Full wwPDB X-ray Structure Validation Report

Mar 20, 2025 – 11:41 AM EDT

PDB ID	:	1PDA
Title	:	STRUCTURE OF PORPHOBILINOGEN DEAMINASE REVEALS A FLEXIBLE MULTIDOMAIN POLYMERASE WITH A SINGLE CATALYTIC SITE
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Deposited on	:	1992-11-17
Resolution	:	1.76 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

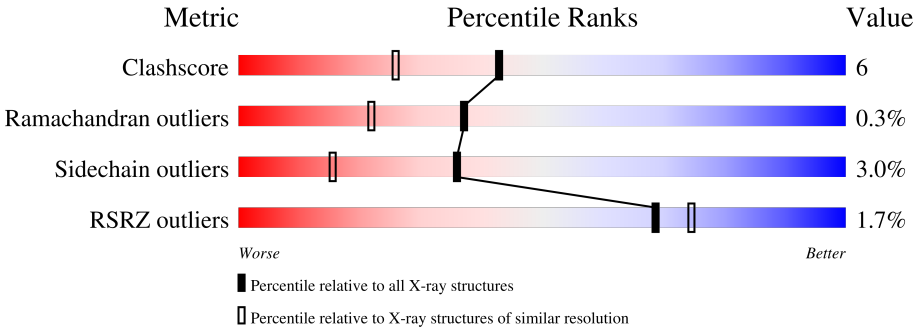
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 1.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	313	2% 68% 24% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	A	315	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2527 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.

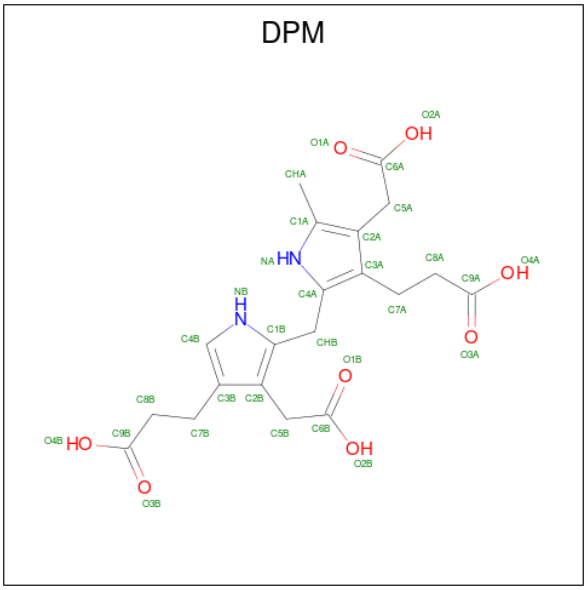
- Molecule 1 is a protein called PORPHOBILINOGEN DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2244	1395	412	428	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

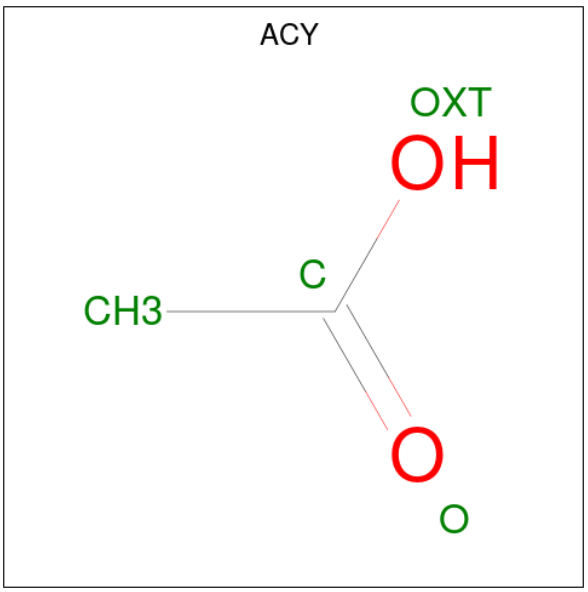
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	ALA	GLY	conflict	UNP P06983
A	261	GLY	ALA	conflict	UNP P06983

