



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:50 AM UTC

PDB ID : 3ECR / pdb_00003ecr
Title : Structure of human porphobilinogen deaminase
Authors : Song, G.; Li, Y.; Cheng, C.; Zhao, Y.; Gao, A.; Zhang, R.; Joachimiak, A.; Shaw, N.; Liu, Z.J.
Deposited on : 2008-09-01
Resolution : 2.18 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

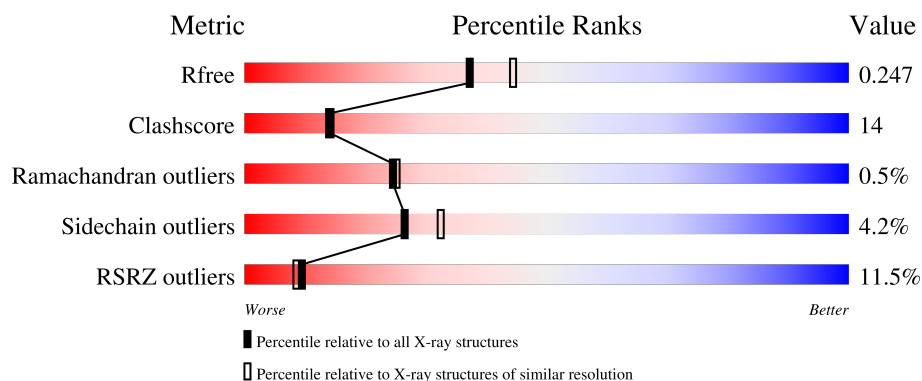
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. 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	364	10% 66% 20% • 13%
1	B	364	10% 68% 15% •• 15%

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
2	DPM	A	365	-	X	-	-
2	DPM	B	365	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4970 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.

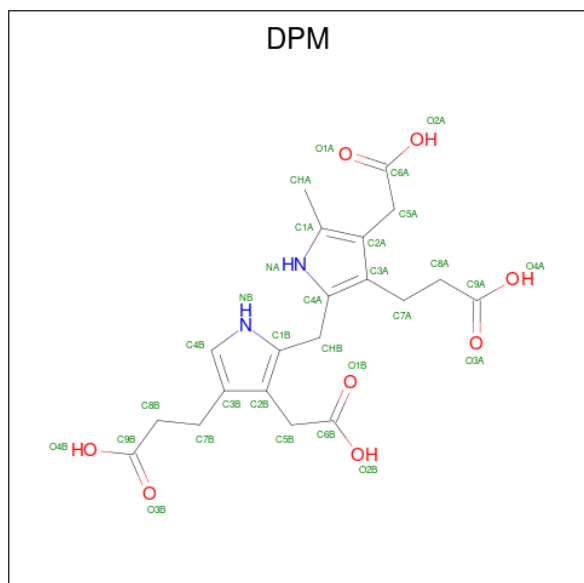
- Molecule 1 is a protein called Porphobilinogen deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2420	1521	445	445	9			
1	B	310	Total	C	N	O	S	0	0	0
			2353	1487	425	432	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P08397
A	2	ASN	-	expression tag	UNP P08397
A	3	ALA	-	expression tag	UNP P08397
B	1	SER	-	expression tag	UNP P08397
B	2	ASN	-	expression tag	UNP P08397
B	3	ALA	-	expression tag	UNP P08397

- 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 (CCD ID: DPM) (formula: C₂₀H₂₄N₂O₈).



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

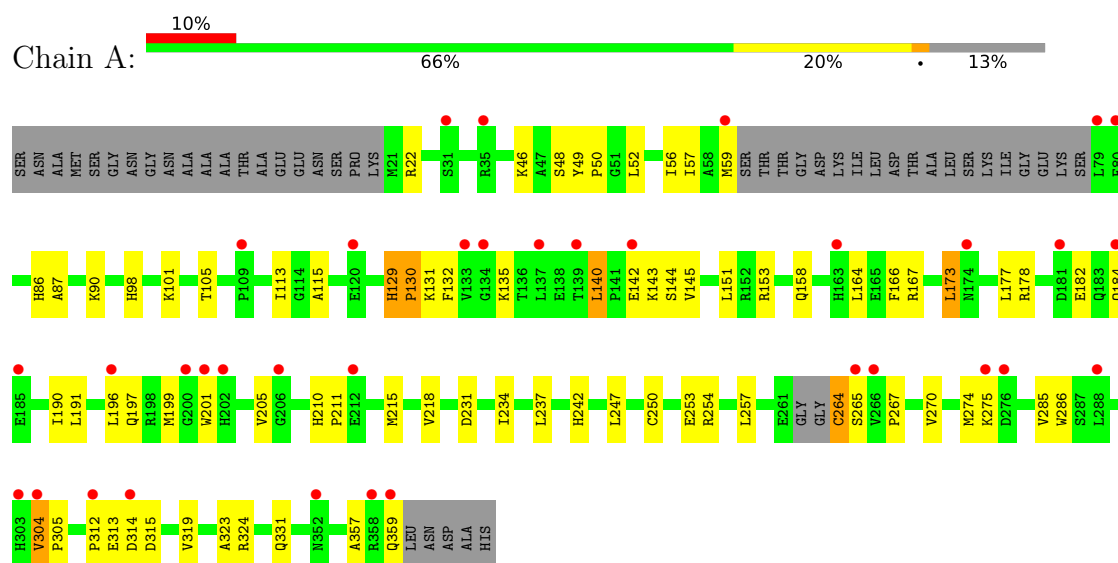
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	60	Total	O	0	0
			60	60		

