



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2017 – 07:02 PM EDT

PDB ID : 5VWU
Title : Crystal structure of oxidized Aspergillus fumigatus UDP-galactopyranose mutase complexed with NADH
Authors : Tanner, J.J.
Deposited on : unknown
Resolution : 2.75 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

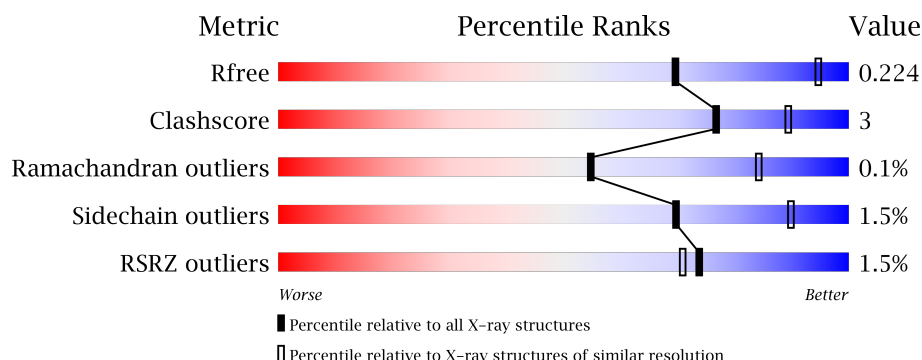
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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.

Mol	Chain	Length	Quality of chain
1	A	513	<div> <div>88%</div> <div>8%</div> <div>•</div> </div>
1	B	513	<div> <div>87%</div> <div>8%</div> <div>• •</div> </div>
1	C	513	<div> <div>3%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
1	D	513	<div> <div>2%</div> <div>92%</div> <div>6%</div> <div>•</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15591 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 UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3777	2409	635	712	21			
1	B	494	Total	C	N	O	S	0	0	0
			3777	2406	633	718	20			
1	C	503	Total	C	N	O	S	0	0	0
			3826	2440	647	720	19			
1	D	504	Total	C	N	O	S	0	0	0
			3827	2442	644	721	20			

There are 24 discrepancies between the modelled and reference sequences:

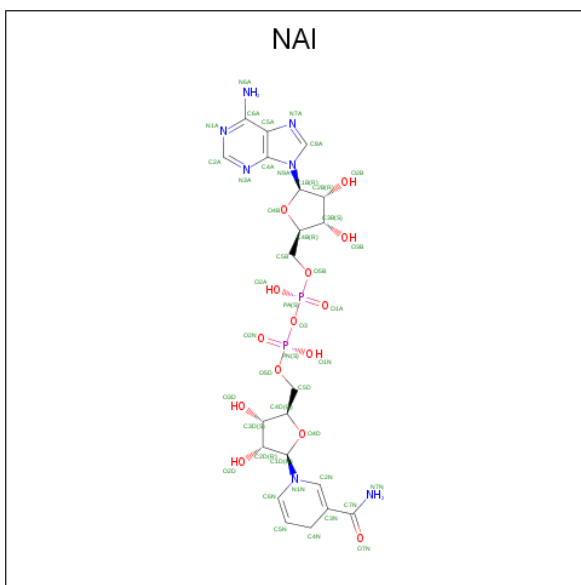
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP Q4W1X2
A	-1	ILE	-	expression tag	UNP Q4W1X2
A	0	ALA	-	expression tag	UNP Q4W1X2
A	344	ALA	LYS	engineered mutation	UNP Q4W1X2
A	345	ALA	LYS	engineered mutation	UNP Q4W1X2
A	429	THR	ALA	conflict	UNP Q4W1X2
B	-2	ALA	-	expression tag	UNP Q4W1X2
B	-1	ILE	-	expression tag	UNP Q4W1X2
B	0	ALA	-	expression tag	UNP Q4W1X2
B	344	ALA	LYS	engineered mutation	UNP Q4W1X2
B	345	ALA	LYS	engineered mutation	UNP Q4W1X2
B	429	THR	ALA	conflict	UNP Q4W1X2
C	-2	ALA	-	expression tag	UNP Q4W1X2
C	-1	ILE	-	expression tag	UNP Q4W1X2
C	0	ALA	-	expression tag	UNP Q4W1X2
C	344	ALA	LYS	engineered mutation	UNP Q4W1X2
C	345	ALA	LYS	engineered mutation	UNP Q4W1X2
C	429	THR	ALA	conflict	UNP Q4W1X2
D	-2	ALA	-	expression tag	UNP Q4W1X2
D	-1	ILE	-	expression tag	UNP Q4W1X2
D	0	ALA	-	expression tag	UNP Q4W1X2

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	344	ALA	LYS	engineered mutation	UNP Q4W1X2
D	345	ALA	LYS	engineered mutation	UNP Q4W1X2
D	429	THR	ALA	conflict	UNP Q4W1X2

