



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:38 PM GMT

PDB ID : 4GDD
Title : Crystal structure of oxidized *Aspergillus fumigatus* UDP-galactopyranose mutase complexed with NADH
Authors : Tanner, J.J.; Dhatwalia, R.D.; Singh, H.
Deposited on : 2012-07-31
Resolution : 2.75 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

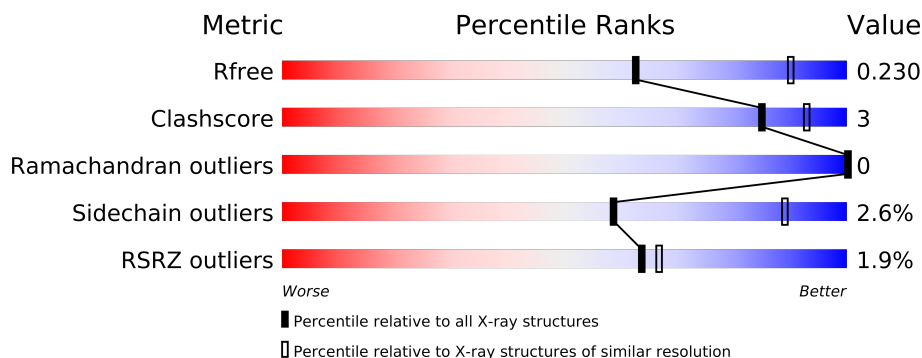
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	513	
1	B	513	
1	C	513	
1	D	513	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	D	603	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15540 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			3776	2409	634	712	21			
1	B	494	Total	C	N	O	S	0	0	0
			3777	2406	633	718	20			
1	C	499	Total	C	N	O	S	0	0	0
			3798	2422	641	716	19			
1	D	502	Total	C	N	O	S	0	0	0
			3813	2434	640	719	20			

There are 24 discrepancies between the modelled and reference sequences:

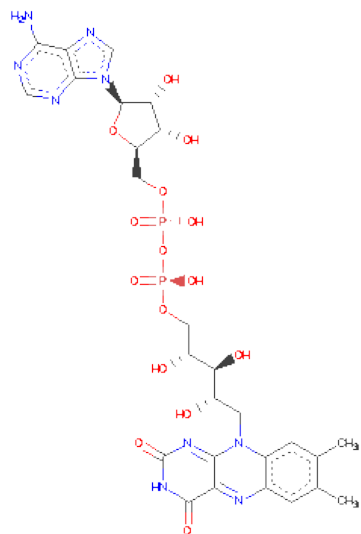
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	EXPRESSION TAG	UNP Q4W1X2
A	-1	ILE	-	EXPRESSION TAG	UNP Q4W1X2
A	0	ALA	-	EXPRESSION TAG	UNP Q4W1X2
A	344	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
A	345	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
A	429	THR	ALA	SEE REMARK 999	UNP Q4W1X2
B	-2	ALA	-	EXPRESSION 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	SEE REMARK 999	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	SEE REMARK 999	UNP Q4W1X2
D	-2	ALA	-	EXPRESSION TAG	UNP Q4W1X2
D	-1	ILE	-	EXPRESSION TAG	UNP Q4W1X2
D	0	ALA	-	EXPRESSION TAG	UNP Q4W1X2

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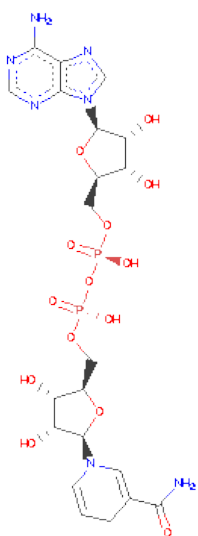
Chain	Residue	Modelled	Actual	Comment	Reference
D	344	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
D	345	ALA	LYS	ENGINEERED MUTATION	UNP Q4W1X2
D	429	THR	ALA	SEE REMARK 999	UNP Q4W1X2

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



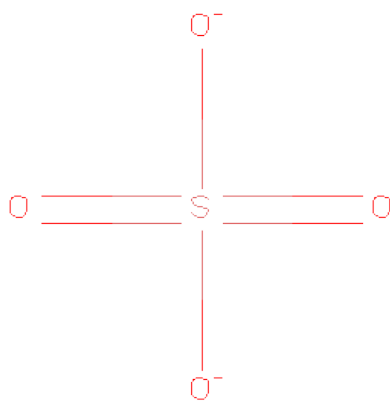
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDEADENINE 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	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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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	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.