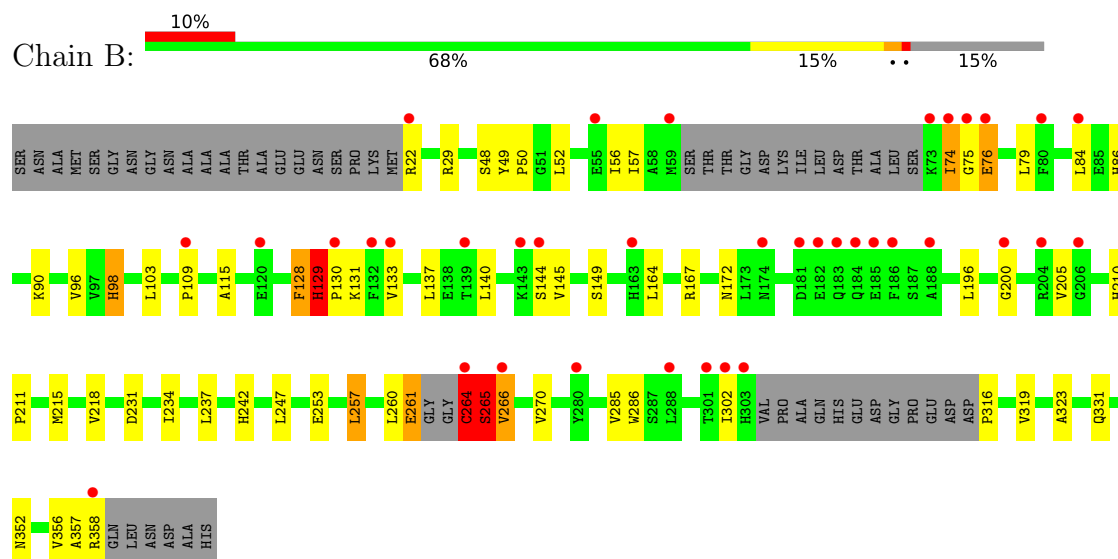
3 Residue-property plots [i](#)

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



• Molecule 1: Porphobilinogen deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.61Å 81.06Å 109.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.28 – 2.18 38.28 – 2.18	Depositor EDS
% Data completeness (in resolution range)	87.6 (38.28-2.18) 87.5 (38.28-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.232 , 0.271 (Not available) , 0.247	Depositor DCC
R_{free} test set	1500 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.928	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4970	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3857e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DPM

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	0.68	2/2460 (0.1%)	0.94	6/3335 (0.2%)
1	B	0.71	1/2388 (0.0%)	0.99	13/3235 (0.4%)
All	All	0.69	3/4848 (0.1%)	0.96	19/6570 (0.3%)

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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	SER	N-CA	-5.49	1.39	1.46
1	A	98	HIS	C-O	-5.21	1.17	1.23
1	B	98	HIS	C-O	-5.21	1.17	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	HIS	CA-C-N	7.72	129.49	119.84
1	A	129	HIS	C-N-CA	7.72	129.49	119.84
1	B	74	ILE	CB-CA-C	-6.94	101.70	111.21
1	A	264	CYS	CA-C-N	6.92	133.47	123.17
1	A	264	CYS	C-N-CA	6.92	133.47	123.17
1	B	264	CYS	CB-CA-C	6.81	123.05	110.10
1	B	128	PHE	CA-C-N	-6.74	110.29	120.60
1	B	128	PHE	C-N-CA	-6.74	110.29	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	PRO	N-CA-CB	6.66	110.32	103.00
1	B	264	CYS	N-CA-CB	-6.29	99.81	110.50
1	B	357	ALA	N-CA-C	-5.96	101.46	110.70
1	B	302	ILE	O-C-N	5.64	129.03	122.99
1	A	22	ARG	CA-C-N	-5.52	115.84	122.90
1	A	22	ARG	C-N-CA	-5.52	115.84	122.90
1	B	22	ARG	CA-C-N	5.42	128.44	120.91
1	B	22	ARG	C-N-CA	5.42	128.44	120.91
1	B	74	ILE	N-CA-C	-5.42	100.64	108.87
1	B	129	HIS	N-CA-C	-5.22	102.59	109.84
1	B	265	SER	N-CA-C	5.19	121.85	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	264	CYS	Mainchain,Peptide