-
- The chemical structure of FAD (Flavin Adenine Dinucleotide) is shown. It consists of a riboflavin moiety (top) and an adenosine moiety (bottom) linked by a pyrophosphate bridge. The riboflavin part includes a ribityl side chain with a terminal phosphate group. The adenosine part includes an adenine base and a ribose sugar. The structure is color-coded: blue for nitrogen atoms, red for oxygen atoms, and green for carbon atoms. The pyrophosphate bridge is shown in red. The riboflavin moiety is labeled with N5A, N7A, C5A, C6A, C7A, C8A, C9A, C10A, C11A, C12A, C13A, C14A, C15A, C16A, C17A, C18A, C19A, C20A, C21A, C22A, C23A, C24A, C25A, C26A, C27A, C28A, C29A, C30A, C31A, C32A, C33A, C34A, C35A, C36A, C37A, C38A, C39A, C40A, C41A, C42A, C43A, C44A, C45A, C46A, C47A, C48A, C49A, C50A, C51A, C52A, C53A, C54A, C55A, C56A, C57A, C58A, C59A, C60A, C61A, C62A, C63A, C64A, C65A, C66A, C67A, C68A, C69A, C70A, C71A, C72A, C73A, C74A, C75A, C76A, C77A, C78A, C79A, C80A, C81A, C82A, C83A, C84A, C85A, C86A, C87A, C88A, C89A, C90A, C91A, C92A, C93A, C94A, C95A, C96A, C97A, C98A, C99A, C100A, C101A, C102A, C103A, C104A, C105A, C106A, C107A, C108A, C109A, C110A, C111A, C112A, C113A, C114A, C115A, C116A, C117A, C118A, C119A, C120A, C121A, C122A, C123A, C124A, C125A, C126A, C127A, C128A, C129A, C130A, C131A, C132A, C133A, C134A, C135A, C136A, C137A, C138A, C139A, C140A, C141A, C142A, C143A, C144A, C145A, C146A, C147A, C148A, C149A, C150A, C151A, C152A, C153A, C154A, C155A, C156A, C157A, C158A, C159A, C160A, C161A, C162A, C163A, C164A, C165A, C166A, C167A, C168A, C169A, C170A, C171A, C172A, C173A, C174A, C175A, C176A, C177A, C178A, C179A, C180A, C181A, C182A, C183A, C184A, C185A, C186A, C187A, C188A, C189A, C190A, C191A, C192A, C193A, C194A, C195A, C196A, C197A, C198A, C199A, C200A, C201A, C202A, C203A, C204A, C205A, C206A, C207A, C208A, C209A, C210A, C211A, C212A, C213A, C214A, C215A, C216A, C217A, C218A, C219A, C220A, C221A, C222A, C223A, C224A, C225A, C226A, C227A, C228A, C229A, C230A, C231A, C232A, C233A, C234A, C235A, C236A, C237A, C238A, C239A, C240A, C241A, C242A, C243A, C244A, C245A, C246A, C247A, C248A, C249A, C250A, C251A, C252A, C253A, C254A, C255A, C256A, C257A, C258A, C259A, C260A, C261A, C262A, C263A, C264A, C265A, C266A, C267A, C268A, C269A, C270A, C271A, C272A, C273A, C274A, C275A, C276A, C277A, C278A, C279A, C280A, C281A, C282A, C283A, C284A, C285A, C286A, C287A, C288A, C289A, C290A, C291A, C292A, C293A, C294A, C295A, C296A, C297A, C298A, C299A, C300A, C301A, C302A, C303A, C304A, C305A, C306A, C307A, C308A, C309A, C310A, C311A, C312A, C313A, C314A, C315A, C316A, C317A, C318A, C319A, C320A, C321A, C322A, C323A, C324A, C325A, C326A, C327A, C328A, C329A, C330A, C331A, C332A, C333A, C334A, C335A, C336A, C337A, C338A, C339A, C340A, C341A, C342A, C343A, C344A, C345A, C346A, C347A, C348A, C349A, C350A, C351A, C352A, C353A, C354A, C355A, C356A, C357A, C358A, C359A, C360A, C361A, C362A, C363A, C364A, C365A, C366A, C367A, C368A, C369A, C370A, C371A, C372A, C373A, C374A, C375A, C376A, C377A, C378A, C379A, C380A, C381A, C382A, C383A, C384A, C385A, C386A, C387A, C388A, C389A, C390A, C391A, C392A, C393A, C394A, C395A, C396A, C397A, C398A, C399A, C400A, C401A, C402A, C403A, C404A, C405A, C406A, C407A, C408A, C409A, C410A, C411A, C412A, C413A, C414A, C415A, C416A, C417A, C418A, C419A, C420A, C421A, C422A, C423A, C424A, C425A, C426A, C427A, C428A, C429A, C430A, C431A, C432A, C433A, C434A, C435A, C436A, C437A, C438A, C439A, C440A, C441A, C442A, C443A, C444A, C445A, C446A, C447A, C448A, C449A, C450A, C451A, C452A, C453A, C454A, C455A, C456A, C457A, C458A, C459A, C460A, C461A, C462A, C463A, C464A, C465A, C466A, C467A, C468A, C469A, C470A, C471A, C472A, C473A, C474A, C475A, C476A, C477A, C478A, C479A, C480A, C481A, C482A, C483A, C484A, C485A, C486A, C487A, C488A, C489A, C490A, C491A, C492A, C493A, C494A, C495A, C496A, C497A, C498A, C499A, C500A, C501A, C502A, C503A, C504A, C505A, C506A, C507A, C508A, C509A, C510A, C511A, C512A, C513A, C514A, C515A, C516A, C517A, C518A, C519A, C520A, C521A, C522A, C523A, C524A, C525A, C526A, C527A, C528A, C529A, C530A, C531A, C532A, C533A, C534A, C535A, C536A, C537A, C538A, C539A, C540A, C541A, C542A, C543A, C544A, C545A, C546A, C547A, C548A, C549A, C550A, C551A, C552A, C553A, C554A, C555A, C556A, C557A, C558A, C559A, C560A, C561A, C562A, C563A, C564A, C565A, C566A, C567A, C568A, C569A, C570A, C571A, C572A, C573A, C574A, C575A, C576A, C577A, C578A, C579A, C580A, C581A, C582A, C583A, C584A, C585A, C586A, C587A, C588A, C589A, C590A, C591A, C592A, C593A, C594A, C595A, C596A, C597A, C598A, C599A, C600A, C601A, C602A, C603A, C604A, C605A, C606A, C607A, C608A, C609A, C610A, C611A, C612A, C613A, C614A, C615A, C616A, C617A, C618A, C619A, C620A, C621A, C622A, C623A, C624A, C625A, C626A, C627A, C628A, C629A, C630A, C631A, C632A, C633A, C634A, C635A, C636A, C637A, C638A, C639A, C640A, C641A, C642A, C643A, C644A, C645A, C646A, C647A, C648A, C649A, C650A, C651A, C652A, C653A, C654A, C655A, C656A, C657A, C658A, C659A, C660A, C661A, C662A, C663A, C664A, C665A, C666A, C667A, C668A, C669A, C670A, C671A, C672A, C673A, C674A, C675A, C

