



# Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2019 – 08:31 AM EDT

PDB ID : 2C14  
Title : 5-(4-Carboxy-2-oxo-butylamino)-4-oxo-pentanoic acid acid bound to Porphobilinogen synthase from Pseudomonas aeruginosa  
Authors : Frere, F.; Nentwich, M.; Gacond, S.; Heinz, D.W.; Neier, R.; Frankenberg-Dinkel, N.  
Deposited on : 2005-09-11  
Resolution : 1.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

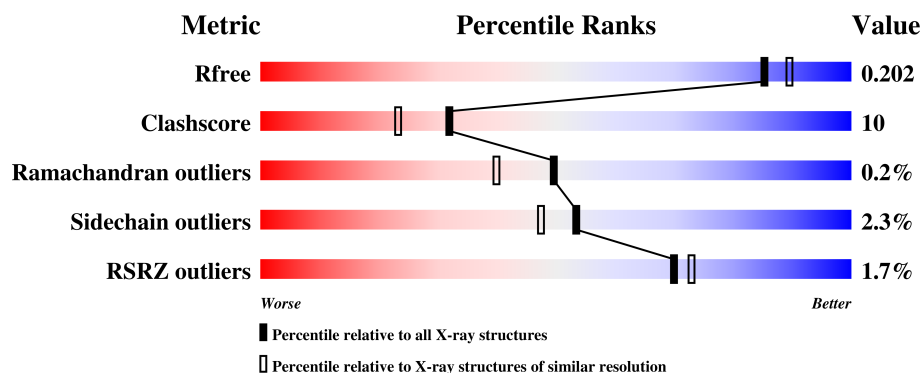
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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  $\geq 3$ , 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	337	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 5px; left: 88%; width: 10%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 5px; left: 98%; width: 10%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>88%</span> <span>11% ..</span> </div> </div>
1	B	337	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 5px; left: 84%; width: 10%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 5px; left: 98%; width: 10%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>84%</span> <span>12% ..</span> </div> </div>

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
1	CYJ	B	205	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6349 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 DELTA-AMINOLEVULINIC ACID DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	25	1
			2822	1764	508	538	12			
1	B	329	Total	C	N	O	S	0	28	1
			2802	1753	499	539	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	VAL	ILE	engineered mutation	UNP Q59643
B	199	VAL	ILE	engineered mutation	UNP Q59643

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

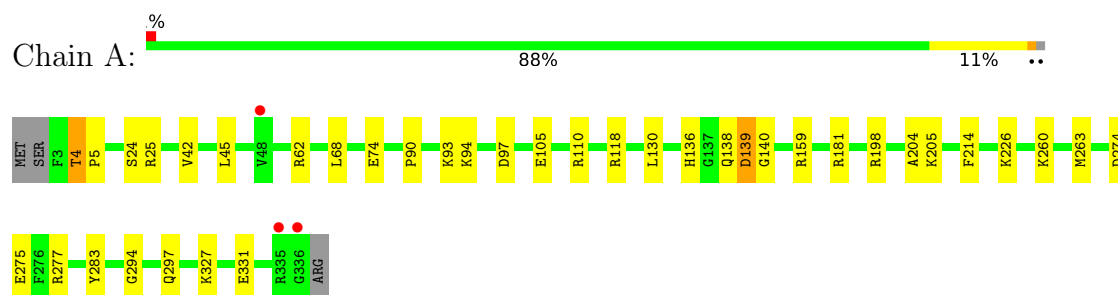
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	356	Total	O	0	0
			356	356		
3	B	367	Total	O	0	0
			367	367		

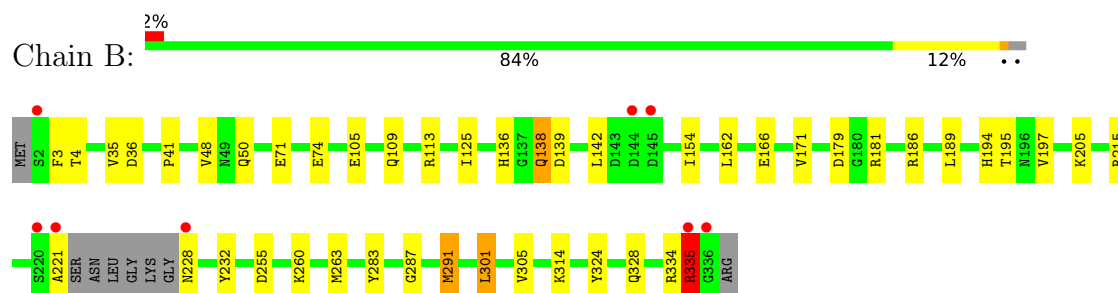
### 3 Residue-property plots [i](#)