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	2420	0	2433	78	0
1	B	2353	0	2384	71	0
2	A	30	0	21	2	0
2	B	30	0	22	1	0
3	A	77	0	0	1	0
3	B	60	0	0	2	0
All	All	4970	0	4860	138	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 14.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PRO:O	1:B:133:VAL:CG2	1.82	1.24
1:B:264:CYS:N	1:B:265:SER:HB2	1.59	1.18
1:A:105:THR:HA	1:A:254:ARG:HH21	1.16	1.11
1:B:130:PRO:O	1:B:133:VAL:HG23	0.93	1.09
1:B:130:PRO:C	1:B:133:VAL:HG23	1.78	1.07
1:B:261:GLU:OE1	1:B:261:GLU:HA	1.56	1.04
1:B:75:GLY:O	1:B:76:GLU:HB3	1.60	1.01
1:B:323:ALA:HB3	1:B:331:GLN:HE22	1.24	1.00
1:A:323:ALA:HB3	1:A:331:GLN:HE22	1.24	0.99
1:A:247:LEU:HD21	1:A:331:GLN:HE21	1.30	0.94
1:B:129:HIS:ND1	1:B:130:PRO:HD2	1.82	0.94
1:B:247:LEU:HD21	1:B:331:GLN:HE21	1.34	0.90
1:B:74:ILE:HG22	1:B:74:ILE:O	1.70	0.90
1:A:59:MET:HE1	1:A:87:ALA:CB	2.04	0.87
1:B:84:LEU:HD13	1:B:96:VAL:HG11	1.56	0.87
1:A:105:THR:HA	1:A:254:ARG:NH2	1.92	0.85
1:B:129:HIS:ND1	1:B:130:PRO:CD	2.39	0.84
1:B:261:GLU:OE1	1:B:261:GLU:CA	2.29	0.79
1:B:129:HIS:CE1	1:B:130:PRO:HD2	2.19	0.78
1:A:314:ASP:H	1:A:324:ARG:HH21	1.32	0.77
1:B:74:ILE:O	1:B:74:ILE:CG2	2.29	0.76
1:A:142:GLU:O	1:A:143:LYS:HG2	1.85	0.75
1:B:323:ALA:HB3	1:B:331:GLN:NE2	2.00	0.74
1:A:247:LEU:HD21	1:A:331:GLN:NE2	2.02	0.73
1:A:323:ALA:CB	1:A:331:GLN:HE22	2.00	0.73
1:B:129:HIS:ND1	1:B:130:PRO:N	2.36	0.73
1:A:86:HIS:NE2	1:A:90:LYS:HE3	2.04	0.72
1:A:59:MET:HE1	1:A:87:ALA:HB2	1.71	0.72
1:A:323:ALA:HB3	1:A:331:GLN:NE2	2.02	0.72
1:B:247:LEU:HD21	1:B:331:GLN:NE2	2.07	0.70
1:A:314:ASP:H	1:A:324:ARG:NH2	1.91	0.68
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.29	0.67
1:B:323:ALA:CB	1:B:331:GLN:HE22	2.02	0.66
1:A:59:MET:CE	1:A:87:ALA:CB	2.74	0.66
1:A:132:PHE:O	1:A:135:LYS:HB2	1.95	0.66
1:B:76:GLU:O	1:B:76:GLU:HG3	1.94	0.66
1:B:86:HIS:NE2	1:B:90:LYS:HE3	2.10	0.66
1:A:59:MET:HE1	1:A:87:ALA:HB3	1.77	0.65
1:B:29:ARG:NH1	1:B:76:GLU:HB2	2.12	0.64
1:A:49:TYR:HB3	1:A:52:LEU:HD13	1.80	0.63
1:A:86:HIS:O	1:A:86:HIS:HD2	1.82	0.63
1:B:84:LEU:HD13	1:B:96:VAL:CG1	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:CE	1:A:87:ALA:HB2	2.29	0.62
1:A:197:GLN:CD	1:B:86:HIS:CE1	2.78	0.61
1:B:86:HIS:HD2	1:B:86:HIS:O	1.83	0.61
1:A:197:GLN:NE2	1:B:86:HIS:HD1	1.99	0.59
1:B:86:HIS:CD2	1:B:86:HIS:C	2.80	0.59
1:A:173:LEU:HD21	1:A:191:LEU:HD13	1.85	0.59
1:B:49:TYR:HB3	1:B:52:LEU:HD13	1.83	0.58
1:A:197:GLN:NE2	1:B:86:HIS:CE1	2.72	0.58
1:B:57:ILE:HD12	1:B:57:ILE:N	2.19	0.57
1:A:275:LYS:HE2	1:B:109:PRO:HA	1.87	0.57
1:A:86:HIS:CD2	1:A:86:HIS:C	2.82	0.57
1:A:197:GLN:CG	1:B:86:HIS:HE1	2.19	0.56
1:A:197:GLN:NE2	1:B:86:HIS:ND1	2.54	0.56
1:A:274:MET:HE2	3:A:384:HOH:O	2.04	0.56
1:A:313:GLU:O	1:A:314:ASP:CG	2.49	0.56
1:A:178:ARG:O	1:A:182:GLU:HB2	2.06	0.56
1:A:144:SER:HB2	1:A:164:LEU:HD22	1.88	0.55
1:B:48:SER:C	1:B:50:PRO:HD3	2.31	0.55
1:A:197:GLN:CG	1:B:86:HIS:CE1	2.90	0.55
1:A:57:ILE:N	1:A:57:ILE:HD12	2.22	0.54
1:A:215:MET:HE3	1:A:286:TRP:HH2	1.70	0.54
1:A:105:THR:CA	1:A:254:ARG:HH21	2.05	0.54
1:B:260:LEU:O	1:B:261:GLU:HB2	2.08	0.54
1:A:177:LEU:HD13	1:A:201:TRP:CE3	2.43	0.54
1:A:101:LYS:HE3	2:A:365:DPM:C4A	2.38	0.53
1:A:275:LYS:HE2	1:B:109:PRO:CA	2.38	0.53
1:A:173:LEU:CD2	1:A:191:LEU:HD13	2.38	0.53