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

Continued on next page...

Continued from previous page...

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

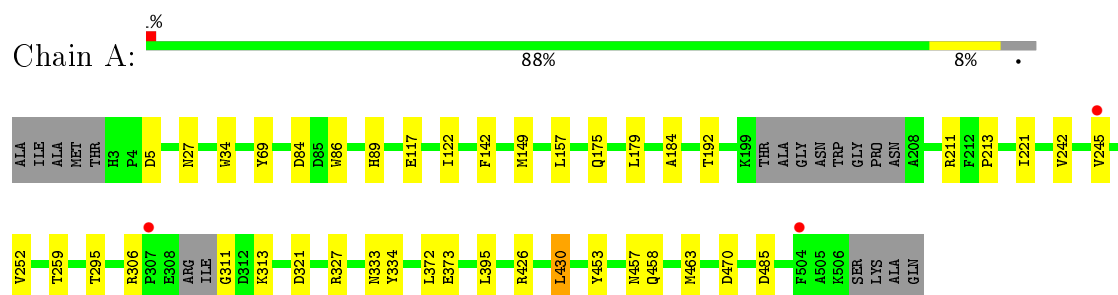
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	7	Total	O	0	0
			7	7		
5	C	5	Total	O	0	0
			5	5		
5	D	5	Total	O	0	0
			5	5		

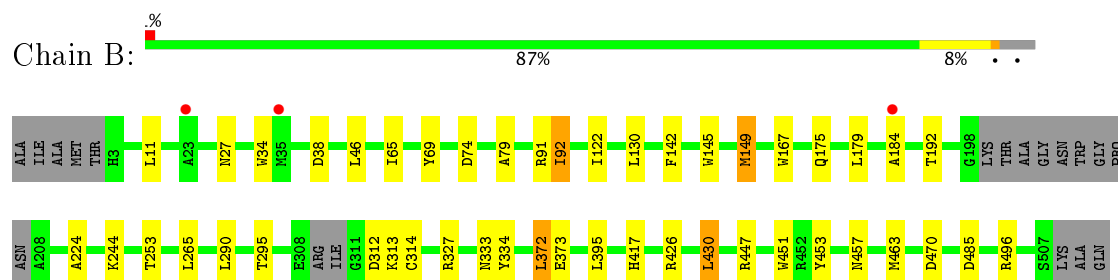
3 Residue-property plots [i](#)