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: DELTA-AMINOLEVULINIC ACID DEHYDRATASE



#### • Molecule 1: DELTA-AMINOLEVULINIC ACID DEHYDRATASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.88Å 126.88Å 86.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.80 – 1.90 40.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (89.80-1.90) 98.9 (40.12-1.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.158 , 0.201 0.157 , 0.202	Depositor DCC
$R_{free}$ test set	2802 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6349	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CYJ, MG

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	0.77	0/2848	0.76	1/3857 (0.0%)
1	B	0.78	0/2826	0.72	1/3831 (0.0%)
All	All	0.77	0/5674	0.74	2/7688 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	97	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	291	MET	CG-SD-CE	5.49	108.98	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ALA	Mainchain

### 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	2822	0	2768	38	1
1	B	2802	0	2735	76	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	356	0	0	8	0
3	B	367	0	0	17	0
All	All	6349	0	5503	107	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 10.

All (107) 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:205:CYJ:C8	1:A:260:LYS:HZ1	0.97	1.54
1:B:205:CYJ:C8	1:B:260:LYS:HZ1	1.18	1.53
1:B:334:ARG:HD3	1:B:335:ARG:NH2	1.29	1.46
1:B:334:ARG:NH1	1:B:335:ARG:HH21	1.11	1.46
1:B:334:ARG:HH11	1:B:335:ARG:NH2	1.01	1.43
1:B:334:ARG:HH11	1:B:335:ARG:CZ	1.39	1.32
1:B:205:CYJ:H8	1:B:260:LYS:NZ	0.92	1.23
1:B:334:ARG:CZ	1:B:335:ARG:HH21	1.55	1.20
1:A:159[B]:ARG:NH2	3:A:2233:HOH:O	1.72	1.20
1:B:136[B]:HIS:CD2	1:B:138[B]:GLN:HB2	1.79	1.17
1:B:195[A]:THR:HG22	3:B:2269:HOH:O	1.00	1.16
1:B:334:ARG:NH1	1:B:335:ARG:NH2	1.72	1.16
1:A:205:CYJ:H8	1:A:260:LYS:NZ	0.81	1.14
1:B:334:ARG:CD	1:B:335:ARG:NH2	2.12	1.11
1:A:205:CYJ:H8	1:A:260:LYS:CE	1.87	1.05
1:B:334:ARG:HD2	3:B:2366:HOH:O	1.57	1.04
1:A:263[B]:MET:HG2	1:B:263[B]:MET:HG2	1.40	1.04
1:B:205:CYJ:C8	1:B:260:LYS:NZ	1.89	1.03
1:A:205:CYJ:H8	1:A:260:LYS:HZ2	1.24	0.98
1:B:205:CYJ:H8	1:B:260:LYS:HZ3	1.24	0.97
1:B:36[B]:ASP:OD2	3:B:2092:HOH:O	1.83	0.96
1:B:136[B]:HIS:HD2	1:B:138[B]:GLN:H	1.12	0.96
1:B:334:ARG:NH1	1:B:335:ARG:CZ	2.21	0.95
1:B:328[A]:GLN:OE1	3:B:2359:HOH:O	1.86	0.93
1:A:159[B]:ARG:CZ	3:A:2233:HOH:O	2.10	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:CYJ:C3	1:A:260:LYS:HZ1	1.83	0.90
1:B:334:ARG:NH1	1:B:335:ARG:NE	2.18	0.90
1:B:334:ARG:HD3	1:B:335:ARG:HH22	1.30	0.90
1:B:205:CYJ:H8	1:B:260:LYS:CE	2.02	0.89
1:B:334:ARG:HH11	1:B:335:ARG:NE	1.70	0.88
1:B:136[B]:HIS:CD2	1:B:138[B]:GLN:H	1.89	0.88
1:B:334:ARG:NH1	1:B:335:ARG:HE	1.71	0.87
1:B:136[B]:HIS:HD2	1:B:138[B]:GLN:HB2	1.40	0.86
1:B:314[B]:LYS:CE	3:B:2351:HOH:O	2.26	0.83
1:B:334:ARG:CD	3:B:2366:HOH:O	2.18	0.81
1:B:314[B]:LYS:HE3	3:B:2351:HOH:O	1.81	0.80
1:A:139[B]:ASP:OD2	3:A:2211:HOH:O	1.98	0.80
1:A:25[B]:ARG:NH2	3:A:2060:HOH:O	2.16	0.79
1:A:263[B]:MET:CG	1:B:263[B]:MET:HG2	2.12	0.79