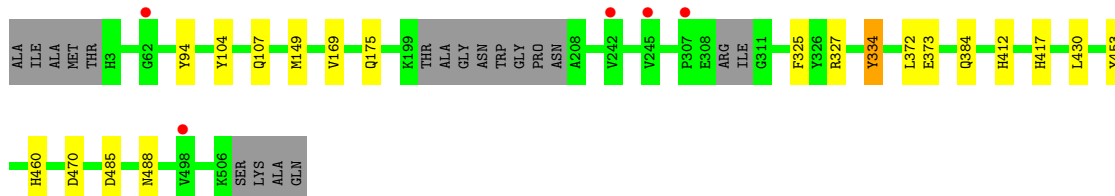
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	7	Total	O	0	0
			7	7		
5	C	7	Total	O	0	0
			7	7		
5	D	8	Total	O	0	0
			8	8		

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.

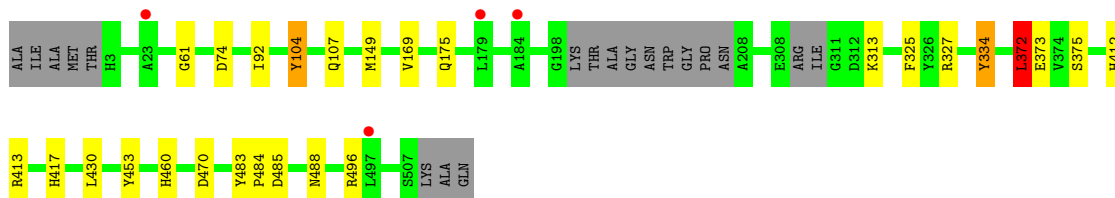
- Molecule 1: UDP-galactopyranose mutase

Chain A: 



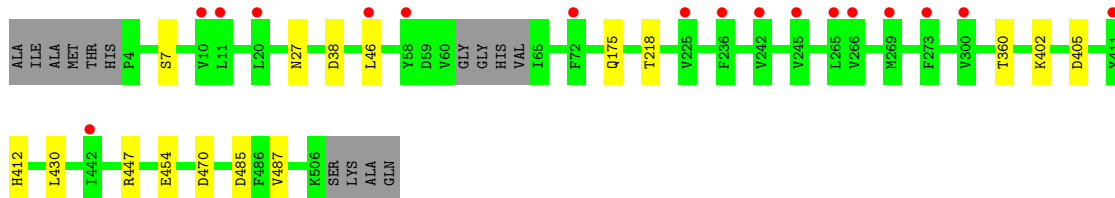
- Molecule 1: UDP-galactopyranose mutase

Chain B: 



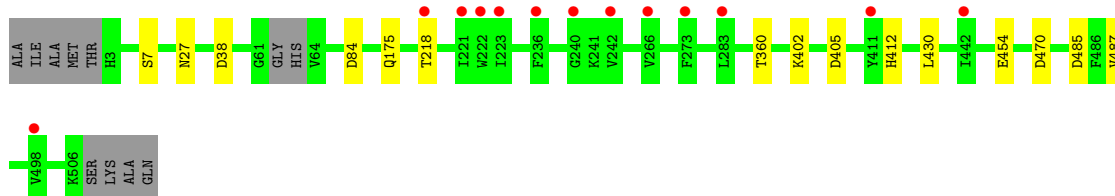
- Molecule 1: UDP-galactopyranose mutase

Chain C: 



- Molecule 1: UDP-galactopyranose mutase

Chain D: 



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)	162.48 – 2.75 162.48 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (162.48-2.75) 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 (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.212 , 0.245 0.198 , 0.230	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 , 27.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 115117 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15540	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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.