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

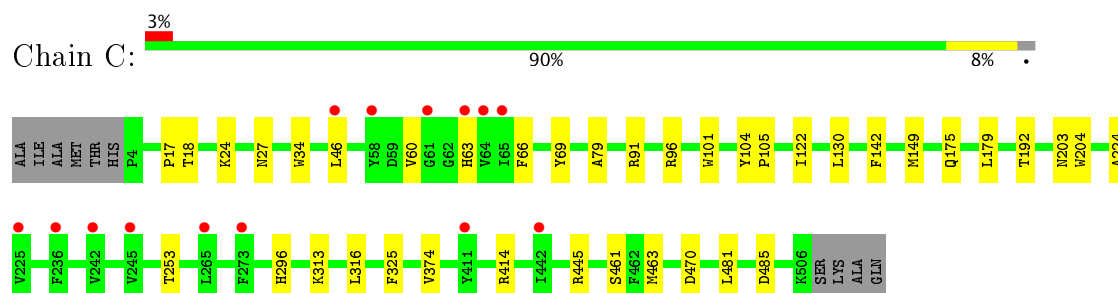
• Molecule 1: UDP-galactopyranose mutase



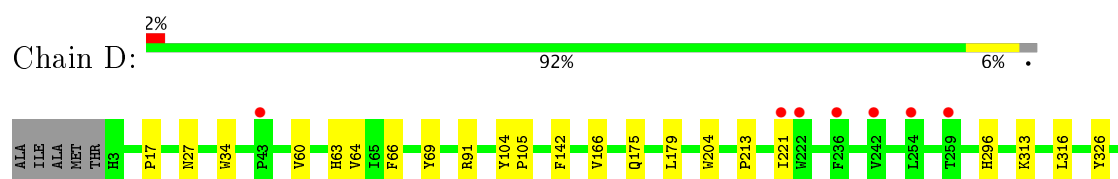
• Molecule 1: UDP-galactopyranose mutase

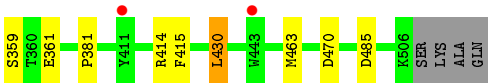


• Molecule 1: UDP-galactopyranose mutase



• Molecule 1: UDP-galactopyranose mutase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.25Å 218.25Å 318.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.59 – 2.75 162.48 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.59-2.75) 99.3 (162.48-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.73Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.194 , 0.227 0.190 , 0.224	Depositor DCC
R_{free} test set	5786 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15591	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: NAI, 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	0.46	0/3870	0.62	0/5277
1	B	0.45	0/3870	0.62	0/5279
1	C	0.42	0/3924	0.59	0/5356
1	D	0.43	0/3925	0.58	0/5356
All	All	0.44	0/15589	0.60	0/21268

