



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2017 – 06:56 PM EDT

PDB ID : 5VWT
Title : Crystal structure of oxidized Aspergillus fumigatus UDP-galactopyranose mutase complexed with NADPH
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

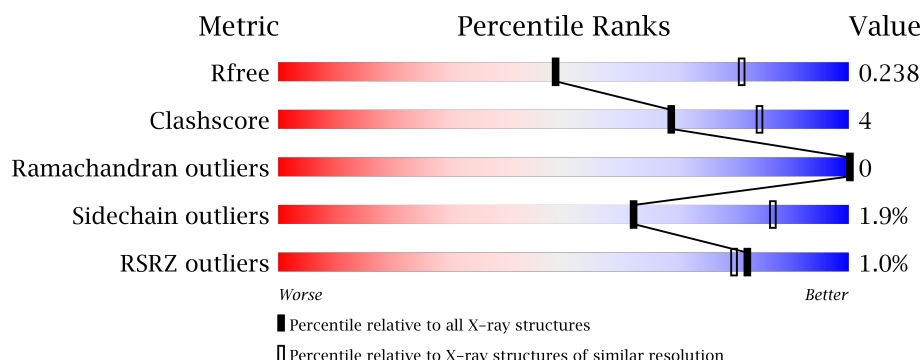
1 Overall quality at a glance

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	
1	B	513	
1	C	513	
1	D	513	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15472 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	495	Total	C	N	O	S	0	0	0
			3756	2396	632	707	21			
1	B	492	Total	C	N	O	S	0	0	0
			3748	2384	633	711	20			
1	C	501	Total	C	N	O	S	0	0	0
			3774	2400	639	716	19			
1	D	499	Total	C	N	O	S	0	0	0
			3740	2380	629	713	18			

There are 24 discrepancies between the modelled and reference sequences:

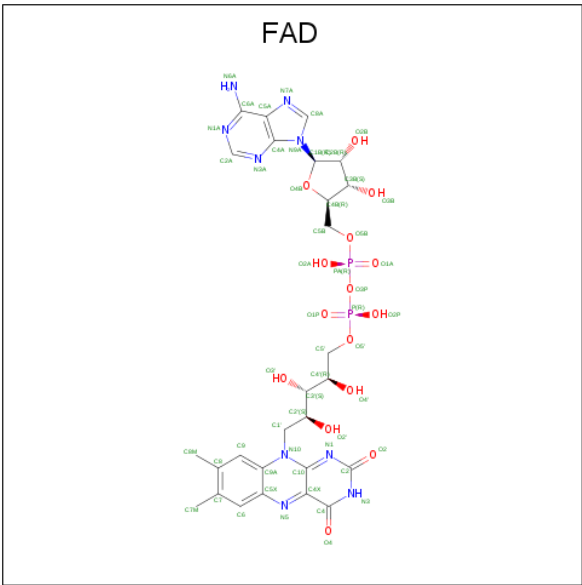
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP Q4W1X2
A	-1	ILE	-	expression tag	UNP Q4W1X2
A	0	ALA	-	expression tag	UNP Q4W1X2
A	344	ALA	LYS	engineered mutation	UNP Q4W1X2
A	345	ALA	LYS	engineered mutation	UNP Q4W1X2
A	429	THR	ALA	conflict	UNP Q4W1X2
B	-2	ALA	-	expression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

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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	conflict	UNP Q4W1X2

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



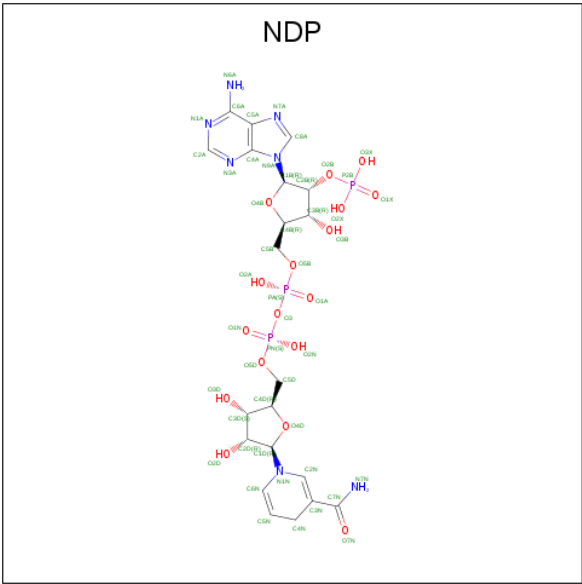
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

