHE:CD1	2.53	0.43
1:B:255:ASP:HB3	1:B:407[B]:VAL:HG12	2.00	0.43
1:B:376:LEU:O	1:B:379:LEU:HB3	2.18	0.43
1:B:531:LYS:HE3	4:B:878:HOH:O	2.18	0.43
1:A:239:ALA:O	1:A:434:GLU:HA	2.19	0.43
1:A:252:SER:HB2	1:A:494:GLU:HB3	2.00	0.43
1:B:490:PRO:HA	1:B:519:SER:HB2	1.99	0.43
1:B:407[B]:VAL:HG13	1:B:407[B]:VAL:O	2.19	0.43
1:A:496:PHE:CG	1:A:499:GLN:HB3	2.54	0.43
1:A:499:GLN:O	1:A:503:GLN:HG3	2.19	0.43
1:A:484:TRP:CD1	1:A:513:ARG:HB2	2.54	0.43
1:A:288:LYS:NZ	4:A:841:HOH:O	2.52	0.42
1:B:279:TRP:CH2	1:B:385:PRO:HD3	2.54	0.42
1:A:523:LYS:CD	1:A:523:LYS:H	2.31	0.42
1:A:541:ARG:HB2	1:A:541:ARG:HH11	1.84	0.42
1:A:532:LEU:HD23	1:A:539:LEU:HD21	2.00	0.42
1:A:241:LEU:O	1:A:432:GLU:N	2.48	0.42
1:A:585:LEU:HD11	1:A:594:TYR:CD2	2.55	0.42
1:B:479:ALA:HA	1:B:480:PRO:HD3	1.88	0.42
1:B:431:GLU:HA	4:B:623:HOH:O	2.18	0.42
1:B:440:GLU:HG2	4:B:847:HOH:O	2.18	0.42
1:A:348:LYS:HG3	1:A:348:LYS:HZ3	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:VAL:HG11	1:B:402:HIS:CE1	2.54	0.42
1:B:556:ASN:ND2	1:B:556:ASN:H	2.18	0.42
1:B:555:ALA:O	1:B:559:ALA:HB3	2.19	0.42
1:B:520:ARG:HE	1:B:523:LYS:HZ3	1.64	0.42
1:B:564:GLN:O	1:B:568:GLU:HG3	2.20	0.42
1:B:319:PHE:CE2	1:B:377:ILE:HG13	2.55	0.42
1:A:464:ILE:HD11	1:A:502:TRP:CZ2	2.54	0.41
1:B:250:ARG:HG3	1:B:250:ARG:H	1.53	0.41
1:B:270:TYR:CE1	1:B:401:VAL:HG13	2.55	0.41
1:A:299:ASP:O	1:A:300:GLU:HB2	2.20	0.41
1:B:294:LEU:O	1:B:295:TRP:HB2	2.20	0.41
1:B:268:LEU:HD21	1:B:439:ILE:CD1	2.49	0.41
1:A:326:ALA:HB1	1:A:351:LEU:HB3	2.01	0.41
1:B:228:THR:HG23	1:B:229:SER:N	2.35	0.41
1:A:332:TYR:OH	1:A:364:VAL:HB	2.20	0.41
1:A:518:TRP:HB2	1:A:521:ASP:HB2	2.03	0.41
1:A:294:LEU:HD12	1:A:369:ALA:O	2.21	0.41
1:A:248:THR:HG23	1:A:256:VAL:HB	2.02	0.41
1:B:311:LEU:HD22	1:B:315:LEU:HD22	2.02	0.41
1:A:431:GLU:O	1:A:432:GLU:HB2	2.21	0.41
1:B:471:MET:CE	1:B:510:VAL:HG22	2.51	0.41
1:B:246:LYS:HA	1:B:257:ARG:HD3	2.02	0.41
1:A:374:GLU:O	1:A:378:ASN:HB2	2.21	0.41
1:B:485:LEU:O	1:B:514:ILE:HA	2.20	0.41
1:A:534:GLU:HG2	1:A:534:GLU:O	2.21	0.40
1:A:279:TRP:CZ3	1:A:385:PRO:HD3	2.56	0.40
1:A:529:GLN:HA	1:A:532:LEU:HD12	2.03	0.40
1:B:504:ARG:HG2	1:B:507:LYS:HE3	2.04	0.40
1:B:482:LYS:HE2	1:B:482:LYS:H	1.86	0.40
3:B:601:FAD:HM82	3:B:601:FAD:HM71	1.88	0.40
1:A:330:GLU:O	1:A:334:THR:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	376/374 (100%)	353 (94%)	14 (4%)	9 (2%)	7 2
1	B	375/374 (100%)	358 (96%)	14 (4%)	3 (1%)	24 15
All	All	751/748 (100%)	711 (95%)	28 (4%)	12 (2%)	12 5