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3777	0	3592	26	0
1	B	3777	0	3583	31	0
1	C	3826	0	3615	23	0
1	D	3827	0	3613	17	0
2	A	53	0	31	5	0
2	B	53	0	31	7	0
2	C	53	0	31	6	0
2	D	53	0	31	3	0
3	A	44	0	26	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	1	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	20	0	0	0	0
4	D	20	0	0	0	0
5	A	2	0	0	0	0
5	B	7	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
All	All	15591	0	14579	104	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 3.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:NE	1:B:373:GLU:OE2	2.25	0.67
1:A:372:LEU:HD21	1:A:395:LEU:HD21	1.78	0.66
1:B:122:ILE:HD12	1:B:192:THR:HG22	1.81	0.63
1:B:149:MET:SD	1:B:184:ALA:HA	2.39	0.62
1:C:46:LEU:O	1:C:60:VAL:HG21	1.99	0.61
1:D:69:TYR:CD1	1:D:463:MET:HG3	2.37	0.60
1:B:244:LYS:HB3	1:B:253:THR:HB	1.84	0.59
1:D:313:LYS:HD3	1:D:316:LEU:HD21	1.85	0.58
1:C:325:PHE:HA	1:C:374:VAL:HG22	1.86	0.57
1:A:327:ARG:NE	1:A:373:GLU:OE2	2.25	0.57
1:C:313:LYS:HD3	1:C:316:LEU:HD21	1.86	0.56
1:B:372:LEU:HD11	1:B:395:LEU:HD21	1.89	0.55
1:B:313:LYS:HG3	1:B:333:ASN:HB3	1.89	0.55
1:B:46:LEU:HD13	2:B:601:FAD:HM81	1.87	0.55
2:B:601:FAD:H2'	2:B:601:FAD:N1	2.23	0.54
1:A:69:TYR:CD1	1:A:463:MET:HG3	2.43	0.54
1:B:453:TYR:CE1	3:B:602:NAI:H42N	2.43	0.54
1:C:296:HIS:CE1	1:C:414:ARG:HD2	2.44	0.53
1:A:457:ASN:HB2	2:A:601:FAD:O2	2.08	0.52
1:D:359:SER:OG	1:D:361:GLU:HG2	2.09	0.52
1:B:92:ILE:HG22	1:B:314:CYS:HB3	1.92	0.52
1:A:149:MET:SD	1:A:184:ALA:HA	2.50	0.51
1:D:166:VAL:HG22	1:D:326:TYR:CD1	2.46	0.51
1:B:290:LEU:HD21	1:B:430:LEU:HD13	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:O	1:C:204:TRP:HB3	2.11	0.51
1:C:17:PRO:HG2	2:C:601:FAD:O3'	2.10	0.51
1:B:142:PHE:CE1	1:B:179:LEU:HD11	2.46	0.50
1:D:91:ARG:O	1:D:204:TRP:HB3	2.10	0.50
1:B:69:TYR:CD1	1:B:463:MET:HG3	2.46	0.50
1:B:74:ASP:OD2	1:B:496:ARG:NE	2.40	0.50
1:B:69:TYR:CG	1:B:463:MET:HG3	2.47	0.50
1:C:66:PHE:HB2	1:C:91:ARG:NH1	2.26	0.50
1:B:290:LEU:HD13	1:B:451:TRP:CD2	2.46	0.50
1:A:313:LYS:HG3	1:A:333:ASN:HB3	1.94	0.50
1:C:69:TYR:CD1	1:C:463:MET:HG3	2.47	0.49
1:B:130:LEU:HD23	1:C:130:LEU:HD23	1.94	0.49
1:B:426:ARG:HG2	1:B:430:LEU:HD22	1.96	0.48
1:A:89:HIS:ND1	1:A:313:LYS:HG2	2.29	0.48
1:D:296:HIS:CE1	1:D:414:ARG:HD2	2.50	0.47
2:A:601:FAD:O2'	2:A:601:FAD:O4'	2.29	0.46
1:C:105:PRO:HD3	1:C:203:ASN:HB3	1.96	0.46
1:B:92:ILE:HG21	1:B:312:ASP:OD1	2.16	0.46
1:D:213:PRO:HG3	1:D:221:ILE:HG13	1.96	0.46
1:A:334:TYR:N	1:A:334:TYR:CD1	2.84	0.46
2:A:601:FAD:H9	2:A:601:FAD:H1'1	1.66	0.46
1:A:245:VAL:HG22	1:A:252:VAL:HG22	1.96	0.46
1:A:306:ARG:HD2	1:A:311:GLY:HA2	1.97	0.45
1:A:86:TRP:CD2	1:A:211:ARG:HD2	2.50	0.45
1:B:167:TRP:HH2	1:B:453:TYR:CD1	2.34	0.45
1:A:242:VAL:HG13	1:A:252:VAL:HG13	1.98	0.45
1:D:60:VAL:HG13	1:D:415:PHE:CE2	2.50	0.45
2:B:601:FAD:H9	2:B:601:FAD:H1'1	1.63	0.45
1:A:117:GLU:OE2	1:A:157:LEU:HD21	2.16	0.45
1:A:69:TYR:CG	1:A:463:MET:HG3	2.51	0.45
1:B:11:LEU:O	1:B:265:LEU:HD12	2.17	0.45
1:C:142:PHE:CE1	1:C:179:LEU:HD11	2.52	0.45
1:C:69:TYR:CG	1:C:463:MET:HG3	2.52	0.45
1:D:430:LEU:HD12	1:D:430:LEU:HA	1.84	0.44
1:B:145:TRP:CD2	1:B:179:LEU:HD13	2.53	0.44
1:A:122:ILE:HD12	1:A:192:THR:HG22	1.99	0.44
1:A:321:ASP:OD1	1:A:321:ASP:N	2.46	0.44
1:B:295:THR:HG21	2:B:601:FAD:C7M	2.47	0.44
1:D:69:TYR:CG	1:D:463:MET:HG3	2.52	0.44
1:A:458:GLN:HA	2:A:601:FAD:O3'	2.17	0.44
1:B:65:ILE:HB	1:B:91:ARG:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:HIS:HB3	2:C:601:FAD:N3	2.32	0.44
1:A:27:ASN:HB2	1:A:34:TRP:CZ2	2.52	0.43
1:B:457:ASN:HB2	2:B:601:FAD:O2	2.18	0.43
1:C:17:PRO:HD2	2:C:601:FAD:H4'	2.00	0.43
1:B:27:ASN:HB2	1:B:34:TRP:CZ2	2.53	0.43
1:C:122:ILE:HD12	1:C:192:THR:HG22	1.99	0.43
1:C:104:TYR:CG	1:C:105:PRO:HA	2.54	0.43
1:B:313:LYS:HD2	1:B:313:LYS:N	2.33	0.43
1:D:66:PHE:HB2	1:D:91:ARG:NH2	2.34	0.43
1:D:63:HIS:HB3	2:D:601:FAD:C4	2.50	0.42
1:D:142:PHE:CE1	1:D:179:LEU:HD11	2.53	0.42
1:C:79:ALA:HB1	1:C:224:ALA:CB	2.49	0.42
1:A:334:TYR:N	1:A:334:TYR:HD1	2.17	0.42
1:A:453:TYR:CE1	3:A:602:NAI:H42N	2.55	0.42
1:C:27:ASN:HB2	1:C:34:TRP:CZ2	2.54	0.42
1:D:69:TYR:CE1	1:D:463:MET:HG3	2.55	0.42
1:A:295:THR:HG21	2:A:601:FAD:C7M	2.50	0.42
1:B:334:TYR:CD1	1:B:334:TYR:N	2.88	0.42
1:A:5:ASP:HB2	1:A:259:THR:O	2.20	0.42
1:B:38:ASP:OD2	2:B:601:FAD:O3B	2.37	0.42
1:D:17:PRO:HD2	2:D:601:FAD:H4'	2.02	0.42
1:A:213:PRO:HG3	1:A:221:ILE:HG13	2.02	0.41
2:C:601:FAD:H1'1	2:C:601:FAD:H9	1.75	0.41
1:A:142:PHE:CE1	1:A:179:LEU:HD11	2.55	0.41
1:B:142:PHE:CD1	1:B:179:LEU:HD11	2.54	0.41
1:C:445:ARG:NE	1:C:481:LEU:HD22	2.35	0.41
1:C:96:ARG:HB2	1:C:101:TRP:CZ3	2.56	0.41
1:A:426:ARG:HG2	1:A:430:LEU:HD22	2.02	0.41
2:C:601:FAD:O4'	2:C:601:FAD:O2'	2.31	0.41
1:D:104:TYR:CG	1:D:105:PRO:HA	2.55	0.41
1:C:18:THR:OG1	1:C:461:SER:HB3	2.20	0.41
1:C:24:LYS:HA	1:C:24:LYS:HD2	1.93	0.41
1:B:79:ALA:HB1	1:B:224:ALA:CB	2.51	0.41
1:C:142:PHE:CD1	1:C:179:LEU:HD11	2.57	0.40
1:A:372:LEU:HD11	1:A:395:LEU:HD11	2.04	0.40
1:D:27:ASN:HB2	1:D:34:TRP:HZ2	1.87	0.40
2:D:601:FAD:H1'1	2:D:601:FAD:H9	1.75	0.40
1:B:447:ARG:HB2	2:B:601:FAD:H5'2	2.04	0.40
2:C:601:FAD:N1	2:C:601:FAD:H2'	2.37	0.40