5 Model quality

5.1 Standard geometry

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	0.45	0/3869	0.60	0/5276
1	B	0.45	0/3870	0.61	1/5279 (0.0%)
1	C	0.41	0/3894	0.56	0/5314
1	D	0.42	0/3909	0.57	0/5333
All	All	0.43	0/15542	0.59	1/21202 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	372	LEU	CA-CB-CG	6.95	131.28	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3776	0	0	10	0
1	B	3777	0	0	17	0
1	C	3798	0	0	7	0
1	D	3813	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	30	1	0
2	B	53	0	30	3	0
2	C	53	0	31	5	0
2	D	53	0	31	2	0
3	A	44	0	27	2	0
3	B	44	0	27	2	0
4	A	10	0	0	0	0
4	B	15	0	0	2	0
4	C	10	0	0	1	0
4	D	15	0	0	0	0
5	A	4	0	0	0	0
5	B	7	0	0	1	0
5	C	7	0	0	0	0
5	D	8	0	0	0	0
All	All	15540	0	176	44	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:453:TYR:CE1	3:B:602:NAI:H42N	2.04	0.92
1:D:38:ASP:OD1	2:D:601:FAD:H1B	1.83	0.78
1:A:453:TYR:CE1	3:A:602:NAI:H42N	2.22	0.73
1:C:38:ASP:OD1	2:C:601:FAD:H1B	1.92	0.70
1:B:327:ARG:NE	1:B:373:GLU:OE2	2.25	0.69
1:B:453:TYR:CZ	3:B:602:NAI:H42N	2.31	0.65
1:A:327:ARG:NE	1:A:373:GLU:OE2	2.31	0.63
1:A:325:PHE:CD1	1:A:372:LEU:CD2	2.91	0.54
1:C:447:ARG:NH1	4:C:603:SO4:O2	2.41	0.54
1:A:412:HIS:C	1:A:412:HIS:CD2	2.81	0.54
1:B:334:TYR:CD1	1:B:334:TYR:N	2.76	0.54
1:C:46:LEU:N	2:C:601:FAD:O1A	2.41	0.53
1:A:107:GLN:OE1	1:A:107:GLN:N	2.42	0.53
1:A:334:TYR:N	1:A:334:TYR:CD1	2.77	0.52
1:B:74:ASP:OD2	1:B:496:ARG:NE	2.44	0.51
1:B:412:HIS:CD2	1:B:412:HIS:C	2.82	0.50
1:B:107:GLN:N	1:B:107:GLN:OE1	2.46	0.49
1:B:325:PHE:CD1	1:B:372:LEU:CD1	2.98	0.47
2:B:601:FAD:O4'	2:B:601:FAD:O2'	2.30	0.47
2:D:601:FAD:H9	2:D:601:FAD:H1'1	1.50	0.47
2:A:601:FAD:H1'1	2:A:601:FAD:H9	1.43	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:601:FAD:H2'	2:C:601:FAD:N1	2.31	0.45
1:B:327:ARG:NH1	4:B:605:SO4:S	2.90	0.45
1:B:104:TYR:C	1:B:104:TYR:CD2	2.90	0.45
2:C:601:FAD:H1'1	2:C:601:FAD:H9	1.52	0.45
1:B:61:GLY:O	2:B:601:FAD:C10	2.66	0.44
1:D:412:HIS:CD2	1:D:412:HIS:C	2.90	0.43
1:D:402:LYS:N	1:D:405:ASP:OD2	2.51	0.43
1:C:412:HIS:C	1:C:412:HIS:CD2	2.89	0.43
1:D:454:GLU:OE1	1:D:454:GLU:N	2.51	0.43
1:B:460:HIS:NE2	1:B:488:ASN:OD1	2.52	0.43
1:A:94:TYR:CD1	1:A:94:TYR:N	2.87	0.42
1:B:327:ARG:NH1	4:B:605:SO4:O1	2.52	0.42
1:A:325:PHE:CE1	1:A:372:LEU:CD2	3.03	0.42
1:A:453:TYR:CZ	3:A:602:NAI:H42N	2.54	0.41
1:B:375:SER:N	5:B:707:HOH:O	2.53	0.41
2:B:601:FAD:H1'1	2:B:601:FAD:H9	1.49	0.41
1:C:454:GLU:N	1:C:454:GLU:OE1	2.54	0.41
1:A:460:HIS:NE2	1:A:488:ASN:OD1	2.54	0.41
1:C:402:LYS:N	1:C:405:ASP:OD2	2.54	0.41
1:B:412:HIS:CD2	1:B:413:ARG:N	2.89	0.40
1:B:483:TYR:N	1:B:484:PRO:CD	2.84	0.40
1:C:447:ARG:CB	2:C:601:FAD:H5'1	2.51	0.40
1:B:313:LYS:CD	1:B:313:LYS:N	2.85	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%)	469 (96%)	19 (4%)	0	100	100
1	B	488/513 (95%)	468 (96%)	20 (4%)	0	100	100
1	C	495/513 (96%)	478 (97%)	17 (3%)	0	100	100
1	D	498/513 (97%)	482 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1969/2052 (96%)	1897 (96%)	72 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	386/432 (89%)	376 (97%)	10 (3%)	59	89
1	B	389/432 (90%)	378 (97%)	11 (3%)	56	87
1	C	383/432 (89%)	374 (98%)	9 (2%)	63	91
1	D	384/432 (89%)	374 (97%)	10 (3%)	59	89
All	All	1542/1728 (89%)	1502 (97%)	40 (3%)	59	89

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	TYR
1	A	149	MET
1	A	169	VAL
1	A	175	GLN
1	A	334	TYR
1	A	384	GLN
1	A	417	HIS
1	A	430	LEU
1	A	470	ASP
1	A	485	ASP
1	B	92	ILE
1	B	104	TYR
1	B	149	MET
1	B	169	VAL
1	B	175	GLN
1	B	334	TYR
1	B	372	LEU
1	B	417	HIS