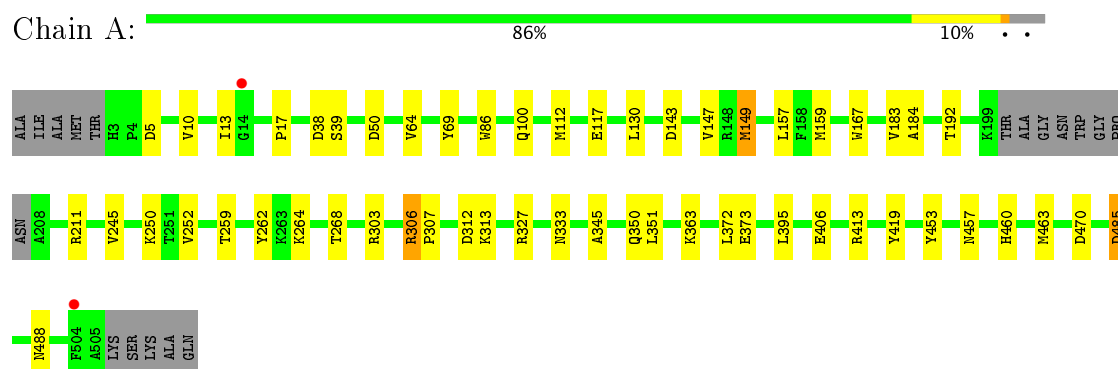
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	4	Total	O	0	0
			4	4		
5	C	2	Total	O	0	0
			2	2		
5	D	1	Total	O	0	0
			1	1		

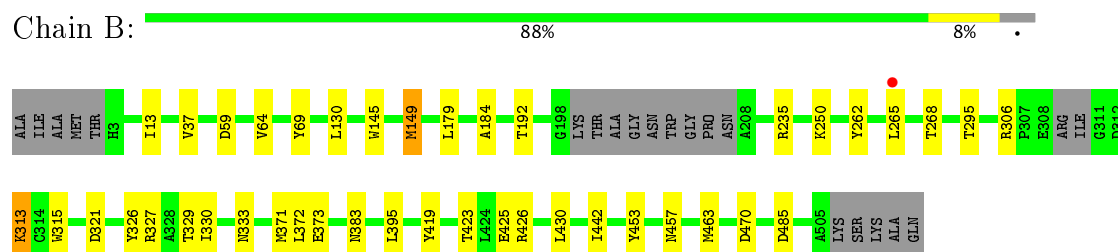
3 Residue-property plots [i](#)

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.

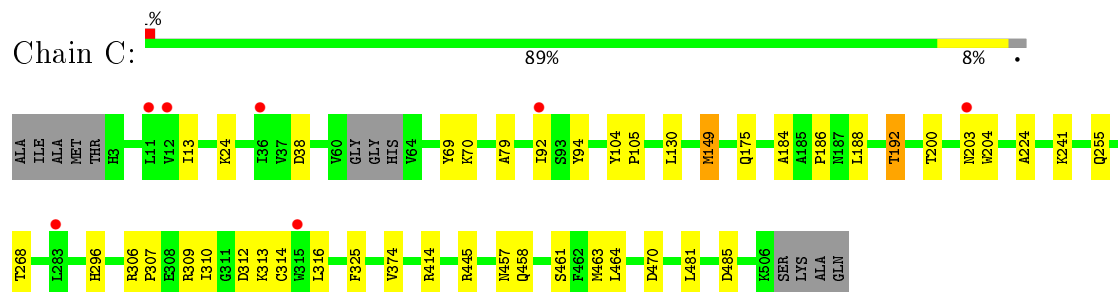
• Molecule 1: UDP-galactopyranose mutase



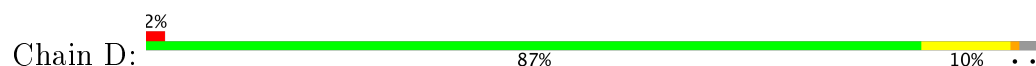
• Molecule 1: UDP-galactopyranose mutase