- Molecule 2 is 3-[5-{[3-(2-carboxyethyl)-4-(carboxymethyl)-5-methyl-1H-pyrrol-2-yl]methyl}-4-(carboxymethyl)-1H-pyrrol-3-yl]propanoic acid (three-letter code: DPM) (formula: $C_{20}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	20	2	8	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

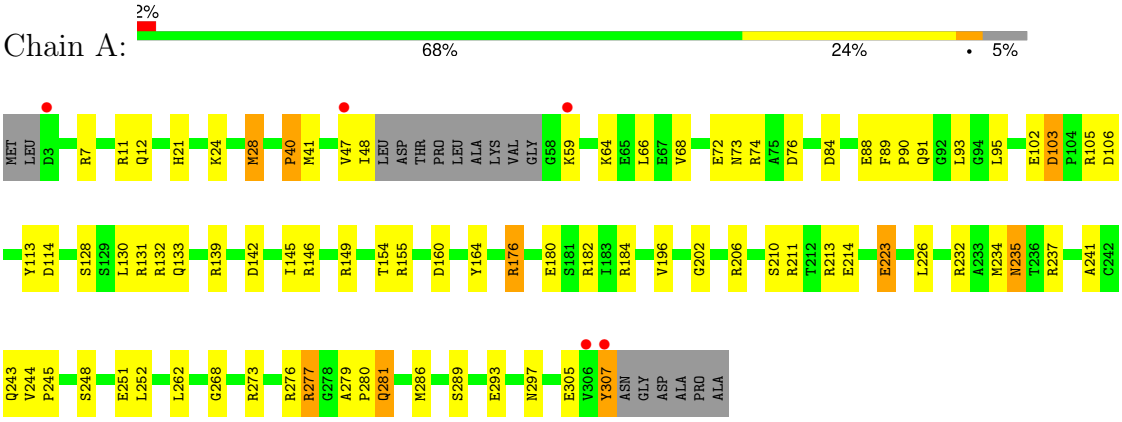
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	249	Total O 249 249	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: PORPHOBILINOGEN DEAMINASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.00Å 75.90Å 50.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.76 57.48 – 1.76	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.76) 98.9 (57.48-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 1.76Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.188 , (Not available) 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 77.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2527	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.09% 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: DPM, ACY

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	1.14	2/2273 (0.1%)	2.14	76/3079 (2.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	GLU	CD-OE1	-5.29	1.19	1.25
1	A	273	ARG	CZ-NH2	5.04	1.39	1.33