There are no symmetry-related clashes.

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	488/513 (95%)	477 (98%)	11 (2%)	0	100	100
1	B	488/513 (95%)	476 (98%)	12 (2%)	0	100	100
1	C	501/513 (98%)	490 (98%)	11 (2%)	0	100	100
1	D	502/513 (98%)	489 (97%)	12 (2%)	1 (0%)	51	81
All	All	1979/2052 (96%)	1932 (98%)	46 (2%)	1 (0%)	55	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/432 (90%)	382 (99%)	5 (1%)	73	91
1	B	389/432 (90%)	381 (98%)	8 (2%)	59	85
1	C	386/432 (89%)	381 (99%)	5 (1%)	73	91
1	D	385/432 (89%)	380 (99%)	5 (1%)	73	91
All	All	1547/1728 (90%)	1524 (98%)	23 (2%)	70	90

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	A	175	GLN
1	A	430	LEU
1	A	470	ASP
1	A	485	ASP
1	B	92	ILE
1	B	149	MET
1	B	175	GLN
1	B	372	LEU
1	B	417	HIS
1	B	430	LEU
1	B	470	ASP
1	B	485	ASP
1	C	149	MET
1	C	175	GLN
1	C	253	THR
1	C	470	ASP
1	C	485	ASP
1	D	175	GLN
1	D	381	PRO
1	D	430	LEU
1	D	470	ASP
1	D	485	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