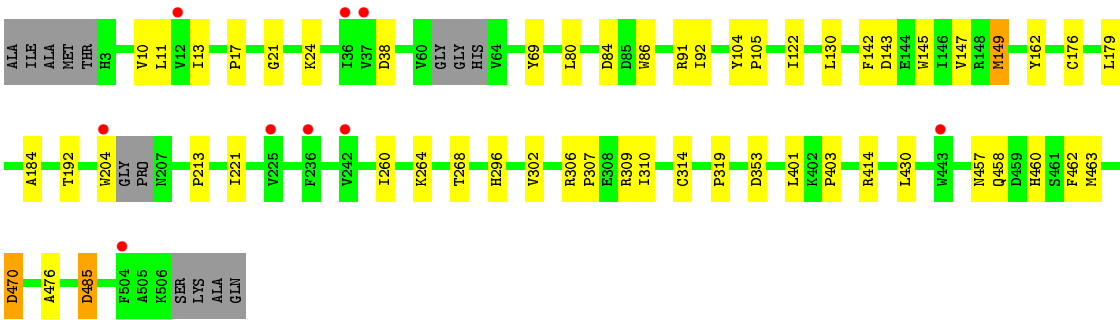


• Molecule 1: UDP-galactopyranose mutase



• 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	218.29 Å 218.29 Å 319.22 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	162.66 – 2.75 162.66 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (162.66-2.75) 99.7 (162.66-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.73 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.239 0.198 , 0.238	Depositor DCC
R_{free} test set	5834 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15472	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: NDP, 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	0/3850	0.61	0/5255
1	B	0.45	0/3840	0.60	1/5240 (0.0%)
1	C	0.43	0/3869	0.59	0/5287
1	D	0.44	0/3834	0.59	0/5243
All	All	0.44	0/15393	0.60	1/21025 (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	321	ASP	CB-CA-C	-5.26	99.88	110.40

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	3756	0	3538	34	0
1	B	3748	0	3543	24	0
1	C	3774	0	3525	28	0
1	D	3740	0	3444	40	0
2	A	53	0	31	8	0
2	B	53	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	6	0
2	D	53	0	31	7	0
3	A	15	0	0	0	0
3	B	20	0	0	1	0
3	C	20	0	0	0	0
3	D	15	0	0	1	0
4	A	48	0	26	2	0
4	B	48	0	26	1	0
4	C	31	0	11	0	0
4	D	31	0	11	0	0
5	A	7	0	0	0	0
5	B	4	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	1	0
All	All	15472	0	14248	129	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 4.