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Mol	Chain	Res	Type
1	B	430	LEU
1	B	470	ASP
1	B	485	ASP
1	C	7	SER
1	C	27	ASN
1	C	175	GLN
1	C	218	THR
1	C	360	THR
1	C	430	LEU
1	C	470	ASP
1	C	485	ASP
1	C	487	VAL
1	D	7	SER
1	D	27	ASN
1	D	84	ASP
1	D	175	GLN
1	D	218	THR
1	D	360	THR
1	D	430	LEU
1	D	470	ASP
1	D	485	ASP
1	D	487	VAL

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 chains 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 ⓘ

16 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	-	58,58,58	2.41	21 (36%)	85,89,89	2.54	28 (32%)
3	NAI	A	602	-	48,48,48	2.01	16 (33%)	73,73,73	2.13	12 (16%)
4	SO4	A	603	-	4,4,4	0.09	0	6,6,6	0.12	0
4	SO4	A	604	-	4,4,4	0.23	0	6,6,6	0.24	0
2	FAD	B	601	-	58,58,58	2.44	20 (34%)	85,89,89	2.24	24 (28%)
3	NAI	B	602	-	48,48,48	2.01	16 (33%)	73,73,73	1.95	12 (16%)
4	SO4	B	603	-	4,4,4	0.14	0	6,6,6	0.28	0
4	SO4	B	604	-	4,4,4	0.15	0	6,6,6	0.26	0
4	SO4	B	605	-	4,4,4	0.28	0	6,6,6	0.16	0
2	FAD	C	601	-	58,58,58	2.27	17 (29%)	85,89,89	2.13	19 (22%)
4	SO4	C	602	-	4,4,4	0.11	0	6,6,6	0.23	0
4	SO4	C	603	-	4,4,4	0.24	0	6,6,6	0.17	0
2	FAD	D	601	-	58,58,58	2.42	18 (31%)	85,89,89	2.21	25 (29%)
4	SO4	D	602	-	4,4,4	0.29	0	6,6,6	0.32	0
4	SO4	D	603	-	4,4,4	0.13	0	6,6,6	0.22	0
4	SO4	D	604	-	4,4,4	0.22	0	6,6,6	0.08	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	-	-	0/34/50/50	0/1/6/6
3	NAI	A	602	-	-	0/30/72/72	0/3/5/5
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
4	SO4	A	604	-	-	0/0/0/0	0/0/0/0
2	FAD	B	601	-	-	0/34/50/50	0/1/6/6
3	NAI	B	602	-	-	0/30/72/72	0/3/5/5
4	SO4	B	603	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/34/50/50	0/1/6/6
4	SO4	C	602	-	-	0/0/0/0	0/0/0/0
4	SO4	C	603	-	-	0/0/0/0	0/0/0/0
2	FAD	D	601	-	-	0/34/50/50	0/1/6/6
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