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	ARG	NE-CZ-NH2	-19.53	110.53	120.30
1	A	237	ARG	NE-CZ-NH1	16.50	128.55	120.30
1	A	11	ARG	NE-CZ-NH2	-15.95	112.33	120.30
1	A	182	ARG	NE-CZ-NH1	15.62	128.11	120.30
1	A	74	ARG	NE-CZ-NH1	14.97	127.78	120.30
1	A	277	ARG	NE-CZ-NH1	-13.58	113.51	120.30
1	A	88	GLU	OE1-CD-OE2	12.81	138.68	123.30
1	A	277	ARG	NE-CZ-NH2	12.40	126.50	120.30
1	A	131	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	A	164	TYR	CB-CG-CD1	11.50	127.90	121.00
1	A	84	ASP	CB-CG-OD1	11.36	128.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	176	ARG	NE-CZ-NH2	-11.27	114.66	120.30
1	A	155	ARG	NE-CZ-NH2	10.28	125.44	120.30
1	A	164	TYR	CG-CD1-CE1	9.82	129.15	121.30
1	A	206	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	A	132	ARG	NE-CZ-NH1	-9.59	115.51	120.30
1	A	276	ARG	NE-CZ-NH2	9.44	125.02	120.30
1	A	251	GLU	OE1-CD-OE2	9.14	134.27	123.30
1	A	28	MET	CG-SD-CE	-8.78	86.14	100.20
1	A	160	ASP	CB-CG-OD1	8.76	126.19	118.30
1	A	28	MET	CA-CB-CG	-8.67	98.56	113.30
1	A	164	TYR	CZ-CE2-CD2	8.34	127.30	119.80
1	A	84	ASP	CB-CG-OD2	-8.26	110.86	118.30
1	A	103	ASP	CB-CG-OD1	8.15	125.63	118.30
1	A	74	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	106	ASP	CB-CG-OD1	7.35	124.91	118.30
1	A	276	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	A	235	ASN	OD1-CG-ND2	7.17	138.40	121.90
1	A	307	TYR	CA-CB-CG	7.16	127.00	113.40
1	A	297	ASN	CB-CG-OD1	-6.96	107.69	121.60
1	A	232	ARG	CD-NE-CZ	6.90	133.26	123.60
1	A	105	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	A	59	LYS	N-CA-CB	6.72	122.69	110.60
1	A	88	GLU	CG-CD-OE1	-6.72	104.86	118.30
1	A	297	ASN	OD1-CG-ND2	6.71	137.34	121.90
1	A	114	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	223	GLU	OE1-CD-OE2	6.62	131.25	123.30
1	A	139	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	A	103	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	211	ARG	CD-NE-CZ	6.36	132.50	123.60
1	A	237	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
1	A	305	GLU	CA-CB-CG	6.29	127.23	113.40
1	A	91	GLN	N-CA-CB	-6.26	99.33	110.60
1	A	160	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	A	234	MET	CA-CB-CG	6.15	123.75	113.30
1	A	184	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	106	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	A	113	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	A	213	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	149	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	A	277	ARG	CD-NE-CZ	-6.04	115.14	123.60
1	A	132	ARG	CD-NE-CZ	5.89	131.85	123.60
1	A	155	ARG	NE-CZ-NH1	-5.83	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	88	GLU	O-C-N	5.79	131.97	122.70
1	A	139	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	A	235	ASN	CB-CG-OD1	-5.74	110.13	121.60
1	A	154	THR	CA-CB-OG1	-5.65	97.13	109.00
1	A	184	ARG	CG-CD-NE	-5.64	99.95	111.80
1	A	289	SER	N-CA-CB	5.62	118.93	110.50
1	A	7	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	176	ARG	NH1-CZ-NH2	5.60	125.56	119.40
1	A	276	ARG	CD-NE-CZ	-5.55	115.83	123.60
1	A	95	LEU	CB-CG-CD1	-5.54	101.58	111.00
1	A	11	ARG	NH1-CZ-NH2	5.51	125.46	119.40
1	A	202	GLY	O-C-N	5.43	131.39	122.70
1	A	76	ASP	O-C-N	5.43	131.38	122.70
1	A	262	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	89	PHE	CB-CG-CD1	5.36	124.56	120.80
1	A	286	MET	CA-CB-CG	5.36	122.42	113.30
1	A	293	GLU	O-C-N	-5.33	114.17	122.70
1	A	268	GLY	O-C-N	5.24	131.08	122.70
1	A	142	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	146	ARG	N-CA-CB	-5.03	101.55	110.60
1	A	130	LEU	O-C-N	5.02	130.74	122.70
1	A	131	ARG	NH1-CZ-NH2	-5.01	113.89	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	PRO	Mainchain

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	2244	0	2267	28	0
2	A	30	0	18	0	0
3	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	249	0	0	6	1
All	All	2527	0	2288	28	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 6.