All (129) 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:D:17:PRO:HD2	2:D:601:FAD:H5'2	1.57	0.86
1:A:17:PRO:HD2	2:A:601:FAD:H5'2	1.58	0.84
1:A:372:LEU:HD21	1:A:395:LEU:HD21	1.65	0.79
1:B:13:ILE:O	1:B:268:THR:HB	1.88	0.73
1:A:268:THR:HG22	2:A:601:FAD:H51A	1.71	0.71
1:A:13:ILE:O	1:A:268:THR:HB	1.92	0.69
1:A:245:VAL:HG22	1:A:252:VAL:HG22	1.78	0.65
1:D:307:PRO:HG2	1:D:310:ILE:HD13	1.79	0.64
1:C:307:PRO:HB2	1:C:309:ARG:HG2	1.78	0.64
1:B:313:LYS:HD2	1:B:313:LYS:H	1.63	0.63
1:B:327:ARG:NE	1:B:373:GLU:OE1	2.22	0.62
1:B:313:LYS:HG3	1:B:333:ASN:HB3	1.80	0.61
1:A:149:MET:SD	1:A:184:ALA:HA	2.41	0.61
1:D:143:ASP:O	1:D:147:VAL:HG23	2.00	0.60
1:B:149:MET:SD	1:B:184:ALA:HA	2.41	0.60
1:D:69:TYR:CD2	1:D:463:MET:HG3	2.36	0.59
1:B:372:LEU:HD21	1:B:395:LEU:HD21	1.83	0.59
1:D:309:ARG:NH1	3:D:603:SO4:O3	2.29	0.59
1:C:13:ILE:O	1:C:268:THR:HB	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ASP:HB3	1:D:476:ALA:HB3	1.87	0.56
1:D:13:ILE:O	1:D:268:THR:HB	2.06	0.56
1:C:38:ASP:OD1	2:C:601:FAD:H1B	2.06	0.55
1:A:192:THR:HG21	1:D:122:ILE:HG21	1.88	0.55
1:B:383:ASN:ND2	3:B:605:SO4:O4	2.34	0.54
1:A:100:GLN:HB3	1:A:112:MET:HE2	1.90	0.54
1:B:130:LEU:HD23	1:C:130:LEU:HD23	1.91	0.54
1:D:457:ASN:HB2	2:D:601:FAD:O2	2.09	0.53
1:C:268:THR:HG22	2:C:601:FAD:H52A	1.91	0.53
1:D:92:ILE:O	1:D:314:CYS:HB2	2.09	0.52
1:B:265:LEU:HD23	1:B:442:ILE:HG12	1.92	0.52
1:C:188:LEU:O	1:C:192:THR:HB	2.10	0.52
1:D:69:TYR:CG	1:D:463:MET:HG3	2.45	0.52
1:A:268:THR:CG2	2:A:601:FAD:H51A	2.40	0.52
1:B:69:TYR:CG	1:B:463:MET:HG3	2.45	0.51
1:A:306:ARG:HB2	1:A:307:PRO:HD2	1.92	0.51
1:B:457:ASN:HB2	2:B:601:FAD:O2	2.12	0.50
1:C:325:PHE:HA	1:C:374:VAL:HG22	1.94	0.50
1:D:80:LEU:HD12	1:D:86:TRP:CZ2	2.47	0.50
1:A:69:TYR:CD2	1:A:463:MET:HG3	2.47	0.50
1:B:453:TYR:CE1	4:B:603:NDP:H42N	2.47	0.50
1:B:313:LYS:HD2	1:B:313:LYS:N	2.26	0.49
1:A:457:ASN:HB3	4:A:604:NDP:H41N	1.94	0.49
1:D:92:ILE:HA	1:D:204:TRP:CE3	2.48	0.49
1:A:457:ASN:HB2	2:A:601:FAD:O2	2.13	0.49
1:A:419:TYR:HE1	2:A:601:FAD:HM73	1.78	0.48
1:C:69:TYR:CG	1:C:463:MET:HG3	2.48	0.48
1:A:5:ASP:HB2	1:A:259:THR:O	2.13	0.48
1:A:69:TYR:CG	1:A:463:MET:HG3	2.47	0.48
1:C:149:MET:SD	1:C:184:ALA:HA	2.54	0.48
1:C:445:ARG:NE	1:C:481:LEU:HD22	2.29	0.47
1:C:458:GLN:HG3	2:C:601:FAD:O2	2.14	0.47
1:D:91:ARG:O	1:D:204:TRP:HB3	2.15	0.47
1:C:92:ILE:O	1:C:314:CYS:HB2	2.15	0.47
1:A:143:ASP:O	1:A:147:VAL:HG23	2.15	0.47
1:C:461:SER:HA	1:C:464:LEU:HD12	1.97	0.46
1:A:485:ASP:N	1:A:485:ASP:OD1	2.42	0.46
1:A:457:ASN:HB2	2:A:601:FAD:C2	2.45	0.46
1:A:250:LYS:HG2	1:A:262:TYR:CE1	2.51	0.46
1:B:145:TRP:CD2	1:B:179:LEU:HD13	2.50	0.46
1:D:192:THR:HG23	5:D:701:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:FAD:H2'	2:B:601:FAD:N1	2.31	0.46
1:A:86:TRP:CD2	1:A:211:ARG:HD2	2.50	0.46
1:D:213:PRO:HG3	1:D:221:ILE:HG13	1.97	0.46
1:D:69:TYR:CE2	1:D:463:MET:HG3	2.51	0.46
1:D:84:ASP:N	1:D:84:ASP:OD1	2.45	0.46
1:D:11:LEU:HD13	1:D:260:ILE:HG21	1.98	0.46
1:A:10:VAL:HA	1:A:264:LYS:O	2.17	0.45
1:A:38:ASP:OD1	1:A:39:SER:N	2.50	0.45
1:B:315:TRP:CE3	1:B:329:THR:HB	2.52	0.45
1:B:37:VAL:HG12	1:B:235:ARG:HB3	1.96	0.45
