WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:10 pm GMT

PDB ID	:	4C74
Title	:	Phenylacetone monooxygenase: Reduced enzyme in complex with APADP
Authors	:	Martinoli, C.; Fraaije, M.W.; Mattevi, A.
Deposited on	:	2013-09-19
Resolution	:	1.97 Å(reported)

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	:	trunk28620
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)	:	recalc28949

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 1.97 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.
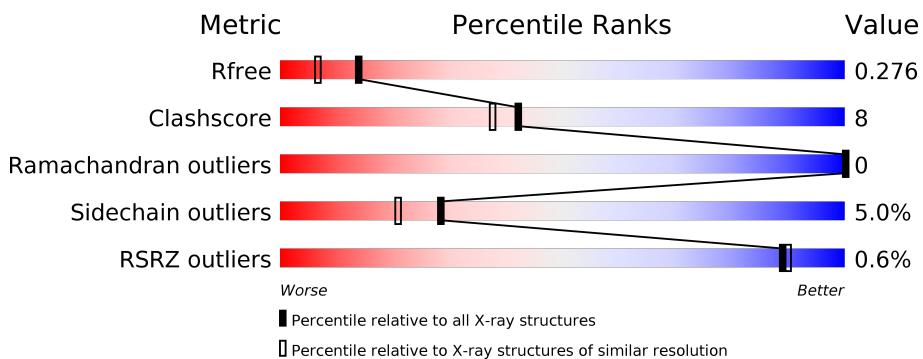
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	9293 (2.00-1.96)
Clashscore	112137	10621 (2.00-1.96)
Ramachandran outliers	110173	10502 (2.00-1.96)
Sidechain outliers	110143	10501 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	542	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4569 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 PHENYLACETONE MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	3	0
			4240	2706	729	795	10			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
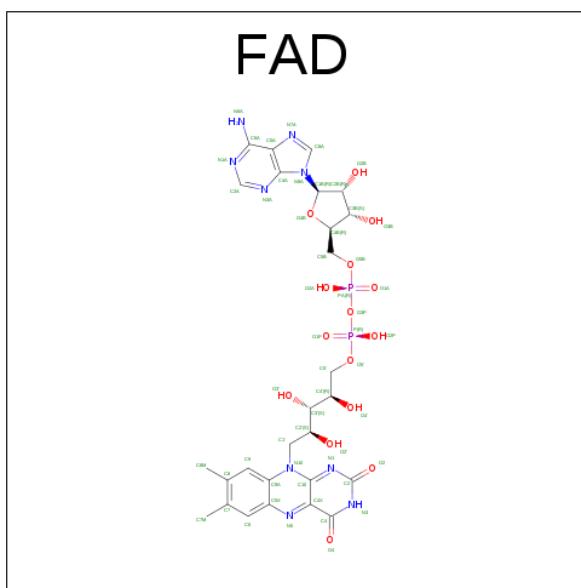
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-ACETYLPYRIDINE ADENINE DINUCLEOTIDE (three-letter code: N01) (formula: $C_{22}H_{26}N_6O_{17}P_3$).
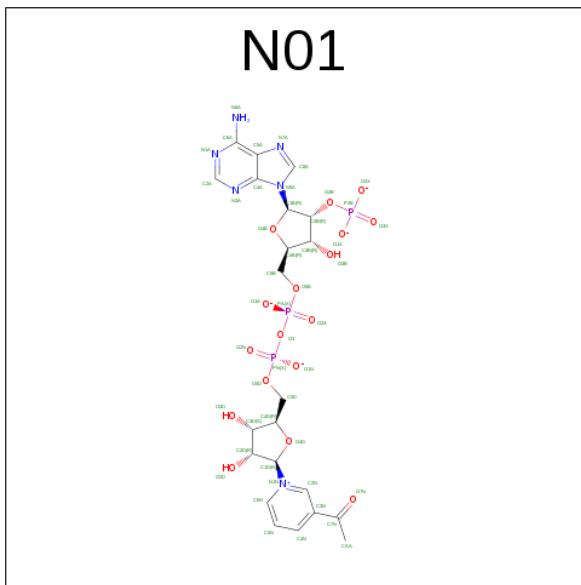
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	22	6	17	3		