All (28) 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:180:GLU:HB2	4:A:557:HOH:O	1.75	0.85
1:A:196:VAL:HG21	1:A:235:ASN:ND2	1.91	0.84
1:A:90:PRO:HG2	1:A:93:LEU:HD12	1.72	0.70
1:A:196:VAL:CG2	1:A:235:ASN:ND2	2.54	0.70
1:A:196:VAL:HG22	1:A:248:SER:HB3	1.78	0.65
1:A:244:VAL:HG11	1:A:307:TYR:CE1	2.34	0.63
1:A:133:GLN:NE2	4:A:561:HOH:O	2.40	0.55
1:A:196:VAL:HG21	1:A:235:ASN:CG	2.27	0.55
1:A:223:GLU:HG3	1:A:252:LEU:HD22	1.88	0.55
1:A:12:GLN:HG2	1:A:40:PRO:HB2	1.88	0.54
1:A:21:HIS:HD2	4:A:541:HOH:O	1.92	0.52
1:A:226:LEU:HD13	1:A:280:PRO:HB3	1.93	0.51
1:A:279:ALA:HB1	1:A:281:GLN:HE22	1.75	0.50
1:A:210:SER:O	1:A:214:GLU:HG3	2.13	0.49
1:A:223:GLU:HG3	1:A:252:LEU:CD2	2.42	0.49
1:A:64:LYS:HD3	1:A:64:LYS:HA	1.52	0.47
1:A:277:ARG:HD3	4:A:592:HOH:O	2.13	0.47
1:A:196:VAL:CG2	1:A:248:SER:HB3	2.46	0.45
1:A:277:ARG:HD3	1:A:277:ARG:HH11	1.32	0.45
1:A:281:GLN:H	1:A:281:GLN:CD	2.21	0.44
1:A:176:ARG:NH1	4:A:627:HOH:O	2.34	0.44
1:A:41:MET:SD	1:A:66:LEU:HD23	2.59	0.43
1:A:24:LYS:HE3	1:A:28:MET:CE	2.48	0.43
1:A:68:VAL:O	1:A:72:GLU:HG2	2.19	0.42
1:A:279:ALA:CB	1:A:281:GLN:HE22	2.32	0.42
1:A:281:GLN:NE2	4:A:586:HOH:O	2.52	0.42
1:A:102:GLU:HG3	1:A:103:ASP:N	2.35	0.41
1:A:133:GLN:HG3	1:A:145:ILE:HG21	2.03	0.41

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:413:HOH:O	4:A:506:HOH:O[3_546]	2.18	0.02

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	292/313 (93%)	288 (99%)	3 (1%)	1 (0%)	37 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	236/251 (94%)	229 (97%)	7 (3%)	36 15

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	47	VAL
1	A	48	ILE
1	A	73	ASN
1	A	128	SER

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Mol	Chain	Res	Type
1	A	243	GLN
1	A	281	GLN

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

Mol	Chain	Res	Type
1	A	19	GLN
1	A	133	GLN
1	A	235	ASN
1	A	243	GLN
1	A	281	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 oligosaccharides in this entry.

5.6 Ligand geometry

2 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	DPM	A	314	1	28,31,31	3.79	9 (32%)	31,43,43	2.64	12 (38%)
3	ACY	A	315	-	3,3,3	2.71	1 (33%)	3,3,3	2.77	2 (66%)

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	DPM	A	314	1	-	5/20/22/22	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	314	DPM	CHB-C1B	-14.09	1.40	1.51
2	A	314	DPM	CHB-C4A	-9.88	1.44	1.51
2	A	314	DPM	C4B-NB	5.62	1.44	1.36
3	A	315	ACY	CH3-C	4.20	1.65	1.49
2	A	314	DPM	C2B-C1B	3.88	1.46	1.39
2	A	314	DPM	C8B-C9B	3.34	1.58	1.50
2	A	314	DPM	C8A-C9A	3.27	1.58	1.50
2	A	314	DPM	C5B-C6B	2.90	1.57	1.51
2	A	314	DPM	C4B-C3B	2.19	1.43	1.37
2	A	314	DPM	O4B-C9B	-2.07	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	314	DPM	C4B-C3B-C2B	10.19	110.39	104.66
2	A	314	DPM	O4A-C9A-C8A	4.58	128.47	114.00
3	A	315	ACY	OXT-C-O	3.82	136.19	122.03
2	A	314	DPM	O2B-C6B-O1B	-3.64	113.96	123.33
2	A	314	DPM	C8B-C7B-C3B	-3.09	104.28	112.71
2	A	314	DPM	C7A-C8A-C9A	-3.04	105.63	113.83
2	A	314	DPM	O4B-C9B-C8B	3.03	123.58	114.00
2	A	314	DPM	O4A-C9A-O3A	-2.93	115.80	123.33
3	A	315	ACY	O-C-CH3	-2.86	110.82	122.53
2	A	314	DPM	O3B-C9B-C8B	-2.69	114.57	123.09
2	A	314	DPM	O3A-C9A-C8A	-2.51	115.13	123.09
2	A	314	DPM	CHB-C1B-C2B	-2.15	122.67	130.17
2	A	314	DPM	CHB-C4A-C3A	-2.07	122.94	130.17
2	A	314	DPM	O2B-C6B-C5B	2.07	121.86	113.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