19 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	601	-	51,58,58	1.02	5 (9%)	54,89,89	2.36	8 (14%)
3	NAI	A	602	-	40,48,48	1.60	4 (10%)	41,73,73	1.30	4 (9%)
4	SO4	A	603	-	4,4,4	0.24	0	6,6,6	0.18	0
4	SO4	A	604	-	4,4,4	0.26	0	6,6,6	0.27	0
2	FAD	B	601	-	51,58,58	1.03	4 (7%)	54,89,89	2.40	7 (12%)
3	NAI	B	602	-	40,48,48	1.64	8 (20%)	41,73,73	1.20	3 (7%)
4	SO4	B	603	-	4,4,4	0.16	0	6,6,6	0.32	0
4	SO4	B	604	-	4,4,4	0.15	0	6,6,6	0.19	0
4	SO4	B	605	-	4,4,4	0.15	0	6,6,6	0.26	0
2	FAD	C	601	-	51,58,58	1.01	4 (7%)	54,89,89	2.35	6 (11%)
4	SO4	C	602	-	4,4,4	0.16	0	6,6,6	0.27	0
4	SO4	C	603	-	4,4,4	0.21	0	6,6,6	0.44	0
4	SO4	C	604	-	4,4,4	0.18	0	6,6,6	0.41	0
4	SO4	C	605	-	4,4,4	0.10	0	6,6,6	0.22	0
2	FAD	D	601	-	51,58,58	1.01	4 (7%)	54,89,89	2.38	8 (14%)
4	SO4	D	602	-	4,4,4	0.21	0	6,6,6	0.30	0
4	SO4	D	603	-	4,4,4	0.18	0	6,6,6	0.24	0
4	SO4	D	604	-	4,4,4	0.21	0	6,6,6	0.37	0
4	SO4	D	605	-	4,4,4	0.14	0	6,6,6	0.30	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
2	FAD	A	601	-	-	0/28/50/50	0/6/6/6
3	NAI	A	602	-	-	0/25/72/72	0/5/5/5
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
4	SO4	A	604	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	601	-	-	0/28/50/50	0/6/6/6
3	NAI	B	602	-	-	0/25/72/72	0/5/5/5
4	SO4	B	603	-	-	0/0/0/0	0/0/0/0
4	SO4	B	604	-	-	0/0/0/0	0/0/0/0
4	SO4	B	605	-	-	0/0/0/0	0/0/0/0
2	FAD	C	601	-	-	0/28/50/50	0/6/6/6
4	SO4	C	602	-	-	0/0/0/0	0/0/0/0
4	SO4	C	603	-	-	0/0/0/0	0/0/0/0
4	SO4	C	604	-	-	0/0/0/0	0/0/0/0
4	SO4	C	605	-	-	0/0/0/0	0/0/0/0
2	FAD	D	601	-	-	0/28/50/50	0/6/6/6
4	SO4	D	602	-	-	0/0/0/0	0/0/0/0
4	SO4	D	603	-	-	0/0/0/0	0/0/0/0
4	SO4	D	604	-	-	0/0/0/0	0/0/0/0
4	SO4	D	605	-	-	0/0/0/0	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAI	O2B-C2B	-3.98	1.33	1.43
3	B	602	NAI	O2B-C2B	-3.93	1.33	1.43
2	A	601	FAD	C1'-N10	-2.83	1.45	1.48
2	D	601	FAD	C1'-N10	-2.78	1.45	1.48
2	C	601	FAD	C4X-N5	-2.50	1.29	1.33
2	C	601	FAD	C1'-N10	-2.49	1.45	1.48
2	D	601	FAD	C4X-N5	-2.39	1.29	1.33
3	B	602	NAI	O2D-C2D	-2.11	1.38	1.43
2	A	601	FAD	C4X-C10	2.03	1.44	1.41
3	A	602	NAI	PA-O5B	2.12	1.68	1.59
2	C	601	FAD	C5X-N5	2.12	1.38	1.35
2	D	601	FAD	C5X-N5	2.22	1.38	1.35
3	B	602	NAI	C2A-N1A	2.28	1.38	1.33
3	B	602	NAI	C7N-N7N	2.29	1.39	1.33
3	A	602	NAI	C4A-N3A	2.32	1.39	1.35
2	B	601	FAD	C4X-C10	2.33	1.45	1.41
3	B	602	NAI	C3D-C4D	2.37	1.59	1.53
3	B	602	NAI	C2B-C1B	2.46	1.57	1.53
2	B	601	FAD	C4-C4X	2.49	1.46	1.41
2	A	601	FAD	C4-N3	2.67	1.37	1.33
2	A	601	FAD	C4-C4X	2.85	1.46	1.41
3	B	602	NAI	C4A-N3A	3.04	1.40	1.35
2	A	601	FAD	C5X-N5	3.10	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	C4-N3	3.26	1.39	1.33
2	B	601	FAD	C4-N3	3.29	1.39	1.33
2	C	601	FAD	C4-N3	3.33	1.39	1.33
2	B	601	FAD	C5X-N5	3.37	1.40	1.35
3	B	602	NAI	PN-O5D	4.68	1.79	1.59
3	A	602	NAI	PN-O5D	5.78	1.83	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4X-C4-N3	-6.94	113.61	123.48
2	B	601	FAD	C4X-C4-N3	-6.87	113.69	123.48
2	C	601	FAD	C4X-C10-N10	-6.50	116.01	120.52
2	D	601	FAD	C4X-C4-N3	-6.46	114.28	123.48
2	C	601	FAD	C4X-C4-N3	-6.17	114.70	123.48
2	B	601	FAD	C4X-C10-N10	-6.08	116.30	120.52
2	D	601	FAD	C4X-C10-N10	-5.94	116.40	120.52
2	A	601	FAD	C4X-C10-N10	-5.81	116.48	120.52
3	A	602	NAI	C4B-O4B-C1B	-3.71	105.82	109.77
2	D	601	FAD	O5'-P-O1P	-3.42	95.45	109.25
2	C	601	FAD	C4-C4X-C10	-3.23	117.35	119.96
2	D	601	FAD	C4-C4X-C10	-3.23	117.35	119.96
3	B	602	NAI	C4B-O4B-C1B	-2.91	106.67	109.77
2	A	601	FAD	C4-C4X-C10	-2.85	117.66	119.96
2	B	601	FAD	C4-C4X-C10	-2.74	117.75	119.96
2	A	601	FAD	C4B-O4B-C1B	-2.31	107.31	109.77
3	A	602	NAI	C2A-N1A-C6A	-2.17	114.97	118.77
3	A	602	NAI	C5B-C4B-C3B	-2.04	107.49	115.29
3	B	602	NAI	O5D-PN-O2N	-2.02	101.09	109.25
2	A	601	FAD	O5B-PA-O1A	2.01	117.35	109.25
3	B	602	NAI	C4A-C5A-N7A	2.09	111.43	109.41
3	A	602	NAI	C4A-C5A-N7A	2.17	111.50	109.41
2	D	601	FAD	O2P-P-O1P	2.28	124.11	112.28
2	A	601	FAD	O3'-C3'-C2'	2.43	114.84	108.82
2	C	601	FAD	O2P-P-O1P	2.43	124.86	112.28
2	D	601	FAD	O2A-PA-O1A	2.78	126.67	112.28
2	A	601	FAD	C10-C4X-N5	3.00	124.04	120.59
2	B	601	FAD	C1'-N10-C10	3.04	121.62	118.50
2	B	601	FAD	C10-C4X-N5	3.36	124.46	120.59
2	B	601	FAD	O3'-C3'-C2'	3.58	117.68	108.82
2	D	601	FAD	C10-C4X-N5	3.63	124.76	120.59
2	C	601	FAD	C10-C4X-N5	3.87	125.05	120.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	C4-N3-C2	12.61	126.19	115.16
2	A	601	FAD	C4-N3-C2	12.62	126.20	115.16
2	C	601	FAD	C4-N3-C2	12.70	126.27	115.16
2	B	601	FAD	C4-N3-C2	12.74	126.30	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	5	0
3	A	602	NAI	1	0
2	B	601	FAD	7	0
3	B	602	NAI	1	0
2	C	601	FAD	6	0
2	D	601	FAD	3	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 ⓘ