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	O4-C4	7.40	1.39	1.24
2	A	601	FAD	O4-C4	7.37	1.39	1.24
2	D	601	FAD	PA-O3P	-7.35	1.46	1.59
2	A	601	FAD	PA-O3P	-7.28	1.46	1.59
2	D	601	FAD	O4-C4	7.18	1.38	1.24
2	B	601	FAD	O2-C2	7.09	1.38	1.23
2	B	601	FAD	PA-O3P	-6.86	1.47	1.59
2	C	601	FAD	O4-C4	6.83	1.37	1.24
2	D	601	FAD	O2-C2	6.67	1.37	1.23
2	A	601	FAD	O2-C2	6.63	1.37	1.23
2	C	601	FAD	O2-C2	6.51	1.37	1.23
2	D	601	FAD	C4-C4X	5.99	1.51	1.41
3	A	602	NAI	PA-O3	-5.93	1.49	1.59
2	C	601	FAD	PA-O3P	-5.78	1.49	1.59
2	A	601	FAD	C4-C4X	5.69	1.50	1.41
3	B	602	NAI	PA-O3	-5.60	1.49	1.59
2	B	601	FAD	C4-C4X	5.52	1.50	1.41
2	C	601	FAD	C4-C4X	4.74	1.49	1.41
2	B	601	FAD	C2B-C1B	-4.11	1.47	1.53
3	A	602	NAI	C4N-C3N	-4.08	1.42	1.50
2	C	601	FAD	C4A-N9A	4.08	1.43	1.37
3	B	602	NAI	C4N-C3N	-4.04	1.42	1.50
3	B	602	NAI	C6N-C5N	3.49	1.40	1.33
3	A	602	NAI	C6N-C5N	3.46	1.40	1.33
2	C	601	FAD	C2-N1	3.41	1.44	1.35
2	A	601	FAD	C2B-C1B	-3.40	1.48	1.53
3	B	602	NAI	C7N-N7N	3.39	1.44	1.33
2	D	601	FAD	C4A-N9A	3.39	1.42	1.37
3	B	602	NAI	C4N-C5N	-3.36	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	O2'-C2'	-3.33	1.35	1.43
3	A	602	NAI	C2N-C3N	3.32	1.41	1.34
2	C	601	FAD	C2B-C1B	-3.32	1.48	1.53
2	A	601	FAD	C2-N1	3.31	1.44	1.35
2	D	601	FAD	C2B-C1B	-3.23	1.48	1.53
2	A	601	FAD	C4A-N9A	3.22	1.42	1.37
3	A	602	NAI	C7N-N7N	3.22	1.43	1.33
2	B	601	FAD	C2-N1	3.19	1.44	1.35
3	A	602	NAI	C4A-N9A	3.19	1.42	1.37
3	B	602	NAI	C6A-N6A	3.18	1.45	1.35
2	B	601	FAD	C4A-N9A	3.16	1.42	1.37
3	A	602	NAI	C4N-C5N	-3.14	1.42	1.49
3	B	602	NAI	C4A-N9A	3.06	1.42	1.37
2	D	601	FAD	C2-N1	3.05	1.43	1.35
3	B	602	NAI	C2N-C3N	3.03	1.40	1.34
2	C	601	FAD	C6A-N6A	2.96	1.44	1.35
2	D	601	FAD	C6A-N6A	2.94	1.44	1.35
2	B	601	FAD	O2'-C2'	-2.94	1.36	1.43
3	A	602	NAI	C2N-N1N	2.94	1.42	1.36
2	B	601	FAD	C5X-N5	2.91	1.39	1.35
2	D	601	FAD	C5X-N5	2.84	1.39	1.35
3	A	602	NAI	C2B-C1B	-2.81	1.49	1.53
3	B	602	NAI	C2N-N1N	2.79	1.41	1.36
2	D	601	FAD	PA-O5B	-2.78	1.46	1.59
2	A	601	FAD	C6A-N6A	2.76	1.43	1.35
2	D	601	FAD	C1'-N10	-2.76	1.45	1.48
3	A	602	NAI	C6A-N6A	2.76	1.43	1.35
2	B	601	FAD	C6A-N6A	2.74	1.43	1.35
2	A	601	FAD	O4'-C4'	-2.67	1.37	1.43
2	D	601	FAD	O2'-C2'	-2.65	1.37	1.43
2	C	601	FAD	C1'-N10	-2.65	1.45	1.48
2	B	601	FAD	O4'-C4'	-2.62	1.37	1.43
3	B	602	NAI	C2B-C1B	-2.59	1.49	1.53
2	B	601	FAD	PA-O5B	-2.56	1.47	1.59
2	C	601	FAD	O4'-C4'	-2.53	1.37	1.43
2	A	601	FAD	C1'-C2'	-2.48	1.49	1.51
2	A	601	FAD	C1'-N10	-2.47	1.45	1.48
3	B	602	NAI	O2D-C2D	-2.47	1.37	1.43
2	C	601	FAD	O2'-C2'	-2.46	1.37	1.43
2	D	601	FAD	O4'-C4'	-2.45	1.37	1.43
2	D	601	FAD	C4X-C10	2.44	1.45	1.40
2	A	601	FAD	PA-O5B	-2.44	1.48	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	C2A-N3A	2.43	1.37	1.32
3	B	602	NAI	PA-O2A	-2.43	1.44	1.55
2	B	601	FAD	C4X-C10	2.41	1.45	1.40
2	C	601	FAD	C2A-N3A	2.39	1.36	1.32
2	C	601	FAD	P-O1P	2.39	1.60	1.51
3	A	602	NAI	C8A-N9A	2.35	1.40	1.36
3	A	602	NAI	O2D-C2D	-2.35	1.37	1.43
2	C	601	FAD	PA-O5B	-2.31	1.48	1.59
2	B	601	FAD	C2B-C3B	-2.29	1.47	1.53
3	B	602	NAI	C2B-C3B	-2.28	1.47	1.53
2	B	601	FAD	PA-O2A	-2.28	1.44	1.55
2	B	601	FAD	C1'-N10	-2.25	1.45	1.48
2	A	601	FAD	C4X-C10	2.23	1.44	1.40
2	A	601	FAD	O2B-C2B	-2.22	1.37	1.43
2	C	601	FAD	C5X-N5	2.22	1.38	1.35
2	B	601	FAD	O3B-C3B	-2.20	1.37	1.43
2	A	601	FAD	C5X-N5	2.20	1.38	1.35
3	B	602	NAI	O2B-C2B	-2.20	1.37	1.43
3	B	602	NAI	PA-O5B	-2.18	1.49	1.59
3	A	602	NAI	C2B-C3B	-2.18	1.47	1.53
3	A	602	NAI	O2B-C2B	-2.17	1.37	1.43
3	A	602	NAI	C2A-N3A	2.16	1.36	1.32
2	A	601	FAD	C2B-C3B	-2.15	1.47	1.53
2	D	601	FAD	P-O1P	2.14	1.59	1.51
2	C	601	FAD	C4X-C10	2.14	1.44	1.40
2	A	601	FAD	PA-O2A	-2.12	1.45	1.55
2	A	601	FAD	C2A-N3A	2.11	1.36	1.32
2	B	601	FAD	P-O1P	2.11	1.59	1.51
2	D	601	FAD	C2B-C3B	-2.11	1.47	1.53
2	D	601	FAD	O4B-C4B	-2.09	1.40	1.45
3	B	602	NAI	C2A-N3A	2.09	1.36	1.32
2	C	601	FAD	O3'-C3'	-2.06	1.38	1.43
2	A	601	FAD	C4'-C3'	-2.03	1.49	1.53
2	B	601	FAD	O2B-C2B	-2.03	1.38	1.43
2	B	601	FAD	C2A-N3A	2.02	1.36	1.32
3	A	602	NAI	PA-O5B	-2.02	1.50	1.59
2	A	601	FAD	O3'-C3'	-2.00	1.38	1.43