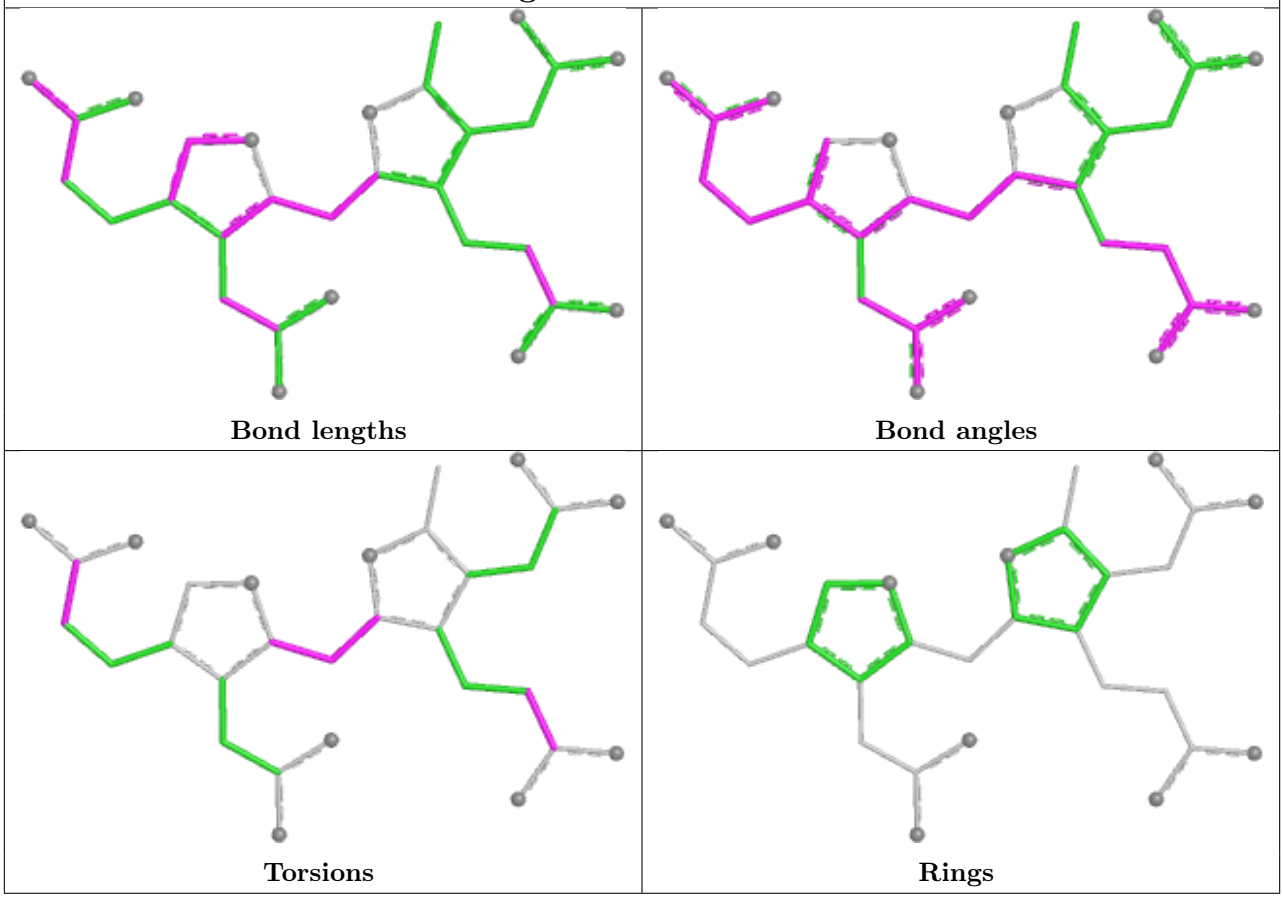
Mol	Chain	Res	Type	Atoms
2	A	314	DPM	C3A-C4A-CHB-C1B
2	A	314	DPM	C2B-C1B-CHB-C4A
2	A	314	DPM	C7B-C8B-C9B-O4B
2	A	314	DPM	C7B-C8B-C9B-O3B
2	A	314	DPM	C7A-C8A-C9A-O4A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DPM A 314



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, 95^{th} 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	296/313 (94%)	-0.45	5 (1%) 69 74	12, 21, 41, 72	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	VAL	3.0
1	A	306	VAL	2.3
1	A	59	LYS	2.3
1	A	307	TYR	2.1
1	A	3	ASP	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 monosaccharides in this entry.