1:B:195[A]:THR:CG2	3:B:2269:HOH:O	1.73	0.78
1:B:136[B]:HIS:HD2	1:B:138[B]:GLN:N	1.82	0.78
1:B:205:CYJ:C9	1:B:260:LYS:HZ1	1.98	0.77
1:B:334:ARG:NE	1:B:335:ARG:HH21	1.83	0.74
1:A:263[B]:MET:SD	1:B:263[B]:MET:SD	2.88	0.72
1:B:189:LEU:HD22	1:B:197[B]:VAL:HG11	1.71	0.71
1:B:314[B]:LYS:NZ	3:B:2351:HOH:O	1.97	0.71
1:A:331:GLU:OE1	3:A:2352:HOH:O	2.09	0.69
1:B:136[B]:HIS:CD2	1:B:138[B]:GLN:CB	2.68	0.68
1:B:334:ARG:NE	3:B:2366:HOH:O	2.26	0.68
1:A:205:CYJ:C7	1:A:260:LYS:NZ	2.57	0.67
1:B:334:ARG:CD	1:B:335:ARG:HH21	1.92	0.67
1:B:138[A]:GLN:HG2	1:B:142:LEU:HD11	1.78	0.65
1:A:139[A]:ASP:HB3	3:A:2211:HOH:O	1.96	0.65
1:A:130:LEU:HD12	1:A:140:GLY:HA2	1.81	0.63
1:A:297[A]:GLN:OE1	3:A:2330:HOH:O	2.16	0.61
1:B:194:HIS:O	1:B:197[B]:VAL:HG12	2.01	0.61
1:B:136[B]:HIS:HD2	1:B:138[B]:GLN:CB	2.10	0.60
1:A:136[A]:HIS:HD2	1:A:138:GLN:H	1.50	0.60
1:A:24:SER:C	1:A:25[B]:ARG:CA	2.63	0.59
1:B:136[B]:HIS:CD2	1:B:138[B]:GLN:N	2.65	0.59
1:A:42[B]:VAL:HG11	1:A:68:LEU:CD1	2.33	0.58
1:B:334:ARG:HD3	1:B:335:ARG:CZ	2.24	0.57
1:A:45:LEU:HD21	1:A:62[A]:ARG:HD3	1.85	0.57
1:A:263[B]:MET:SD	1:B:263[B]:MET:HG2	2.46	0.56
1:B:35[A]:VAL:HG21	3:B:2153:HOH:O	2.05	0.56
1:A:294:GLY:O	1:A:297[B]:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:HD13	1:B:197[B]:VAL:HG13	1.90	0.54
1:B:287:GLY:O	1:B:291:MET:HG3	2.07	0.54
1:B:139:ASP:OD2	1:B:232:TYR:OH	2.28	0.52
1:B:71[A]:GLU:OE2	3:B:2144:HOH:O	2.17	0.52
1:A:275[B]:GLU:CD	1:B:3:PHE:HB3	2.31	0.51
1:B:301:LEU:HG	1:B:305:VAL:HG11	1.92	0.51
1:A:42[B]:VAL:HG11	1:A:68:LEU:HD13	1.93	0.50
1:A:94[B]:LYS:NZ	3:A:2157:HOH:O	2.45	0.50
1:A:263[B]:MET:HG2	1:B:263[B]:MET:CG	2.26	0.50
1:A:74[B]:GLU:HG2	1:A:327:LYS:HE3	1.93	0.50
1:B:205:CYJ:C3	1:B:260:LYS:NZ	2.71	0.50
1:B:205:CYJ:C7	1:B:260:LYS:HZ1	2.13	0.50
1:B:74[A]:GLU:OE2	3:B:2149:HOH:O	2.19	0.50
1:A:274:ASP:O	1:A:277[B]:ARG:NH1	2.45	0.50
1:B:205:CYJ:C4	1:B:260:LYS:HZ3	2.24	0.50
1:A:263[B]:MET:SD	1:B:263[B]:MET:CG	3.00	0.49
1:B:105[B]:GLU:OE1	1:B:113[B]:ARG:NH2	2.46	0.49
1:A:226:LYS:HE2	1:A:226:LYS:HA	1.95	0.48
1:B:205:CYJ:C7	1:B:260:LYS:NZ	2.74	0.48
1:A:105:GLU:O	1:A:110[A]:ARG:HD3	2.14	0.47
1:B:136[B]:HIS:NE2	1:B:138[B]:GLN:HB2	2.25	0.47
1:B:166[A]:GLU:OE1	3:B:2253:HOH:O	2.19	0.47
1:B:335:ARG:HG3	1:B:335:ARG:O	2.15	0.46
1:A:205:CYJ:C8	1:A:260:LYS:HZ2	1.99	0.46
1:B:195[A]:THR:HG21	3:B:2274:HOH:O	2.15	0.46
1:B:113[B]:ARG:NH2	3:B:2200:HOH:O	2.49	0.45
1:B:48[A]:VAL:O	1:B:50:GLN:HG2	2.16	0.44
1:B:186[B]:ARG:NH2	1:B:255:ASP:OD2	2.51	0.44
1:A:90:PRO:HD2	1:A:93:LYS:HD2	1.99	0.44
1:B:136[B]:HIS:HD2	1:B:138[B]:GLN:CA	2.30	0.44
1:B:154:ILE:HD11	1:B:179:ASP:O	2.18	0.44
1:B:215:ARG:CB	1:B:221:ALA:HB2	2.48	0.44
1:B:74[A]:GLU:CD	3:B:2149:HOH:O	2.57	0.43
1:A:4:THR:HA	1:A:5:PRO:HD3	1.91	0.43
1:A:226:LYS:HA	1:A:226:LYS:CE	2.48	0.42
1:B:109:GLN:O	1:B:113[B]:ARG:HG3	2.18	0.42
1:B:125:ILE:HG12	1:B:171:VAL:HB	2.01	0.42
1:B:162:LEU:O	1:B:166[B]:GLU:HG3	2.19	0.42
1:A:205:CYJ:H7C2	1:A:214:PHE:CZ	2.56	0.41
1:B:41:PRO:HB2	1:B:324:TYR:CE1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275[B]:GLU:OE1	1:B:4:THR:OG1[3_645]	2.12	0.08