1:A:313:GLU:HA	1:A:324:ARG:NE	2.23	0.53
1:B:130:PRO:CA	1:B:133:VAL:HG23	2.38	0.53
1:B:149:SER:HB2	2:B:365:DPM:O3A	2.09	0.53
1:B:356:VAL:C	1:B:358:ARG:H	2.17	0.52
1:A:199:MET:HB3	1:A:201:TRP:CD1	2.44	0.52
1:A:48:SER:C	1:A:50:PRO:HD3	2.35	0.52
1:A:135:LYS:HD3	1:A:140:LEU:HD12	1.91	0.52
1:B:129:HIS:ND1	1:B:129:HIS:C	2.68	0.52
1:A:145:VAL:HG11	1:A:167:ARG:HD3	1.91	0.51
1:A:145:VAL:CG1	1:A:167:ARG:HD3	2.41	0.51
1:A:129:HIS:ND1	1:A:130:PRO:HD2	2.26	0.50
1:B:128:PHE:O	1:B:129:HIS:C	2.47	0.50
1:B:356:VAL:HG12	1:B:356:VAL:O	2.12	0.50
1:A:113:ILE:HD11	1:A:254:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:CYS:O	1:A:254:ARG:HG3	2.11	0.50
1:B:98:HIS:CD2	1:B:103:LEU:HD21	2.48	0.49
1:B:144:SER:HB2	1:B:164:LEU:HD22	1.94	0.49
1:B:210:HIS:HB3	1:B:211:PRO:HD2	1.95	0.49
1:B:145:VAL:CG1	1:B:167:ARG:HD3	2.42	0.49
1:A:115:ALA:HA	1:A:242:HIS:CE1	2.47	0.49
1:A:142:GLU:O	1:A:143:LYS:CG	2.58	0.49
1:A:153:ARG:HD3	1:A:190:ILE:CG2	2.43	0.48
1:A:129:HIS:C	1:A:131:LYS:H	2.19	0.48
1:A:86:HIS:O	1:A:86:HIS:CD2	2.64	0.48
1:A:210:HIS:HB3	1:A:211:PRO:HD2	1.95	0.48
1:A:113:ILE:CD1	1:A:254:ARG:HH12	2.26	0.47
1:B:145:VAL:HG11	1:B:167:ARG:HD3	1.95	0.47
1:B:215:MET:HE3	1:B:286:TRP:HH2	1.78	0.47
1:A:142:GLU:C	1:A:143:LYS:HG2	2.39	0.47
1:A:231:ASP:CG	1:A:234:ILE:HG12	2.40	0.47
1:B:86:HIS:O	1:B:86:HIS:CD2	2.66	0.46
1:B:172:ASN:HB2	3:B:424:HOH:O	2.14	0.46
1:B:131:LYS:C	1:B:133:VAL:H	2.24	0.46
1:A:113:ILE:CD1	1:A:254:ARG:NH1	2.79	0.46
1:B:260:LEU:O	1:B:261:GLU:CB	2.63	0.46
1:B:265:SER:HB3	1:B:266:VAL:HG22	1.96	0.46
1:A:267:PRO:HG2	1:A:357:ALA:HB1	1.98	0.46
1:B:218:VAL:HG21	1:B:257:LEU:HB2	1.98	0.46
1:A:199:MET:O	1:A:201:TRP:CD1	2.68	0.46
1:B:56:ILE:C	1:B:57:ILE:HD12	2.42	0.45
1:B:200:GLY:HA2	3:B:366:HOH:O	2.15	0.45
1:B:352:ASN:O	1:B:356:VAL:HG23	2.17	0.45
1:A:158:GLN:HG3	1:A:166:PHE:CD1	2.51	0.45
1:A:197:GLN:CD	1:B:86:HIS:ND1	2.75	0.45
1:B:115:ALA:HA	1:B:242:HIS:CE1	2.52	0.45
1:B:129:HIS:CE1	1:B:131:LYS:H	2.35	0.45
1:B:356:VAL:C	1:B:358:ARG:N	2.74	0.45
1:A:132:PHE:HD1	1:A:135:LYS:HD2	1.83	0.44
1:A:215:MET:HE3	1:A:286:TRP:CH2	2.50	0.44
1:A:101:LYS:HE3	2:A:365:DPM:NA	2.33	0.43
1:A:196:LEU:HD13	1:A:205:VAL:HG22	1.99	0.43
1:B:196:LEU:HD13	1:B:205:VAL:HG22	2.00	0.43
1:B:253:GLU:HG2	1:B:270:VAL:HG21	2.00	0.43
1:A:304:VAL:HA	1:A:305:PRO:HD3	1.90	0.43
1:A:218:VAL:HG21	1:A:257:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASP:CG	1:B:234:ILE:HG12	2.44	0.43
1:A:314:ASP:C	1:A:314:ASP:OD2	2.62	0.42
1:A:197:GLN:HG3	1:B:86:HIS:HE1	1.83	0.42
1:B:215:MET:HE3	1:B:286:TRP:CH2	2.54	0.42
1:A:312:PRO:HB2	1:A:315:ASP:OD2	2.20	0.42
1:B:264:CYS:CA	1:B:265:SER:HB2	2.38	0.41
1:B:57:ILE:N	1:B:57:ILE:CD1	2.83	0.41
1:A:129:HIS:HA	1:A:130:PRO:HD3	1.87	0.41
1:A:205:VAL:O	1:B:79:LEU:HD21	2.19	0.41
1:B:356:VAL:O	1:B:356:VAL:CG1	2.68	0.41
1:A:151:LEU:HD11	1:A:359:GLN:CB	2.50	0.41
1:A:254:ARG:HE	1:A:254:ARG:HB3	1.66	0.40
1:A:253:GLU:HG2	1:A:270:VAL:HG21	2.03	0.40
1:A:56:ILE:C	1:A:57:ILE:HD12	2.46	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	312/364 (86%)	303 (97%)	8 (3%)	1 (0%)	36	39
1	B	302/364 (83%)	289 (96%)	11 (4%)	2 (1%)	18	17
All	All	614/728 (84%)	592 (96%)	19 (3%)	3 (0%)	24	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	GLU
1	B	265	SER
1	A	130	PRO