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).
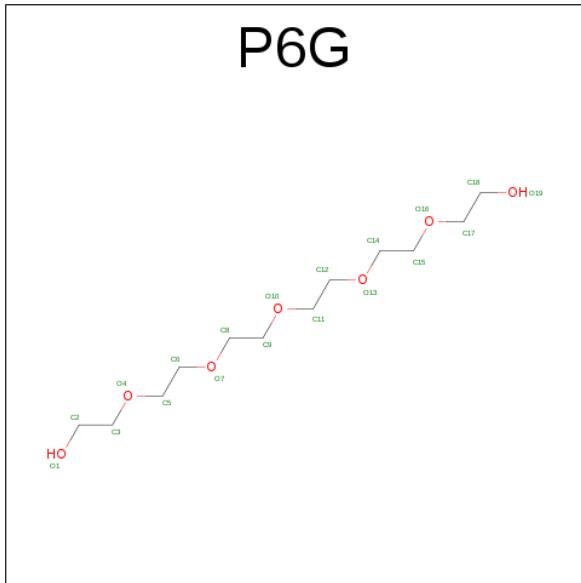
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total 218	O 218	0	0

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 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: PHENYLACETONE MONOOXYGENASE
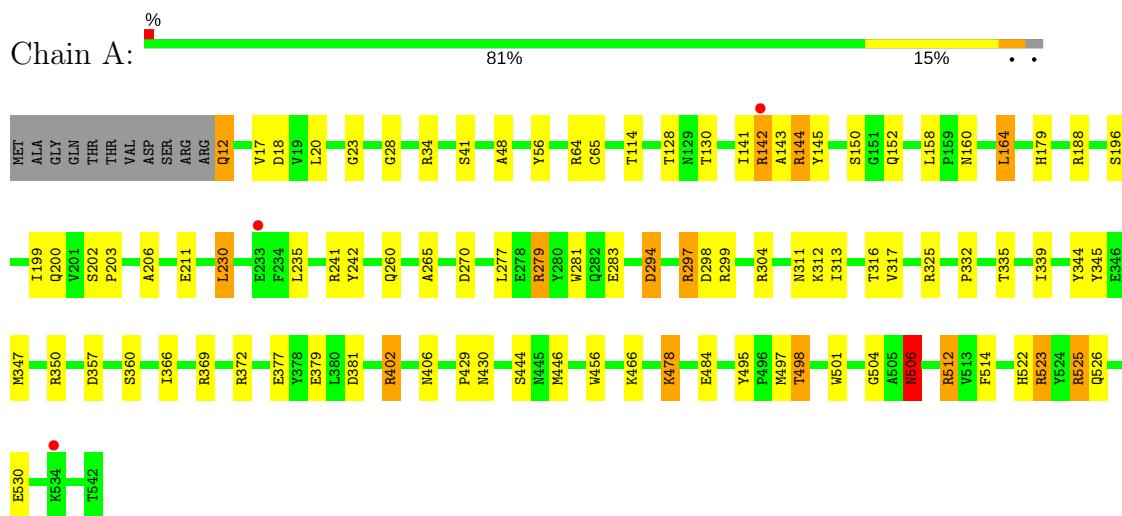
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	107.62Å 107.62Å 106.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.22 – 1.97 70.13 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.7 (70.22-1.97) 98.7 (70.13-1.97)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.235 , 0.278 0.234 , 0.276	Depositor DCC
R_{free} test set	2571 reflections (5.42%)	DCC
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4569	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: N01, FAD, P6G