6.4 Ligands

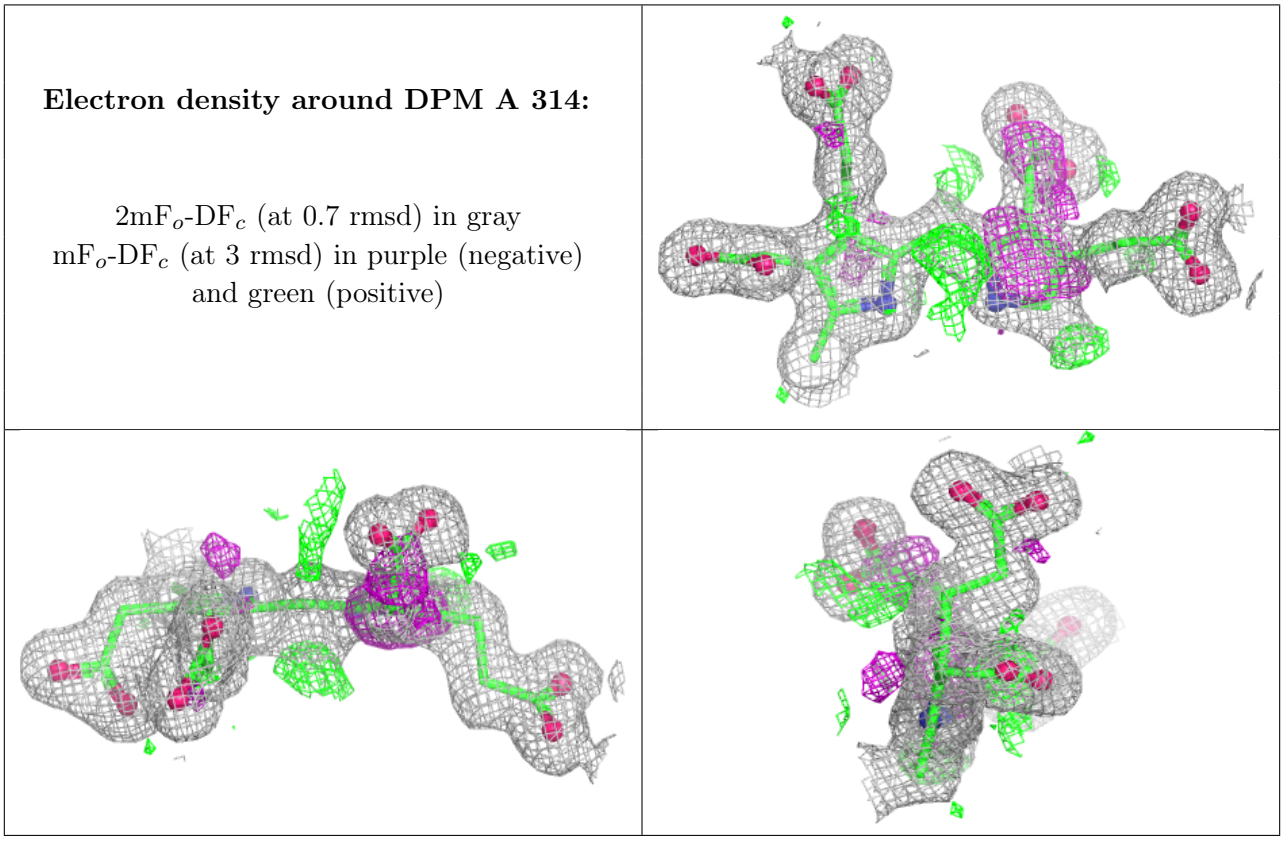
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACY	A	315	4/4	0.90	0.14	25,39,47,57	0
2	DPM	A	314	30/30	0.92	0.07	15,18,25,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DPM A 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.