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	244/301 (81%)	235 (96%)	9 (4%)	30	38
1	B	206/301 (68%)	196 (95%)	10 (5%)	22	26
All	All	450/602 (75%)	431 (96%)	19 (4%)	26	32

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	140	LEU
1	A	173	LEU
1	A	184	GLN
1	A	237	LEU
1	A	264	CYS
1	A	285	VAL
1	A	304	VAL
1	A	319	VAL
1	B	129	HIS
1	B	137	LEU
1	B	140	LEU
1	B	237	LEU
1	B	257	LEU
1	B	261	GLU
1	B	265	SER
1	B	266	VAL
1	B	285	VAL
1	B	319	VAL

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

Mol	Chain	Res	Type
1	A	86	HIS
1	A	91	ASN
1	A	184	GLN

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	202	HIS
1	A	295	GLN
1	A	331	GLN
1	B	271	HIS
1	B	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	365	-	31,31,31	4.15	15 (48%)	39,43,43	2.77	21 (53%)
2	DPM	A	365	-	31,31,31	4.28	16 (51%)	39,43,43	2.50	19 (48%)

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	B	365	-	-	7/22/22/22	0/2/2/2
2	DPM	A	365	-	-	7/22/22/22	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	365	DPM	C4B-C3B	10.37	1.52	1.38
2	A	365	DPM	C1B-NB	10.30	1.51	1.37
2	A	365	DPM	C4B-C3B	9.77	1.51	1.38
2	B	365	DPM	C1B-NB	9.72	1.50	1.37
2	A	365	DPM	O4B-C9B	-7.53	1.05	1.30
2	A	365	DPM	C1B-C2B	7.11	1.57	1.39
2	B	365	DPM	C1B-C2B	7.08	1.57	1.39
2	B	365	DPM	C4B-NB	6.65	1.49	1.36
2	A	365	DPM	C4B-NB	6.32	1.48	1.36
2	A	365	DPM	O3B-C9B	6.11	1.42	1.22
2	A	365	DPM	O3A-C9A	5.98	1.41	1.22
2	B	365	DPM	O3B-C9B	5.84	1.41	1.22
2	B	365	DPM	O3A-C9A	5.68	1.40	1.22
2	B	365	DPM	O1A-C6A	5.37	1.39	1.22
2	B	365	DPM	O1B-C6B	5.18	1.39	1.22
2	A	365	DPM	O1B-C6B	4.96	1.38	1.22
2	B	365	DPM	C4A-C3A	4.89	1.51	1.39
2	A	365	DPM	O1A-C6A	4.79	1.37	1.22
2	A	365	DPM	C4A-C3A	4.77	1.51	1.39
2	B	365	DPM	C3B-C2B	4.02	1.54	1.42
2	B	365	DPM	C1A-NA	3.65	1.47	1.37
2	A	365	DPM	C3B-C2B	3.49	1.52	1.42
2	A	365	DPM	O4A-C9A	3.26	1.41	1.30
2	B	365	DPM	O4A-C9A	3.14	1.41	1.30
2	B	365	DPM	O2A-C6A	3.14	1.41	1.30
2	A	365	DPM	O2B-C6B	3.03	1.40	1.30
2	B	365	DPM	O2B-C6B	2.94	1.40	1.30
2	B	365	DPM	O4B-C9B	2.74	1.39	1.30
2	A	365	DPM	O2A-C6A	2.63	1.39	1.30
2	A	365	DPM	C1A-NA	2.52	1.44	1.37
2	A	365	DPM	CHA-C1A	2.15	1.53	1.49

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	365	DPM	CHA-C1A-C2A	-6.03	121.02	131.20
2	B	365	DPM	O2B-C6B-O1B	-5.28	109.76	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	365	DPM	O3B-C9B-C8B	-5.13	106.83	123.09
2	A	365	DPM	O4A-C9A-O3A	-5.01	110.45	123.33
2	B	365	DPM	C5B-C2B-C1B	-4.70	121.73	126.54
2	B	365	DPM	C7B-C3B-C4B	-4.43	118.31	127.16
2	A	365	DPM	O2A-C6A-O1A	-4.28	112.33	123.33
2	B	365	DPM	CHB-C4A-C3A	-4.24	121.97	130.07
2	A	365	DPM	C5B-C2B-C1B	-4.22	122.22	126.54
2	B	365	DPM	O4B-C9B-O3B	-4.15	112.65	123.33
2	B	365	DPM	CHB-C4A-NA	3.97	130.11	122.04
2	B	365	DPM	C1B-C2B-C3B	-3.91	101.88	107.52
2	A	365	DPM	O2B-C6B-O1B	-3.83	113.48	123.33
2	B	365	DPM	C4B-C3B-C2B	-3.74	102.02	107.04
2	B	365	DPM	CHA-C1A-NA	3.72	128.93	121.36
2	A	365	DPM	O3A-C9A-C8A	-3.60	111.67	123.09
2	B	365	DPM	O1B-C6B-C5B	-3.54	112.03	122.11
2	A	365	DPM	C1A-C2A-C3A	3.46	109.11	107.61
2	B	365	DPM	O2A-C6A-O1A	-3.43	114.50	123.33
2	A	365	DPM	C7B-C3B-C4B	-3.40	120.36	127.16
2	A	365	DPM	CHA-C1A-C2A	-3.12	125.94	131.20
2	A	365	DPM	C8B-C7B-C3B	3.11	119.25	112.94
2	A	365	DPM	C7B-C8B-C9B	3.09	121.85	113.67
2	B	365	DPM	C7B-C8B-C9B	3.08	121.82	113.67
2	A	365	DPM	O1B-C6B-C5B	-3.03	113.47	122.11
2	A	365	DPM	C2B-C1B-NB	-2.92	106.46	109.84
2	A	365	DPM	C5B-C2B-C3B	-2.91	116.48	124.65
2	B	365	DPM	O4A-C9A-O3A	-2.77	116.21	123.33
2	A	365	DPM	O4B-C9B-O3B	2.76	130.43	123.33
2	B	365	DPM	C2A-C1A-NA	2.71	110.05	108.13
2	B	365	DPM	C3B-C4B-NB	-2.64	105.83	109.22
2	B	365	DPM	O1A-C6A-C5A	-2.61	114.69	122.11
2	A	365	DPM	O1A-C6A-C5A	-2.55	114.85	122.11
2	A	365	DPM	C7A-C8A-C9A	2.41	120.05	113.67
2	B	365	DPM	C2B-C1B-NB	-2.40	107.06	109.84
2	B	365	DPM	C5B-C2B-C3B	-2.36	118.03	124.65
2	B	365	DPM	O3A-C9A-C8A	-2.30	115.81	123.09
2	B	365	DPM	O3B-C9B-C8B	-2.27	115.89	123.09
2	A	365	DPM	CHA-C1A-NA	2.16	125.75	121.36
2	A	365	DPM	CHB-C4A-C3A	-2.11	126.04	130.07

There are no chirality outliers.