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	HIS
1	A	228	THR
1	A	299	ASP
1	A	399	ASN
1	A	430	GLU
1	A	576	MET
1	B	228	THR
1	B	250	ARG
1	A	300	GLU
1	A	348	LYS
1	B	522	GLN
1	A	450	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	320/316 (101%)	265 (83%)	55 (17%)	2 1
1	B	319/316 (101%)	275 (86%)	44 (14%)	4 2
All	All	639/632 (101%)	540 (84%)	99 (16%)	3 1

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR

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Mol	Chain	Res	Type
1	A	247	ILE
1	A	251	ASN
1	A	288	LYS
1	A	291	VAL
1	A	294	LEU
1	A	297	LYS
1	A	299	ASP
1	A	302	VAL
1	A	311	LEU
1	A	334	THR
1	A	337	ARG
1	A	342	LEU
1	A	348	LYS
1	A	357	THR
1	A	370	GLN
1	A	371	LEU
1	A	376	LEU
1	A	377	ILE
1	A	380	LEU
1	A	387	LEU
1	A	397	VAL
1	A	403	VAL
1	A	407	VAL
1	A	411	ASP
1	A	431	GLU
1	A	452	GLU
1	A	455	VAL
1	A	478	GLU
1	A	493	THR
1	A	496	PHE
1	A	499	GLN
1	A	510	VAL
1	A	513	ARG
1	A	514	ILE
1	A	516	LEU
1	A	519	SER
1	A	521	ASP
1	A	523	LYS
1	A	524	GLU
1	A	534	GLU
1	A	539	LEU
1	A	541	ARG

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Mol	Chain	Res	Type
1	A	556	ASN
1	A	557[A]	ARG
1	A	557[B]	ARG
1	A	561	ASP
1	A	564	GLN
1	A	567	LEU
1	A	572	GLU
1	A	576	MET
1	A	587	GLU
1	A	588	LEU
1	A	592	ARG
1	A	596	ARG
1	B	227	HIS
1	B	248	THR
1	B	250	ARG
1	B	253	GLU
1	B	286	LEU
1	B	290	LEU
1	B	292	GLU
1	B	294	LEU
1	B	311	LEU
1	B	315	LEU
1	B	317	TRP
1	B	320	GLU
1	B	327[A]	ASN
1	B	327[B]	ASN
1	B	341	LEU
1	B	342	LEU
1	B	348	LYS
1	B	357	THR
1	B	372	ASP
1	B	374	GLU
1	B	376	LEU
1	B	380	LEU
1	B	383	LEU
1	B	384	THR
1	B	398	GLU
1	B	401	VAL
1	B	437	VAL
1	B	452	GLU
1	B	453	THR
1	B	482	LYS

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Mol	Chain	Res	Type
1	B	493	THR
1	B	507	LYS
1	B	510	VAL
1	B	519	SER
1	B	523	LYS
1	B	524	GLU
1	B	525	LYS
1	B	531	LYS
1	B	545	ASP
1	B	557	ARG
1	B	564	GLN
1	B	583	GLU
1	B	588	LEU
1	B	589	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	316	GLN
1	A	318	HIS
1	A	441	HIS
1	A	499	GLN
1	B	227	HIS
1	B	281	GLN
1	B	316	GLN
1	B	489	ASN

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 (i)

3 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	$\#\|Z\| > 2$
3	FAD	A	600	-	48,58,58	2.36	14 (29%)	54,89,89	3.14	17 (31%)
3	FAD	B	601	-	48,58,58	2.18	12 (25%)	54,89,89	3.22	19 (35%)
2	SO4	B	602	-	4,4,4	1.01	0	6,6,6	0.28	0