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	494/513 (96%)	0.28	3 (0%) 89 87	31, 49, 78, 108	0
1	B	494/513 (96%)	0.26	3 (0%) 89 87	33, 50, 81, 118	0
1	C	503/513 (98%)	0.42	14 (2%) 53 48	31, 56, 86, 106	0
1	D	504/513 (98%)	0.39	9 (1%) 69 65	30, 58, 90, 111	0
All	All	1995/2052 (97%)	0.34	29 (1%) 74 71	30, 53, 85, 118	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	HIS	4.5
1	B	184	ALA	3.6
1	C	273	PHE	3.6
1	C	265	LEU	2.8
1	C	64	VAL	2.8
1	D	236	PHE	2.8
1	C	236	PHE	2.8
1	C	65	ILE	2.6
1	D	259	THR	2.6
1	C	242	VAL	2.5
1	A	245	VAL	2.5
1	B	23	ALA	2.4
1	C	46	LEU	2.4
1	C	411	TYR	2.3
1	D	43	PRO	2.3
1	D	411	TYR	2.3
1	D	221	ILE	2.3
1	C	61	GLY	2.3
1	C	245	VAL	2.2
1	A	504	PHE	2.2
1	D	443	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	35	MET	2.2
1	D	242	VAL	2.2
1	C	442	ILE	2.1
1	A	307	PRO	2.1
1	D	222	TRP	2.1
1	D	254	LEU	2.1
1	C	58	TYR	2.1
1	C	225	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	605	5/5	0.95	0.23	0.59	81,82,84,87	0
2	FAD	B	601	53/53	0.98	0.20	0.13	24,46,54,55	0
3	NAI	B	602	44/44	0.97	0.20	0.09	41,57,65,66	0
4	SO4	C	605	5/5	0.98	0.28	0.05	56,58,66,71	5
4	SO4	D	605	5/5	0.99	0.25	-0.05	55,55,55,70	5
2	FAD	A	601	53/53	0.97	0.21	-0.09	38,48,59,76	0
2	FAD	D	601	53/53	0.95	0.22	-0.21	37,60,73,84	0
3	NAI	A	602	44/44	0.95	0.20	-0.60	40,63,69,76	0
2	FAD	C	601	53/53	0.95	0.21	-0.68	40,60,72,86	0
4	SO4	B	603	5/5	0.91	0.13	-	85,86,92,97	5
4	SO4	D	602	5/5	0.89	0.20	-	84,84,89,89	5
4	SO4	A	604	5/5	0.90	0.20	-	86,91,93,97	0
4	SO4	C	603	5/5	0.93	0.22	-	73,77,80,83	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	C	602	5/5	0.93	0.18	-	70,71,76,83	5
4	SO4	A	603	5/5	0.96	0.17	-	59,64,73,78	5
4	SO4	D	603	5/5	0.95	0.28	-	67,77,79,85	5
4	SO4	C	604	5/5	0.86	0.27	-	83,88,91,99	5
4	SO4	B	604	5/5	0.95	0.20	-	66,72,78,78	5
4	SO4	D	604	5/5	0.91	0.19	-	67,68,77,79	5

6.5 Other polymers [i](#)

There are no such residues in this entry.