All (14) torsion outliers are listed below:

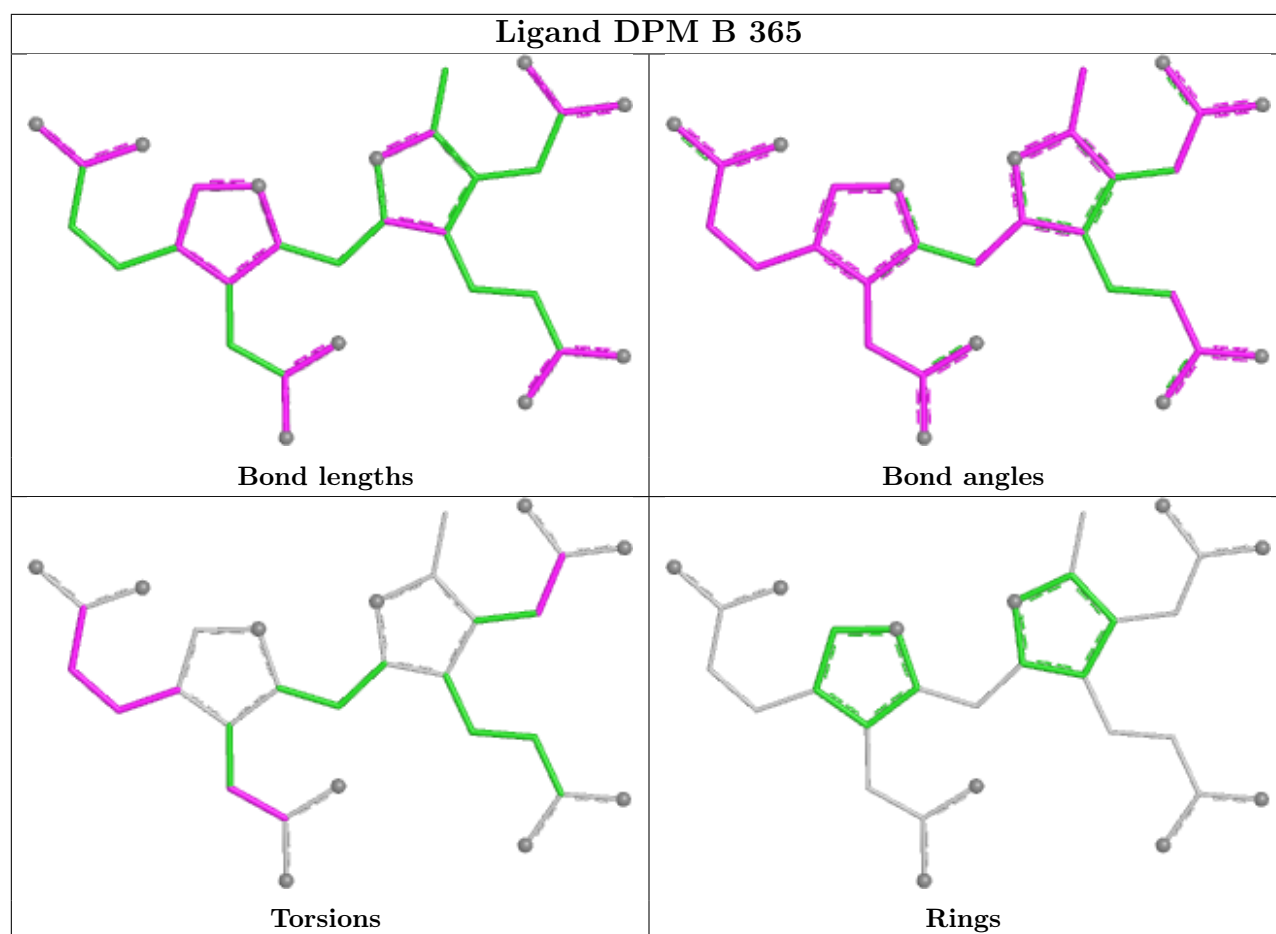
Mol	Chain	Res	Type	Atoms
2	A	365	DPM	C4B-C3B-C7B-C8B
2	B	365	DPM	C4B-C3B-C7B-C8B
2	B	365	DPM	C3B-C7B-C8B-C9B
2	B	365	DPM	C2B-C5B-C6B-O2B
2	A	365	DPM	C2A-C5A-C6A-O2A
2	A	365	DPM	C2B-C5B-C6B-O2B
2	B	365	DPM	C2A-C5A-C6A-O1A
2	A	365	DPM	C2A-C5A-C6A-O1A
2	B	365	DPM	C2A-C5A-C6A-O2A
2	A	365	DPM	C7A-C8A-C9A-O4A
2	B	365	DPM	C7B-C8B-C9B-O4B
2	B	365	DPM	C7B-C8B-C9B-O3B
2	A	365	DPM	C7B-C8B-C9B-O3B
2	A	365	DPM	C7A-C8A-C9A-O3A