1:C:457:ASN:HB2	2:C:601:FAD:O2	2.17	0.45
1:B:426:ARG:O	1:B:430:LEU:HB2	2.17	0.45
1:B:295:THR:HG21	2:B:601:FAD:C7M	2.46	0.45
1:D:296:HIS:CE1	1:D:414:ARG:HD2	2.52	0.45
1:C:104:TYR:CG	1:C:105:PRO:HA	2.52	0.45
1:C:458:GLN:HA	2:C:601:FAD:O3'	2.17	0.45
1:D:457:ASN:HB2	2:D:601:FAD:C2	2.48	0.44
1:A:460:HIS:NE2	1:A:488:ASN:OD1	2.46	0.44
1:C:310:ILE:O	1:C:313:LYS:HG3	2.18	0.44
1:B:69:TYR:CD1	1:B:463:MET:HG3	2.52	0.44
1:D:142:PHE:HA	1:D:176:CYS:HB3	1.99	0.44
1:D:149:MET:SD	1:D:184:ALA:HA	2.57	0.44
1:A:117:GLU:OE2	1:A:157:LEU:HD21	2.18	0.44
1:C:92:ILE:HG22	1:C:94:TYR:HE1	1.82	0.44
2:D:601:FAD:H1'1	2:D:601:FAD:H9	1.78	0.44
2:B:601:FAD:H9	2:B:601:FAD:H1'1	1.63	0.43
1:D:38:ASP:OD1	2:D:601:FAD:H1B	2.18	0.43
1:C:92:ILE:HD12	1:C:312:ASP:O	2.18	0.43
1:B:423:THR:HB	1:B:425:GLU:OE1	2.17	0.43
1:C:296:HIS:CE1	1:C:414:ARG:HD2	2.52	0.43
2:C:601:FAD:H1'1	2:C:601:FAD:H9	1.78	0.43
1:D:10:VAL:HA	1:D:264:LYS:O	2.19	0.43
1:B:250:LYS:HB3	1:B:262:TYR:O	2.19	0.43
1:D:457:ASN:OD1	1:D:460:HIS:ND1	2.51	0.43
1:B:419:TYR:HE1	2:B:601:FAD:HM73	1.82	0.43
1:D:458:GLN:HG3	2:D:601:FAD:O2	2.19	0.43
1:D:353:ASP:HB3	1:D:403:PRO:HB3	2.01	0.43
1:B:59:ASP:H	1:B:371:MET:HE1	1.83	0.42
1:C:79:ALA:HB1	1:C:224:ALA:CB	2.48	0.42
2:A:601:FAD:O2'	2:A:601:FAD:H9	2.19	0.42
4:A:604:NDP:H71N	4:A:604:NDP:H2N	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLN:HG3	1:A:351:LEU:O	2.19	0.42
1:C:69:TYR:CD1	1:C:463:MET:HG3	2.54	0.42
1:A:327:ARG:NE	1:A:373:GLU:OE1	2.40	0.42
1:D:145:TRP:CD2	1:D:179:LEU:HD13	2.55	0.42
1:D:430:LEU:HD12	1:D:430:LEU:HA	1.88	0.42
1:C:313:LYS:HD2	1:C:316:LEU:HD21	2.02	0.42
1:D:307:PRO:HB2	1:D:309:ARG:HG2	2.02	0.42
1:A:50:ASP:OD2	1:A:413:ARG:NH1	2.47	0.41
1:D:162:TYR:HB2	1:D:319:PRO:HB3	2.01	0.41
1:D:104:TYR:CG	1:D:105:PRO:HA	2.55	0.41
1:D:24:LYS:HA	1:D:24:LYS:HD2	1.88	0.41
1:C:24:LYS:HA	1:C:24:LYS:HD2	1.90	0.41
1:A:130:LEU:HD23	1:D:130:LEU:HD23	2.03	0.41
1:C:241:LYS:HB3	1:C:255:GLN:HB2	2.02	0.41
1:A:419:TYR:CE1	2:A:601:FAD:HM73	2.55	0.41
1:A:313:LYS:HG3	1:A:333:ASN:HB3	2.03	0.40
1:A:345:ALA:HA	1:A:363:LYS:O	2.21	0.40
1:B:326:TYR:CZ	1:B:373:GLU:HB3	2.56	0.40
1:D:302:VAL:HG21	1:D:401:LEU:HD21	2.02	0.40
1:A:303:ARG:NE	1:A:406:GLU:OE1	2.50	0.40
1:D:21:GLY:HA2	1:D:462:PHE:CE1	2.56	0.40
1:D:485:ASP:OD1	1:D:485:ASP:N	2.43	0.40
1:D:17:PRO:CD	2:D:601:FAD:H5'2	2.40	0.40
1:C:149:MET:O	1:C:186:PRO:HB3	2.20	0.40
1:C:105:PRO:HD3	1:C:203:ASN:HB3	2.03	0.40
1:C:92:ILE:HA	1:C:204:TRP:CE3	2.56	0.40
1:A:167:TRP:HH2	1:A:453:TYR:CG	2.39	0.40
1:D:142:PHE:CE1	1:D:179:LEU:HD11	2.56	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	491/513 (96%)	479 (98%)	12 (2%)	0	100	100
1	B	486/513 (95%)	470 (97%)	16 (3%)	0	100	100
1	C	497/513 (97%)	482 (97%)	15 (3%)	0	100	100
1	D	493/513 (96%)	478 (97%)	15 (3%)	0	100	100
All	All	1967/2052 (96%)	1909 (97%)	58 (3%)	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	378/432 (88%)	370 (98%)	8 (2%)	59	85
1	B	383/432 (89%)	375 (98%)	8 (2%)	59	85
1	C	378/432 (88%)	370 (98%)	8 (2%)	59	85
1	D	368/432 (85%)	364 (99%)	4 (1%)	78	92
All	All	1507/1728 (87%)	1479 (98%)	28 (2%)	62	87