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	1.02	4/4362 (0.1%)	1.07	20/5935 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	525	ARG	CZ-NH1	6.63	1.41	1.33
1	A	506	ASN	CB-CG	5.26	1.63	1.51
1	A	283	GLU	CD-OE1	5.24	1.31	1.25
1	A	456	TRP	CE3-CZ3	5.19	1.47	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	A	64	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	34	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	64	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	279	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	294	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	270	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	158	LEU	C-N-CD	7.01	143.13	128.40
1	A	144	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	402	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	A	230	LEU	CA-CB-CG	5.83	128.71	115.30
1	A	34	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	372	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	381	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	446	MET	CG-SD-CE	-5.46	91.46	100.20
1	A	525	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	523	ARG	NE-CZ-NH2	-5.25	117.67	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	ASN	N-CA-CB	-5.14	101.34	110.60
1	A	144	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	277	LEU	CB-CG-CD2	5.11	119.68	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4240	0	4096	63	0
2	A	53	0	31	2	0
3	A	48	0	26	1	0
4	A	10	0	13	6	1
5	A	218	0	0	17	0
All	All	4569	0	4166	67	1

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 8.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASN:HB3	5:A:2135:HOH:O	1.31	1.27
4:A:1543:P6G:H92	5:A:2218:HOH:O	1.36	1.26
1:A:530:GLU:HB3	5:A:2216:HOH:O	1.51	1.10
1:A:12:GLN:HB3	5:A:2012:HOH:O	1.59	1.00
1:A:506:ASN:OD1	1:A:506:ASN:N	2.04	0.90
1:A:402:ARG:HD2	1:A:406:ASN:HD21	1.41	0.84
1:A:325:ARG:HD2	1:A:357:ASP:HB2	1.60	0.82
1:A:523:ARG:HD3	5:A:2212:HOH:O	1.79	0.82
1:A:402:ARG:HD2	1:A:406:ASN:ND2	1.99	0.77
1:A:279:ARG:HB3	4:A:1543:P6G:H51	1.66	0.76
1:A:200:GLN:NE2	3:A:701:N01:HAAB	2.02	0.75
1:A:313:ILE:O	1:A:316:THR:HG22	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TRP:CD2	1:A:312[B]:LYS:HD3	2.23	0.73
1:A:335:THR:OG1	1:A:498:THR:HG21	1.89	0.73
1:A:369:ARG:HD3	1:A:379:GLU:OE2	1.92	0.70
1:A:325:ARG:HD3	5:A:2138:HOH:O	1.90	0.70
1:A:65[A]:CYS:SG	2:A:700:FAD:O4	2.49	0.70
1:A:311:ASN:CB	5:A:2135:HOH:O	2.05	0.69
1:A:281:TRP:CE2	1:A:312[B]:LYS:HD3	2.31	0.66
1:A:152:GLN:HE22	2:A:700:FAD:H5'2	1.60	0.66
1:A:512:ARG:HH11	1:A:512:ARG:HB3	1.60	0.66
1:A:332:PRO:HD2	1:A:498:THR:CG2	2.27	0.65
1:A:199:ILE:HD12	1:A:339:ILE:HD13	1.80	0.63