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	A	600	-	2/2/9/9	0/30/50/50	0/6/6/6
3	FAD	B	601	-	3/3/9/9	0/30/50/50	0/6/6/6
2	SO4	B	602	-	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	FAD	C1'-N10	-7.29	1.40	1.48
3	A	600	FAD	C1'-N10	-7.05	1.41	1.48
3	B	601	FAD	PA-O2A	-4.58	1.35	1.54
3	A	600	FAD	C10-N10	-4.42	1.34	1.39
3	A	600	FAD	PA-O2A	-4.42	1.36	1.54
3	B	601	FAD	C10-N10	-3.94	1.34	1.39
3	A	600	FAD	P-O1P	-3.42	1.38	1.51
3	B	601	FAD	P-O1P	-3.17	1.39	1.51
3	A	600	FAD	P-O5'	-2.46	1.47	1.59
3	B	601	FAD	P-O5'	-2.39	1.48	1.59
3	A	600	FAD	O3B-C3B	-2.37	1.37	1.43
3	B	601	FAD	PA-O5B	-2.07	1.49	1.59
3	A	600	FAD	C2'-C3'	-2.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	FAD	C9A-N10	2.10	1.41	1.38
3	A	600	FAD	C4-C4X	2.31	1.45	1.41
3	B	601	FAD	C9A-N10	2.43	1.42	1.38
3	B	601	FAD	C4-C4X	2.47	1.46	1.41
3	A	600	FAD	C2B-C3B	2.75	1.60	1.53
3	B	601	FAD	C5'-C4'	3.12	1.56	1.51
3	B	601	FAD	O4'-C4'	3.31	1.50	1.43
3	A	600	FAD	C4X-C10	3.54	1.47	1.41
3	B	601	FAD	C4X-C10	3.64	1.47	1.41
3	A	600	FAD	C5'-C4'	3.64	1.57	1.51
3	A	600	FAD	O4'-C4'	3.77	1.51	1.43
3	B	601	FAD	O4B-C1B	4.97	1.47	1.41
3	A	600	FAD	O4B-C1B	6.97	1.50	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	FAD	C4B-O4B-C1B	-9.92	98.81	109.72
3	A	600	FAD	N3A-C2A-N1A	-7.99	122.78	128.89
3	B	601	FAD	C4X-C4-N3	-7.75	112.99	123.59
3	A	600	FAD	O2B-C2B-C3B	-7.44	87.62	111.83
3	B	601	FAD	N3A-C2A-N1A	-7.23	123.36	128.89
3	B	601	FAD	O2B-C2B-C3B	-6.77	89.81	111.83
3	A	600	FAD	C4X-C4-N3	-6.53	114.65	123.59
3	A	600	FAD	C2B-C3B-C4B	-6.41	89.44	102.61
3	A	600	FAD	C4B-O4B-C1B	-6.40	102.68	109.72
3	A	600	FAD	O4'-C4'-C5'	-4.28	100.86	110.19
3	A	600	FAD	C1B-N9A-C4A	-4.24	120.55	126.94
3	B	601	FAD	O4B-C4B-C3B	-3.78	97.54	105.15
3	A	600	FAD	O2'-C2'-C1'	-3.61	101.07	109.94
3	B	601	FAD	O4'-C4'-C5'	-3.14	103.35	110.19
3	B	601	FAD	O2'-C2'-C1'	-2.97	102.64	109.94
3	B	601	FAD	C8M-C8-C7	-2.34	115.60	120.73
3	B	601	FAD	C7M-C7-C8	-2.33	115.62	120.73
3	A	600	FAD	O5B-C5B-C4B	-2.32	100.57	109.12
3	A	600	FAD	C4X-C10-N10	-2.31	119.16	120.52
3	B	601	FAD	C4X-C10-N10	-2.17	119.24	120.52
3	B	601	FAD	C2B-C3B-C4B	-2.05	98.40	102.61
3	B	601	FAD	C1B-N9A-C4A	-2.01	123.91	126.94
3	B	601	FAD	C8M-C8-C9	2.13	126.08	120.28
3	A	600	FAD	C2A-N1A-C6A	2.16	122.62	118.77
3	A	600	FAD	O2A-PA-O1A	2.41	125.60	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	FAD	O3P-P-O5'	2.81	110.38	102.94
3	A	600	FAD	C4X-N5-C5X	2.86	120.06	116.76
3	B	601	FAD	C4X-N5-C5X	2.96	120.17	116.76
3	B	601	FAD	O3'-C3'-C4'	3.41	117.34	108.75
3	A	600	FAD	O3'-C3'-C4'	3.74	118.18	108.75
3	A	600	FAD	P-O3P-PA	3.82	143.46	132.73
3	B	601	FAD	C2A-N1A-C6A	4.00	125.91	118.77
3	B	601	FAD	C4-N3-C2	6.11	120.53	115.25
3	A	600	FAD	C4-N3-C2	8.49	122.58	115.25
3	A	600	FAD	O4B-C1B-N9A	8.53	125.96	108.10
3	B	601	FAD	O4B-C1B-N9A	11.26	131.67	108.10

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	601	FAD	C4B
3	B	601	FAD	C2B
3	B	601	FAD	C3B
3	A	600	FAD	C4B
3	A	600	FAD	C2B

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FAD	1	0
3	B	601	FAD	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.