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAI	N3A-C2A-N1A	-11.10	119.43	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAI	N3A-C2A-N1A	-11.08	119.45	128.71
2	A	601	FAD	N3A-C2A-N1A	-9.91	120.43	128.71
2	B	601	FAD	N3A-C2A-N1A	-9.60	120.69	128.71
2	D	601	FAD	N3A-C2A-N1A	-9.41	120.84	128.71
2	C	601	FAD	N3A-C2A-N1A	-9.36	120.89	128.71
3	A	602	NAI	O4B-C1B-N9A	8.44	116.29	108.44
2	B	601	FAD	O4B-C1B-N9A	7.30	115.23	108.44
2	A	601	FAD	O4B-C1B-N9A	7.18	115.12	108.44
2	A	601	FAD	C1'-N10-C9A	-6.87	112.19	118.87
2	C	601	FAD	O4B-C1B-N9A	6.00	114.02	108.44
2	A	601	FAD	C2'-C1'-N10	5.85	120.21	112.45
2	D	601	FAD	C2-N1-C10	5.78	120.80	114.98
2	B	601	FAD	C2-N1-C10	5.62	120.65	114.98
2	C	601	FAD	N3A-C4A-N9A	5.56	135.47	125.43
2	A	601	FAD	C2-N1-C10	5.54	120.56	114.98
2	D	601	FAD	O2P-P-O3P	-5.45	79.28	105.14
2	C	601	FAD	C4X-C10-N10	-5.37	117.83	120.51
2	D	601	FAD	O4B-C1B-N9A	5.36	113.43	108.44
2	D	601	FAD	N3A-C4A-N9A	5.10	134.63	125.43
2	A	601	FAD	C4X-C10-N10	-5.04	118.00	120.51
3	B	602	NAI	O4B-C1B-N9A	5.02	113.11	108.44
2	A	601	FAD	N3A-C4A-N9A	5.02	134.49	125.43
2	C	601	FAD	C2-N1-C10	4.99	120.01	114.98
2	A	601	FAD	C4B-O4B-C1B	-4.72	104.62	109.75
2	B	601	FAD	N3A-C4A-N9A	4.71	133.93	125.43
2	B	601	FAD	C1'-N10-C9A	-4.70	114.30	118.87
2	A	601	FAD	C1'-N10-C10	4.47	125.51	119.17
3	B	602	NAI	N3A-C4A-N9A	4.42	133.42	125.43
2	D	601	FAD	C1'-N10-C9A	-4.23	114.76	118.87
2	A	601	FAD	C4X-N5-C5X	4.22	121.43	116.69
2	D	601	FAD	C4X-N5-C5X	4.18	121.39	116.69
3	A	602	NAI	N3A-C4A-N9A	4.09	132.82	125.43
2	C	601	FAD	O2P-P-O5'	-3.99	88.39	108.51
2	B	601	FAD	C4X-C10-N10	-3.88	118.58	120.51
3	B	602	NAI	O4D-C1D-N1N	3.83	116.17	108.05
2	C	601	FAD	C4X-N5-C5X	3.81	120.97	116.69
2	B	601	FAD	C4X-N5-C5X	3.72	120.86	116.69
2	B	601	FAD	C2'-C1'-N10	3.69	117.35	112.45
2	D	601	FAD	C1'-N10-C10	3.66	124.36	119.17
2	C	601	FAD	C5X-C9A-N10	3.46	120.20	116.80
2	A	601	FAD	P-O3P-PA	-3.39	121.73	131.68
2	B	601	FAD	C5X-C9A-N10	3.35	120.11	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C5A-C4A-N3A	-3.35	118.42	125.70
2	B	601	FAD	C1'-N10-C10	3.33	123.90	119.17
3	A	602	NAI	O4D-C1D-N1N	3.32	115.08	108.05
2	A	601	FAD	C5X-C9A-N10	3.32	120.07	116.80
3	A	602	NAI	C4B-O4B-C1B	-3.28	106.19	109.75
2	C	601	FAD	C1'-N10-C9A	-3.22	115.74	118.87
2	A	601	FAD	C5'-C4'-C3'	-3.14	106.13	112.06
2	A	601	FAD	C5A-C4A-N3A	-3.10	118.95	125.70
2	C	601	FAD	O5'-P-O1P	3.09	121.50	109.37
2	B	601	FAD	O3'-C3'-C2'	3.06	116.46	108.74