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	149	MET
1	A	159	MET
1	A	183	VAL
1	A	306	ARG
1	A	312	ASP
1	A	470	ASP
1	A	485	ASP
1	B	64	VAL
1	B	149	MET
1	B	192	THR
1	B	306	ARG
1	B	313	LYS

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Mol	Chain	Res	Type
1	B	330	ILE
1	B	470	ASP
1	B	485	ASP
1	C	70	LYS
1	C	149	MET
1	C	175	GLN
1	C	192	THR
1	C	200	THR
1	C	306	ARG
1	C	470	ASP
1	C	485	ASP
1	D	149	MET
1	D	306	ARG
1	D	470	ASP
1	D	485	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	B	175	GLN
1	B	279	ASN
1	C	246	ASN
1	D	246	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

22 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	1.05	3 (5%)	54,89,89	2.50	10 (18%)
3	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.38	0
3	SO4	A	603	-	4,4,4	0.21	0	6,6,6	0.11	0
4	NDP	A	604	-	43,52,52	2.53	7 (16%)	49,80,80	1.40	7 (14%)
3	SO4	A	605	-	4,4,4	0.28	0	6,6,6	0.44	0
2	FAD	B	601	-	51,58,58	0.94	3 (5%)	54,89,89	2.37	7 (12%)
3	SO4	B	602	-	4,4,4	0.22	0	6,6,6	0.43	0
4	NDP	B	603	-	43,52,52	2.82	8 (18%)	49,80,80	1.33	6 (12%)
3	SO4	B	604	-	4,4,4	0.13	0	6,6,6	0.36	0
3	SO4	B	605	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	B	606	-	4,4,4	0.20	0	6,6,6	0.29	0
2	FAD	C	601	-	51,58,58	0.92	3 (5%)	54,89,89	2.27	5 (9%)
4	NDP	C	602	-	28,33,52	3.69	4 (14%)	32,52,80	1.76	10 (31%)
3	SO4	C	603	-	4,4,4	0.21	0	6,6,6	0.39	0
3	SO4	C	604	-	4,4,4	0.19	0	6,6,6	0.21	0
3	SO4	C	605	-	4,4,4	0.18	0	6,6,6	0.23	0
3	SO4	C	606	-	4,4,4	0.13	0	6,6,6	0.25	0
2	FAD	D	601	-	51,58,58	1.01	4 (7%)	54,89,89	2.32	6 (11%)
3	SO4	D	602	-	4,4,4	0.23	0	6,6,6	0.43	0
3	SO4	D	603	-	4,4,4	0.20	0	6,6,6	0.31	0
4	NDP	D	604	-	28,33,52	3.44	4 (14%)	32,52,80	1.79	12 (37%)
3	SO4	D	605	-	4,4,4	0.12	0	6,6,6	0.23	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
4	NDP	A	604	-	-	0/30/77/77	0/5/5/5
3	SO4	A	605	-	-	0/0/0/0	0/0/0/0
2	FAD	B	601	-	-	0/28/50/50	0/6/6/6
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
4	NDP	B	603	-	-	0/30/77/77	0/5/5/5
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	605	-	-	0/0/0/0	0/0/0/0
3	SO4	B	606	-	-	0/0/0/0	0/0/0/0
2	FAD	C	601	-	-	0/28/50/50	0/6/6/6
4	NDP	C	602	-	-	0/17/37/77	0/3/3/5
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
3	SO4	C	604	-	-	0/0/0/0	0/0/0/0
3	SO4	C	605	-	-	0/0/0/0	0/0/0/0
3	SO4	C	606	-	-	0/0/0/0	0/0/0/0
2	FAD	D	601	-	-	0/28/50/50	0/6/6/6
3	SO4	D	602	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
4	NDP	D	604	-	-	0/17/37/77	0/3/3/5
3	SO4	D	605	-	-	0/0/0/0	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4X-N5	-3.67	1.28	1.33
4	A	604	NDP	O2B-C2B	-2.87	1.33	1.44
4	D	604	NDP	O2B-C2B	-2.59	1.34	1.44
4	B	603	NDP	O2B-C2B	-2.45	1.34	1.44
4	C	602	NDP	O2B-C2B	-2.39	1.35	1.44
4	B	603	NDP	O3D-C3D	-2.14	1.38	1.43
4	B	603	NDP	C7N-N7N	2.04	1.39	1.33
4	B	603	NDP	C6N-N1N	2.08	1.43	1.37
4	A	604	NDP	C7N-N7N	2.15	1.39	1.33
2	C	601	FAD	C4-N3	2.19	1.37	1.33
4	C	602	NDP	C2A-N1A	2.22	1.38	1.33
4	A	604	NDP	C2A-N1A	2.22	1.38	1.33
4	A	604	NDP	C4A-N3A	2.27	1.38	1.35
2	B	601	FAD	C4X-C10	2.27	1.45	1.41
4	D	604	NDP	C2A-N1A	2.39	1.38	1.33
4	B	603	NDP	C4A-N3A	2.43	1.39	1.35
2	D	601	FAD	C4X-C10	2.49	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C5X-N5	2.55	1.39	1.35
2	C	601	FAD	C4-C4X	2.60	1.46	1.41
2	C	601	FAD	C5X-N5	2.63	1.39	1.35
4	B	603	NDP	C2A-N1A	2.78	1.39	1.33
2	A	601	FAD	C9A-N10	2.84	1.42	1.38
2	D	601	FAD	C4-N3	2.86	1.38	1.33
4	A	604	NDP	C3D-C4D	2.89	1.60	1.53
2	B	601	FAD	C4-N3	2.92	1.38	1.33
2	D	601	FAD	C5X-N5	3.02	1.39	1.35
2	D	601	FAD	C4-C4X	3.06	1.47	1.41
2	A	601	FAD	C4-N3	3.32	1.39	1.33
4	B	603	NDP	PN-O5D	4.20	1.77	1.59
4	A	604	NDP	PN-O5D	5.09	1.80	1.59
4	C	602	NDP	PN-O5D	6.82	1.82	1.54
4	D	604	NDP	PN-O1N	7.53	1.76	1.50
4	A	604	NDP	P2B-O2B	13.69	1.83	1.59
4	D	604	NDP	P2B-O2B	15.34	1.86	1.59
4	B	603	NDP	P2B-O2B	16.29	1.88	1.59
4	C	602	NDP	P2B-O2B	17.28	1.89	1.59