## 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	357/337 (106%)	350 (98%)	7 (2%)	0	100	100
1	B	352/337 (104%)	342 (97%)	9 (3%)	1 (0%)	43	33
All	All	709/674 (105%)	692 (98%)	16 (2%)	1 (0%)	49	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	335	ARG

### 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	291/268 (109%)	284 (98%)	7 (2%)	52	45
1	B	290/268 (108%)	283 (98%)	7 (2%)	52	45
All	All	581/536 (108%)	567 (98%)	14 (2%)	53	45

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	118	ARG
1	A	139[A]	ASP
1	A	139[B]	ASP
1	A	181	ARG
1	A	198	ARG
1	A	283	TYR
1	B	138[A]	GLN
1	B	138[B]	GLN
1	B	181	ARG
1	B	228	ASN
1	B	283	TYR
1	B	301	LEU
1	B	335	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	50	GLN
1	B	7	ASN
1	B	50	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CYJ	A	205	1	17,24,25	1.01	2 (11%)	9,30,32	2.42	5 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CYJ	B	205	1	17,24,25	1.12	1 (5%)	9,30,32	2.67	3 (33%)

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
1	CYJ	A	205	1	-	0/11/33/35	0/1/1/1
1	CYJ	B	205	1	-	0/11/33/35	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	CYJ	CA-C	2.05	1.52	1.50
1	A	205	CYJ	C3-C4	2.44	1.53	1.51
1	B	205	CYJ	C3-C4	3.08	1.54	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	CYJ	CG-CD-CE	-2.00	106.26	113.49
1	A	205	CYJ	C3-C4-NZ	2.06	124.83	119.23
1	A	205	CYJ	CE-NZ-C4	2.27	128.98	122.49
1	A	205	CYJ	CD-CE-NZ	2.27	114.20	110.72
1	B	205	CYJ	CE-NZ-C4	2.69	130.18	122.49
1	B	205	CYJ	C5-C4-C3	2.91	118.72	115.28
1	A	205	CYJ	C2-C3-C4	5.18	120.50	112.42
1	B	205	CYJ	C2-C3-C4	6.37	122.36	112.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	205	CYJ	8	0
1	B	205	CYJ	10	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	333/337 (98%)	-0.32	3 (0%) 84 86	10, 15, 25, 49	2 (0%)
1	B	328/337 (97%)	-0.33	8 (2%) 59 62	10, 15, 29, 45	4 (1%)
All	All	661/674 (98%)	-0.33	11 (1%) 70 73	10, 15, 27, 49	6 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	GLY	11.1
1	B	336	GLY	9.6
1	B	221	ALA	5.7
1	B	2	SER	4.4
1	B	335	ARG	3.7
1	A	335	ARG	3.4
1	B	220	SER	2.7
1	B	144	ASP	2.6
1	A	48	VAL	2.5
1	B	228	ASN	2.4
1	B	145	ASP	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CYJ	B	205	24/25	0.94	0.13	10,13,20,33	0
1	CYJ	A	205	24/25	0.95	0.12	10,12,17,21	0

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MG	A	1336	1/1	0.98	0.08	17,17,17,17	0
2	MG	B	1336	1/1	1.00	0.07	14,14,14,14	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.