1:A:316:THR:HG23	1:A:317:VAL:HG23	1.80	0.63
1:A:260:GLN:HG2	5:A:2113:HOH:O	1.97	0.63
1:A:294:ASP:HA	1:A:297:ARG:HG3	1.82	0.61
1:A:144:ARG:HG2	1:A:145:TYR:CE2	2.36	0.61
1:A:12:GLN:N	5:A:2001:HOH:O	2.33	0.60
1:A:311:ASN:CG	5:A:2135:HOH:O	2.37	0.58
1:A:299:ARG:HH12	1:A:497:MET:HG3	1.68	0.57
1:A:332:PRO:HD2	1:A:498:THR:HG21	1.86	0.57
1:A:316:THR:CG2	1:A:345:TYR:HB3	2.35	0.57
1:A:206:ALA:O	1:A:350:ARG:NH2	2.37	0.57
1:A:501:TRP:HA	1:A:506:ASN:OD1	2.05	0.56
1:A:12:GLN:CB	5:A:2012:HOH:O	2.33	0.56
1:A:202:SER:HB2	1:A:203:PRO:HD3	1.86	0.55
1:A:316:THR:HG21	1:A:345:TYR:HB3	1.89	0.55
1:A:128:THR:HG21	1:A:142:ARG:HH22	1.73	0.54
1:A:332:PRO:HD2	1:A:498:THR:HG22	1.91	0.52
4:A:1543:P6G:C5	5:A:2119:HOH:O	2.56	0.52
1:A:23:GLY:O	1:A:28:GLY:HA3	2.10	0.51
1:A:523:ARG:HA	1:A:526:GLN:HE21	1.76	0.51
1:A:128:THR:O	1:A:130:THR:HG23	2.12	0.50
1:A:495:TYR:HB3	1:A:514:PHE:CE1	2.47	0.50
1:A:316:THR:CG2	1:A:317:VAL:HG23	2.43	0.49
1:A:241:ARG:HD2	5:A:2106:HOH:O	2.12	0.48
1:A:265:ALA:O	1:A:304:ARG:NH1	2.45	0.48
1:A:512:ARG:NH1	1:A:512:ARG:HB3	2.25	0.48
1:A:164:LEU:HD13	1:A:366:ILE:HG13	1.97	0.47
1:A:512:ARG:HD3	5:A:2205:HOH:O	2.13	0.47
1:A:12:GLN:HG3	1:A:114:THR:HG23	1.97	0.45
1:A:402:ARG:CD	1:A:406:ASN:ND2	2.75	0.45
1:A:429:PRO:O	1:A:430:ASN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1543:P6G:H52	5:A:2120:HOH:O	2.17	0.45
1:A:279:ARG:CZ	4:A:1543:P6G:H21	2.47	0.45
1:A:504:GLY:C	1:A:506:ASN:OD1	2.56	0.44
1:A:48:ALA:HB1	1:A:56:TYR:CE1	2.54	0.43
1:A:478:LYS:HE2	1:A:478:LYS:HB3	1.67	0.42
1:A:17:VAL:O	1:A:143:ALA:HA	2.19	0.42
1:A:18:ASP:HB2	1:A:41:SER:O	2.19	0.42
1:A:316:THR:HG23	1:A:345:TYR:HB3	2.02	0.42
1:A:344:TYR:O	1:A:347:MET:HB3	2.20	0.41
1:A:350:ARG:H	1:A:350:ARG:HG3	1.72	0.41
1:A:20:LEU:HD13	1:A:141:ILE:HG21	2.02	0.41
4:A:1543:P6G:C9	5:A:2218:HOH:O	2.20	0.41
1:A:525:ARG:NH1	5:A:2214:HOH:O	2.54	0.40
1:A:188:ARG:NH1	1:A:211:GLU:HG3	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1543:P6G:O10	4:A:1543:P6G:O10[6_555]	1.92	0.28

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	532/542 (98%)	516 (97%)	16 (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	444/453 (98%)	422 (95%)	22 (5%)	28	21

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	142	ARG
1	A	150	SER
1	A	160	ASN
1	A	164	LEU
1	A	179	HIS
1	A	196	SER
1	A	230	LEU
1	A	235	LEU
1	A	242	TYR
1	A	297	ARG
1	A	298	ASP
1	A	360	SER
1	A	377	GLU
1	A	444	SER
1	A	466	LYS
1	A	478	LYS
1	A	484	GLU
1	A	498	THR
1	A	506	ASN
1	A	512	ARG
1	A	522	HIS

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

Mol	Chain	Res	Type
1	A	58	ASN
1	A	129	ASN
1	A	152	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	160	ASN
1	A	170	ASN
1	A	204	GLN
1	A	315	ASN
1	A	406	ASN
1	A	526	GLN