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	C4X-C4-N3	-7.24	113.17	123.48
2	C	601	FAD	C4X-C4-N3	-6.93	113.62	123.48
2	B	601	FAD	C4X-C4-N3	-6.75	113.87	123.48
2	A	601	FAD	C4X-C4-N3	-6.70	113.95	123.48
2	B	601	FAD	C4X-C10-N10	-6.22	116.20	120.52
2	D	601	FAD	C4X-C10-N10	-5.52	116.69	120.52
2	C	601	FAD	C4X-C10-N10	-5.41	116.76	120.52
2	A	601	FAD	C4X-C10-N10	-4.89	117.12	120.52
4	C	602	NDP	C4B-O4B-C1B	-4.32	105.17	109.77
2	A	601	FAD	C4B-O4B-C1B	-4.30	105.19	109.77
4	A	604	NDP	O2B-P2B-O1X	-3.47	95.65	109.26
4	D	604	NDP	C4B-O4B-C1B	-3.35	106.20	109.77
2	A	601	FAD	C4-C4X-C10	-3.01	117.53	119.96
4	D	604	NDP	O5D-PN-O1N	-2.99	98.79	110.50
4	C	602	NDP	C3B-C2B-C1B	-2.87	97.14	102.75
4	D	604	NDP	C3B-C2B-C1B	-2.84	97.20	102.75
2	C	601	FAD	C4-C4X-C10	-2.78	117.71	119.96
4	C	602	NDP	O5D-PN-O1N	-2.71	99.89	110.50
2	B	601	FAD	C4-C4X-C10	-2.69	117.79	119.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C1'-N10-C10	-2.68	115.76	118.50
2	D	601	FAD	C4-C4X-C10	-2.59	117.87	119.96
4	C	602	NDP	O3X-P2B-O2B	-2.57	94.30	106.00
4	C	602	NDP	O2B-P2B-O1X	-2.54	99.31	109.26
4	D	604	NDP	C2A-N1A-C6A	-2.31	114.73	118.77
4	B	603	NDP	O3X-P2B-O2B	-2.25	95.76	106.00
4	D	604	NDP	C1B-N9A-C4A	-2.17	122.89	126.64
4	C	602	NDP	C5B-C4B-C3B	-2.11	107.23	115.29
4	D	604	NDP	O2N-PN-O1N	-2.11	102.23	110.50
4	A	604	NDP	C2A-N1A-C6A	-2.08	115.13	118.77
4	B	603	NDP	O2B-P2B-O1X	-2.08	101.12	109.26
4	D	604	NDP	O2X-P2B-O2B	-2.03	96.78	106.00
4	A	604	NDP	C3N-C2N-N1N	-2.00	120.17	123.08
4	B	603	NDP	C2A-N1A-C6A	-2.00	115.27	118.77
4	B	603	NDP	C4A-C5A-N7A	2.00	111.34	109.41
2	A	601	FAD	O4'-C4'-C5'	2.01	114.47	110.00
4	A	604	NDP	O4D-C1D-N1N	2.05	112.19	108.07
4	C	602	NDP	O4B-C4B-C3B	2.09	109.32	105.17
4	D	604	NDP	O4B-C4B-C3B	2.11	109.36	105.17
4	D	604	NDP	C4A-C5A-N7A	2.11	111.45	109.41
2	A	601	FAD	O2'-C2'-C1'	2.15	114.75	109.79
2	D	601	FAD	C4'-C3'-C2'	2.21	118.16	113.41
4	B	603	NDP	O4D-C1D-N1N	2.22	112.55	108.07
4	A	604	NDP	O4B-C4B-C3B	2.23	109.61	105.17
4	A	604	NDP	C4A-C5A-N7A	2.27	111.61	109.41
4	B	603	NDP	O3X-P2B-O2X	2.42	117.36	107.61
4	C	602	NDP	O3X-P2B-O2X	2.42	117.38	107.61
4	C	602	NDP	C4A-C5A-N7A	2.43	111.76	109.41
4	A	604	NDP	O3X-P2B-O2X	2.43	117.42	107.61
4	D	604	NDP	O3X-P2B-O2X	2.47	117.58	107.61
4	D	604	NDP	N3A-C2A-N1A	2.59	131.11	128.86
2	B	601	FAD	C1'-N10-C10	2.64	121.21	118.50
4	C	602	NDP	O2N-PN-O1N	2.76	121.30	110.50
2	D	601	FAD	C10-C4X-N5	3.09	124.14	120.59