2	C	601	FAD	C1'-N10-C10	3.05	123.50	119.17
2	D	601	FAD	P-O3P-PA	-3.00	122.89	131.68
2	A	601	FAD	O5B-PA-O1A	2.97	121.01	109.37
2	B	601	FAD	O2P-P-O3P	-2.95	91.16	105.14
2	D	601	FAD	C2'-C1'-N10	2.90	116.29	112.45
3	B	602	NAI	C4B-O4B-C1B	-2.85	106.65	109.75
2	D	601	FAD	C5A-C4A-N3A	-2.80	119.60	125.70
2	B	601	FAD	P-O3P-PA	-2.73	123.69	131.68
3	B	602	NAI	O2A-PA-O5B	-2.71	94.83	108.51
2	B	601	FAD	C5A-C4A-N3A	-2.71	119.80	125.70
2	A	601	FAD	O2P-P-O5'	-2.69	94.93	108.51
2	D	601	FAD	C4A-C5A-N7A	-2.64	107.26	109.52
2	D	601	FAD	C5X-C9A-N10	2.64	119.40	116.80
2	A	601	FAD	O2P-P-O3P	-2.63	92.67	105.14
2	A	601	FAD	C4A-C5A-N7A	-2.56	107.33	109.52
3	A	602	NAI	O2A-PA-O3	-2.55	93.03	105.14
3	A	602	NAI	C5N-C4N-C3N	2.54	119.48	112.60
2	B	601	FAD	C6-C5X-N5	2.54	121.93	118.97
2	A	601	FAD	C4X-C10-N1	-2.52	120.21	122.73
3	A	602	NAI	C1B-N9A-C4A	-2.52	122.28	126.64
3	B	602	NAI	C5N-C4N-C3N	2.51	119.40	112.60
2	A	601	FAD	O2A-PA-O5B	-2.50	95.91	108.51
2	A	601	FAD	O5'-P-O1P	2.49	119.12	109.37
2	D	601	FAD	C4X-C10-N1	-2.47	120.26	122.73
3	A	602	NAI	PN-O3-PA	-2.44	124.52	131.68
2	D	601	FAD	O5B-PA-O1A	2.42	118.85	109.37
2	C	601	FAD	C5'-C4'-C3'	-2.42	107.50	112.06
2	D	601	FAD	O2A-PA-O1A	2.41	125.66	112.21
2	A	601	FAD	O2A-PA-O3P	-2.40	93.74	105.14
2	B	601	FAD	O5'-P-O1P	2.39	118.73	109.37
2	A	601	FAD	C2A-N3A-C4A	2.38	120.78	114.01
3	B	602	NAI	C3N-C2N-N1N	-2.38	119.67	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C2A-N3A-C4A	2.34	120.67	114.01
2	D	601	FAD	C4X-C10-N10	-2.33	119.35	120.51
2	A	601	FAD	C1'-C2'-C3'	-2.33	103.17	109.82
2	B	601	FAD	O2P-P-O5'	-2.32	96.82	108.51
2	D	601	FAD	C4-N3-C2	-2.32	120.63	125.39
3	A	602	NAI	C2A-N3A-C4A	2.32	120.61	114.01
2	C	601	FAD	O5B-PA-O1A	2.31	118.43	109.37
3	B	602	NAI	O5B-PA-O1A	2.31	118.42	109.37
2	B	601	FAD	O2'-C2'-C1'	-2.30	103.99	109.71
3	A	602	NAI	C4A-C5A-N7A	-2.29	107.56	109.52
2	A	601	FAD	C4-N3-C2	-2.27	120.73	125.39
2	C	601	FAD	C4A-C5A-N7A	-2.26	107.59	109.52
3	B	602	NAI	C2A-N3A-C4A	2.25	120.43	114.01
2	C	601	FAD	C4-N3-C2	-2.23	120.82	125.39
3	A	602	NAI	C5A-C4A-N3A	-2.22	120.86	125.70
2	A	601	FAD	C6-C5X-N5	2.22	121.56	118.97
2	A	601	FAD	N1-C10-N10	2.21	121.78	115.97
3	B	602	NAI	C5A-C4A-N3A	-2.21	120.89	125.70
2	A	601	FAD	O5B-C5B-C4B	2.20	117.01	108.94
2	B	601	FAD	O2A-PA-O3P	-2.18	94.81	105.14
3	B	602	NAI	O4B-C1B-C2B	2.17	110.10	106.77
2	D	601	FAD	C5'-C4'-C3'	-2.17	107.96	112.06
2	B	601	FAD	C4-N3-C2	-2.16	120.96	125.39