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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	P6G	A	1543	-	9,9,18	0.78	0	8,8,17	0.93	0
2	FAD	A	700	-	51,58,58	1.32	5 (9%)	54,89,89	2.00	8 (14%)
3	N01	A	701	-	44,52,52	1.70	8 (18%)	51,80,80	2.05	13 (25%)

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
4	P6G	A	1543	-	-	0/7/7/16	0/0/0/0
2	FAD	A	700	-	-	0/28/50/50	0/6/6/6
3	N01	A	701	-	-	0/27/67/67	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	N01	CAA-C7N	-3.37	1.39	1.49
2	A	700	FAD	C4A-N3A	-2.38	1.32	1.35
2	A	700	FAD	C4-C4X	-2.12	1.37	1.41
3	A	701	N01	C4A-N3A	-2.06	1.32	1.35
2	A	700	FAD	C2A-N1A	2.26	1.38	1.33
2	A	700	FAD	C4X-N5	2.57	1.37	1.33
3	A	701	N01	C5N-C4N	3.11	1.44	1.38
3	A	701	N01	C2N-C3N	3.24	1.43	1.39
3	A	701	N01	C2D-C1D	3.31	1.58	1.53
3	A	701	N01	C4N-C3N	3.36	1.44	1.39
3	A	701	N01	P2B-O2B	4.37	1.67	1.59
2	A	700	FAD	C5X-N5	4.79	1.42	1.35
3	A	701	N01	O4D-C1D	4.91	1.48	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	N01	N3A-C2A-N1A	-8.59	121.37	128.86
2	A	700	FAD	N3A-C2A-N1A	-7.75	122.11	128.86
2	A	700	FAD	C4X-C4-N3	-4.05	117.72	123.48
3	A	701	N01	C1B-N9A-C4A	-3.94	119.83	126.64
3	A	701	N01	C3B-C2B-C1B	-3.50	95.91	102.75
3	A	701	N01	O5B-C5B-C4B	-2.83	98.95	109.00
3	A	701	N01	O2B-P2B-O3X	-2.80	98.28	109.26
3	A	701	N01	O3B-C3B-C4B	-2.73	103.12	111.09
3	A	701	N01	C4B-O4B-C1B	-2.52	107.08	109.77
3	A	701	N01	O2D-C2D-C1D	-2.28	104.50	111.61
2	A	700	FAD	C4-C4X-N5	-2.22	116.25	118.68
2	A	700	FAD	O2'-C2'-C1'	-2.04	105.06	109.79
2	A	700	FAD	C10-C4X-N5	2.38	123.33	120.59
3	A	701	N01	C3N-C2N-N1N	2.61	123.05	120.43
3	A	701	N01	C2A-N1A-C6A	2.72	123.53	118.77
3	A	701	N01	O2X-P2B-O1X	2.85	119.10	107.61
3	A	701	N01	N6A-C6A-N1A	3.05	124.81	118.77

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	FAD	C5X-C9A-N10	3.58	120.31	117.66
3	A	701	N01	CAA-C7N-C3N	3.92	127.33	119.27
2	A	700	FAD	C1'-N10-C9A	5.14	123.06	118.35
2	A	700	FAD	C4-N3-C2	6.42	120.77	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1543	P6G	6	1
2	A	700	FAD	2	0
3	A	701	N01	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	531/542 (97%)	-0.01	3 (0%)	89	90	19, 31, 51, 71	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ARG	2.1
1	A	534	LYS	2.1
1	A	233	GLU	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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	P6G	A	1543	10/19	0.82	0.15	1.19	40,44,46,53	0
2	FAD	A	700	53/53	0.98	0.10	0.02	18,22,29,34	0
3	N01	A	701	48/48	0.98	0.10	-0.58	18,24,31,41	0

6.5 Other polymers (i)

There are no such residues in this entry.