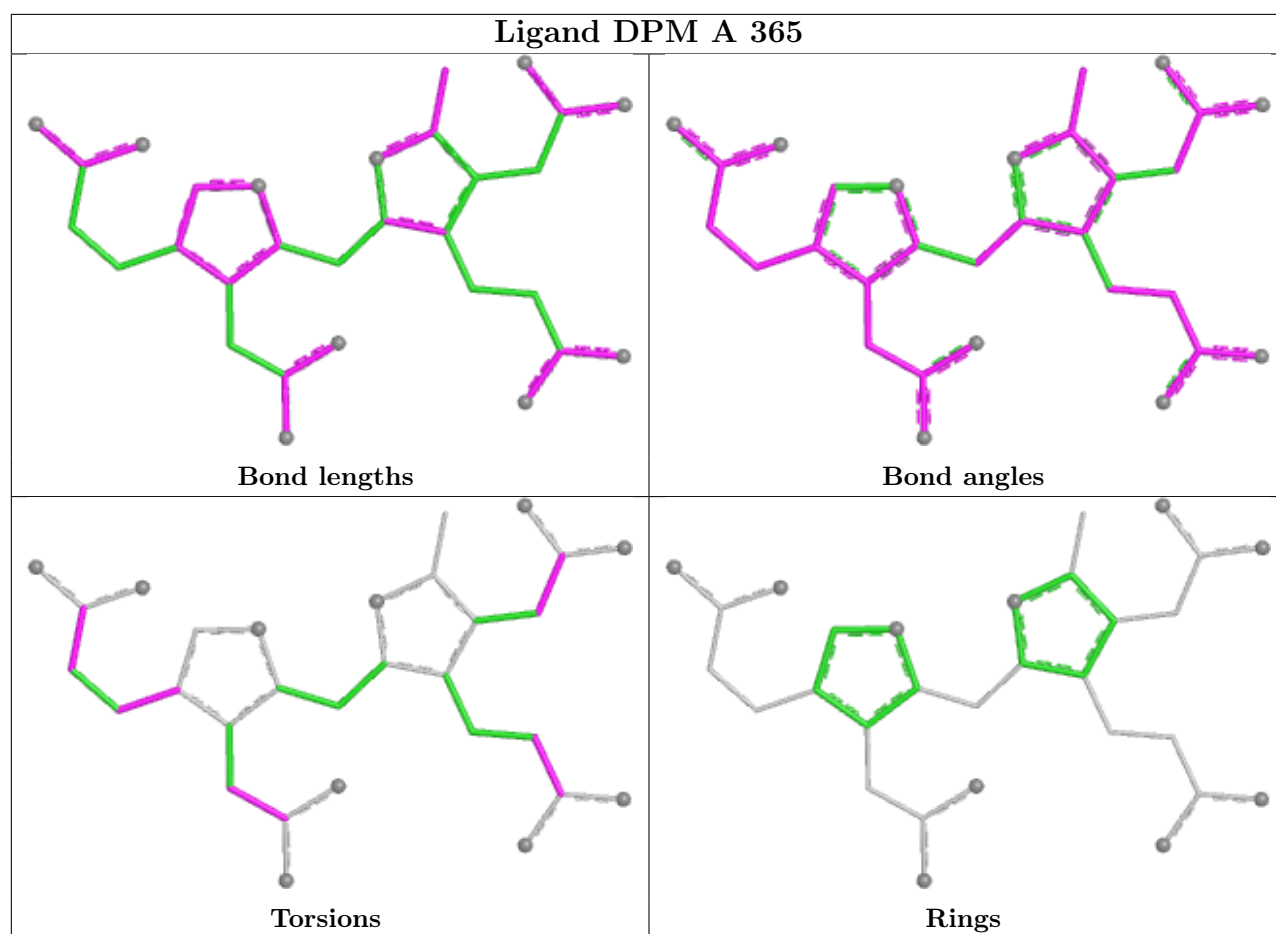
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	365	DPM	1	0
2	A	365	DPM	2	0

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 than 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.





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	318/364 (87%)	0.87	35 (11%) 10 9	21, 37, 59, 77	0
1	B	310/364 (85%)	0.87	37 (11%) 9 8	21, 36, 57, 69	0
All	All	628/728 (86%)	0.87	72 (11%) 9 8	21, 36, 58, 77	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	TRP	6.7
1	A	80	PHE	5.1
1	B	133	VAL	4.6
1	B	76	GLU	4.5
1	A	59	MET	4.5
1	B	75	GLY	4.3
1	B	74	ILE	4.2
1	A	133	VAL	4.1
1	B	303	HIS	3.9
1	A	184	GLN	3.9
1	B	59	MET	3.9
1	B	288	LEU	3.9
1	A	139	THR	3.6
1	B	139	THR	3.6
1	A	174	ASN	3.5
1	A	288	LEU	3.5
1	A	265	SER	3.5
1	A	276	ASP	3.4
1	A	200	GLY	3.4
1	B	182	GLU	3.3
1	B	132	PHE	3.1
1	A	359	GLN	3.1
1	A	314	ASP	3.0
1	A	79	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	174	ASN	2.9
1	A	163	HIS	2.9
1	B	22	ARG	2.8
1	B	143	LYS	2.8
1	A	303	HIS	2.8
1	B	200	GLY	2.8
1	B	264	CYS	2.8
1	B	266	VAL	2.8
1	A	212	GLU	2.7
1	B	109	PRO	2.7
1	B	120	GLU	2.7
1	B	84	LEU	2.7
1	B	302	ILE	2.7
1	A	137	LEU	2.6
1	B	130	PRO	2.6
1	A	358	ARG	2.5
1	B	188	ALA	2.5
1	B	80	PHE	2.5
1	A	304	VAL	2.5
1	B	280	TYR	2.5
1	A	120	GLU	2.5
1	A	35	ARG	2.4
1	B	206	GLY	2.4
1	A	181	ASP	2.4
1	A	109	PRO	2.4
1	A	134	GLY	2.3
1	A	185	GLU	2.3
1	B	358	ARG	2.3
1	A	142	GLU	2.3
1	A	202	HIS	2.3
1	A	312	PRO	2.2
1	B	301	THR	2.2
1	B	184	GLN	2.2
1	B	144	SER	2.2
1	B	204	ARG	2.2
1	B	55	GLU	2.2
1	B	183	GLN	2.2
1	A	266	VAL	2.2
1	A	275	LYS	2.2
1	B	186	PHE	2.1
1	A	31	SER	2.1
1	A	196	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	352	ASN	2.1
1	B	163	HIS	2.1
1	B	185	GLU	2.0
1	B	73	LYS	2.0
1	B	181	ASP	2.0
1	A	206	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