2	D	601	FAD	C4B-O4B-C1B	-2.15	107.41	109.75
2	D	601	FAD	O2P-P-O1P	2.15	124.21	112.21
2	B	601	FAD	O5B-PA-O1A	2.11	117.66	109.37
2	C	601	FAD	N1-C10-N10	2.11	121.53	115.97
2	B	601	FAD	C4B-O4B-C1B	-2.10	107.46	109.75
2	B	601	FAD	C2A-N3A-C4A	2.10	120.00	114.01
2	C	601	FAD	C4X-C10-N1	-2.10	120.63	122.73
2	D	601	FAD	C2A-N3A-C4A	2.10	119.99	114.01
2	B	601	FAD	C5'-C4'-C3'	-2.10	108.10	112.06
2	D	601	FAD	O3'-C3'-C2'	2.08	114.00	108.74
2	D	601	FAD	O2A-PA-O5B	-2.06	98.10	108.51
2	D	601	FAD	C5B-C4B-C3B	-2.06	106.95	115.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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%)	0.32	5 (1%) 79 81	25, 46, 76, 103	0
1	B	494/513 (96%)	0.31	4 (0%) 83 85	24, 47, 77, 121	0
1	C	499/513 (97%)	0.43	17 (3%) 43 46	24, 53, 84, 106	0
1	D	502/513 (97%)	0.40	13 (2%) 53 57	23, 54, 86, 104	0
All	All	1989/2052 (96%)	0.36	39 (1%) 64 65	23, 50, 81, 121	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	VAL	3.5
1	D	236	PHE	3.2
1	C	245	VAL	3.0
1	B	184	ALA	3.0
1	C	273	PHE	2.9
1	A	62	GLY	2.7
1	B	497	LEU	2.7
1	D	218	THR	2.6
1	D	273	PHE	2.5
1	C	442	ILE	2.5
1	C	411	TYR	2.5
1	D	222	TRP	2.5
1	D	221	ILE	2.5
1	A	498	VAL	2.4
1	A	245	VAL	2.4
1	C	20	LEU	2.4
1	C	11	LEU	2.4
1	C	300	VAL	2.3
1	C	46	LEU	2.3
1	C	58	TYR	2.3
1	D	266	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	72	PHE	2.2
1	A	307	PRO	2.2
1	C	265	LEU	2.2
1	D	411	TYR	2.2
1	C	266	VAL	2.2
1	D	240	GLY	2.2
1	C	236	PHE	2.2
1	D	442	ILE	2.2
1	A	242	VAL	2.1
1	C	10	VAL	2.1
1	D	223	ILE	2.1
1	C	225	VAL	2.1
1	D	242	VAL	2.0
1	C	269	MET	2.0
1	D	498	VAL	2.0
1	B	179	LEU	2.0
1	D	283	LEU	2.0
1	B	23	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	D	603	5/5	0.20	2.52	80,89,94,94	5
4	SO4	C	603	5/5	0.25	1.12	46,49,61,87	5
4	SO4	D	604	5/5	0.22	0.85	51,102,114,116	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	604	5/5	0.23	0.72	53,68,89,90	0
4	SO4	B	605	5/5	0.22	0.54	70,74,84,89	0
4	SO4	D	602	5/5	0.22	0.14	30,31,55,82	5
3	NAI	B	602	44/44	0.21	0.01	29,48,63,71	0
4	SO4	B	604	5/5	0.20	-0.01	45,66,73,76	5
2	FAD	B	601	53/53	0.20	-0.04	18,43,62,66	0
2	FAD	D	601	53/53	0.20	-0.26	26,57,91,107	0
2	FAD	A	601	53/53	0.20	-0.31	25,44,63,69	0
2	FAD	C	601	53/53	0.20	-0.56	24,60,86,96	0
4	SO4	C	602	5/5	0.16	-0.59	63,74,90,102	0
3	NAI	A	602	44/44	0.19	-0.93	22,54,71,78	0
4	SO4	A	603	5/5	0.17	-0.93	29,37,66,74	5
4	SO4	B	603	5/5	0.12	-3.05	68,94,101,101	0

6.5 Other polymers ⓘ

There are no such residues in this entry.