2	C	601	FAD	C10-C4X-N5	3.17	124.23	120.59
2	B	601	FAD	C10-C4X-N5	3.54	124.67	120.59
2	B	601	FAD	O3'-C3'-C2'	3.58	117.69	108.82
2	A	601	FAD	C10-C4X-N5	3.58	124.72	120.59
4	D	604	NDP	O5D-PN-O2N	3.62	122.21	107.61
2	A	601	FAD	C1'-N10-C9A	5.02	122.94	118.35
2	B	601	FAD	C4-N3-C2	12.34	125.96	115.16
2	A	601	FAD	C4-N3-C2	12.46	126.06	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C4-N3-C2	12.76	126.32	115.16
2	D	601	FAD	C4-N3-C2	12.83	126.38	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	8	0
4	A	604	NDP	2	0
2	B	601	FAD	5	0
4	B	603	NDP	1	0
3	B	605	SO4	1	0
2	C	601	FAD	6	0
2	D	601	FAD	7	0
3	D	603	SO4	1	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	495/513 (96%)	0.17	2 (0%) 92 91	28, 44, 74, 101	0
1	B	492/513 (95%)	0.16	1 (0%) 94 95	28, 47, 78, 106	0
1	C	501/513 (97%)	0.30	7 (1%) 75 72	29, 55, 82, 102	0
1	D	499/513 (97%)	0.32	9 (1%) 69 65	27, 56, 91, 107	0
All	All	1987/2052 (96%)	0.24	19 (0%) 82 80	27, 50, 83, 107	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	VAL	3.8
1	D	236	PHE	3.6
1	D	204	TRP	3.3
1	D	242	VAL	3.1
1	D	37	VAL	3.1
1	C	11	LEU	3.0
1	C	12	VAL	3.0
1	D	36	ILE	2.9
1	D	12	VAL	2.6
1	D	504	PHE	2.5
1	A	504	PHE	2.5
1	C	283	LEU	2.2
1	D	443	TRP	2.2
1	A	14	GLY	2.1
1	C	36	ILE	2.1
1	B	265	LEU	2.1
1	C	203	ASN	2.1
1	C	315	TRP	2.1
1	C	92	ILE	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
3	SO4	C	606	5/5	0.95	0.30	1.87	76,78,80,81	5
3	SO4	D	605	5/5	0.97	0.25	0.71	59,66,73,74	5
4	NDP	D	604	31/48	0.90	0.23	0.65	42,68,87,95	31
4	NDP	B	603	48/48	0.97	0.21	0.63	35,48,60,68	0
2	FAD	B	601	53/53	0.98	0.20	0.09	23,36,47,50	0
2	FAD	A	601	53/53	0.98	0.20	-0.30	17,37,50,63	0
2	FAD	D	601	53/53	0.95	0.21	-0.36	40,60,74,91	0
2	FAD	C	601	53/53	0.96	0.20	-0.40	28,60,73,86	0
4	NDP	C	602	31/48	0.91	0.20	-0.52	38,58,69,72	31
4	NDP	A	604	48/48	0.97	0.18	-1.25	41,56,70,74	0
3	SO4	B	605	5/5	0.91	0.14	-1.47	76,80,81,82	5
3	SO4	C	605	5/5	0.93	0.16	-	69,73,79,86	5
3	SO4	D	603	5/5	0.94	0.18	-	69,73,76,78	5
3	SO4	C	603	5/5	0.93	0.17	-	58,63,71,80	5
3	SO4	D	602	5/5	0.94	0.14	-	64,64,69,71	5
3	SO4	C	604	5/5	0.95	0.25	-	65,77,83,86	5
3	SO4	B	604	5/5	0.95	0.17	-	68,71,72,74	5
3	SO4	B	606	5/5	0.97	0.19	-	71,72,74,76	0
3	SO4	A	605	5/5	0.95	0.16	-	67,75,79,82	0
3	SO4	A	602	5/5	0.95	0.17	-	51,61,72,74	5
3	SO4	B	602	5/5	0.93	0.14	-	62,74,81,87	5
3	SO4	A	603	5/5	0.94	0.14	-	78,80,86,90	5

6.5 Other polymers [i](#)

There are no such residues in this entry.