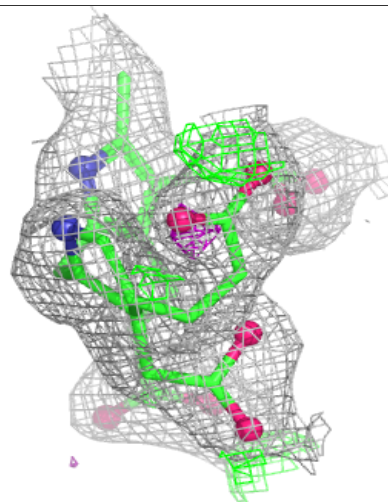
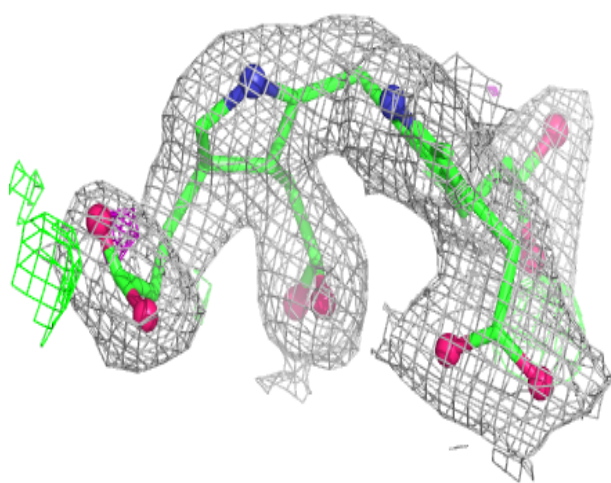
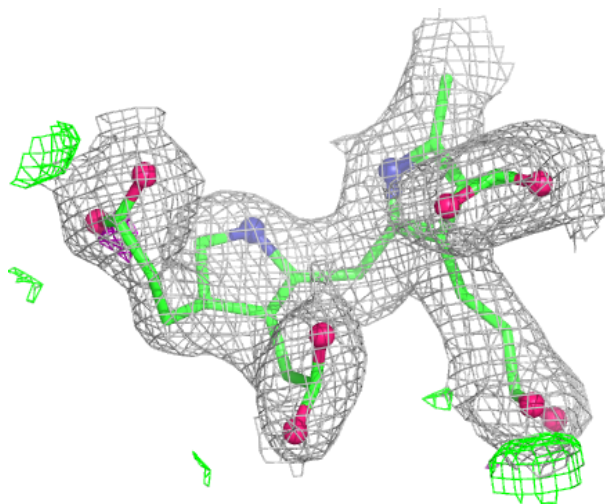
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DPM	A	365	30/30	0.92	0.08	19,23,35,42	0
2	DPM	B	365	30/30	0.93	0.08	22,32,41,54	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.

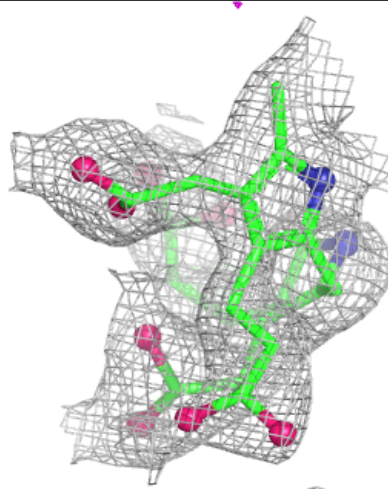
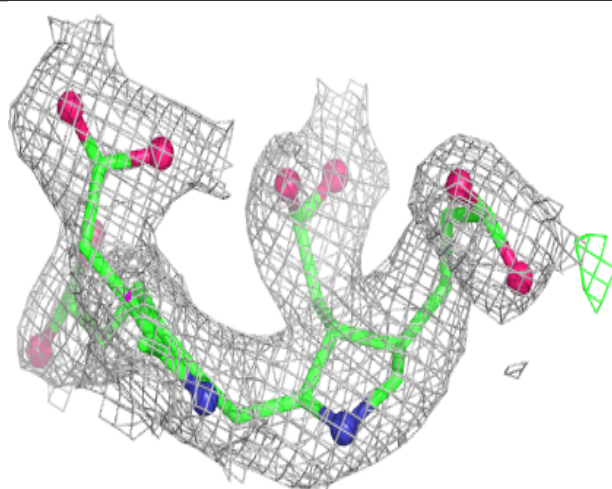
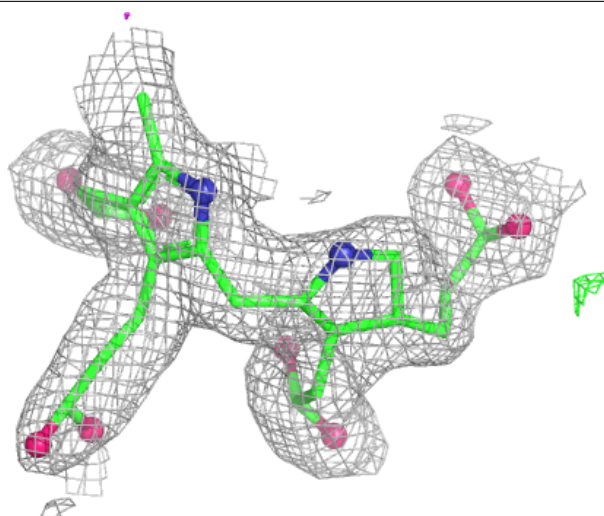
Electron density around DPM A 365:

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



Electron density around DPM B 365:

$2mF_o-DF_c$ (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.