



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:43 AM GMT

PDB ID : 2J56  
Title : X-RAY REDUCED PARACCOCUS DENITRIFICANS METHYLAMINE  
DEHYDROGENASE N-SEMIQUINONE IN COMPLEX WITH AMI-  
CYANIN.  
Authors : Pearson, A.R.; Pahl, R.; Davidson, V.L.; Wilmot, C.M.  
Deposited on : 2006-09-12  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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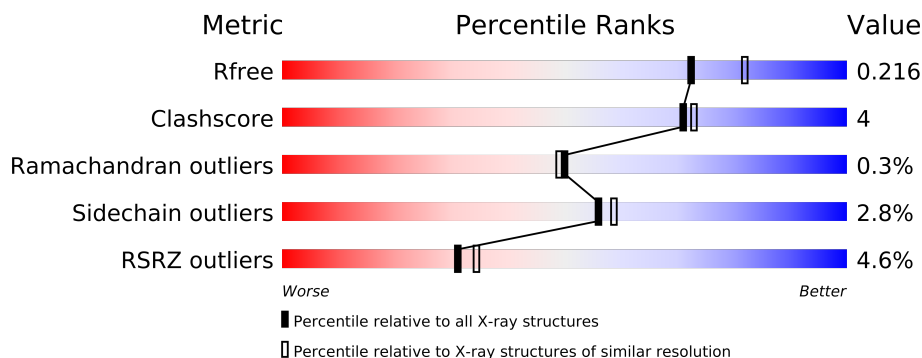
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	105	
1	B	105	
2	H	386	
2	J	386	
3	L	131	
3	M	131	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10400 atoms, of which 0 are hydrogen and 0 are deuterium.

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 AMICYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			806	516	132	152	6			
1	B	105	Total	C	N	O	S	0	0	0
			806	516	132	152	6			

- Molecule 2 is a protein called METHYLAMINE DEHYDROGENASE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	375	Total	C	N	O	S	0	2	0
			2929	1857	501	563	8			
2	J	375	Total	C	N	O	S	0	0	0
			2910	1846	500	556	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	312	PHE	LEU	SEE REMARK 999	UNP P29894
H	313	VAL	LEU	SEE REMARK 999	UNP P29894
J	312	PHE	LEU	SEE REMARK 999	UNP P29894
J	313	VAL	LEU	SEE REMARK 999	UNP P29894

- Molecule 3 is a protein called METHYLAMINE DEHYDROGENASE LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	125	Total	C	N	O	S	0	0	0
			956	590	162	191	13			
3	M	125	Total	C	N	O	S	0	0	1
			950	587	162	188	13			

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cu 1 1	0	0
4	A	1	Total Cu 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 6 3 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total Na 1 1	0	0
6	M	1	Total Na 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	49	Total O 49 49	0	0
7	B	99	Total O 99 99	0	0

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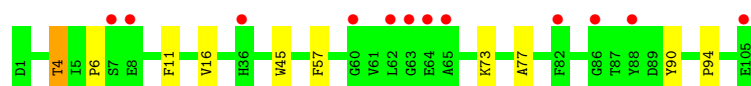
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	417	Total 417	O 417	0	0
7	J	278	Total 278	O 278	0	0
7	L	91	Total 91	O 91	0	0
7	M	99	Total 99	O 99	0	0

### 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 errors 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: AMICYANIN

Chain A: 



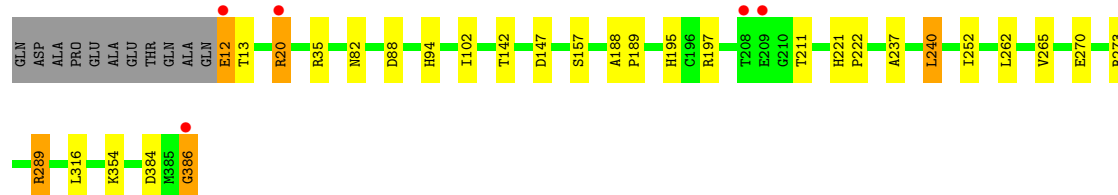
- Molecule 1: AMICYANIN

Chain B: 



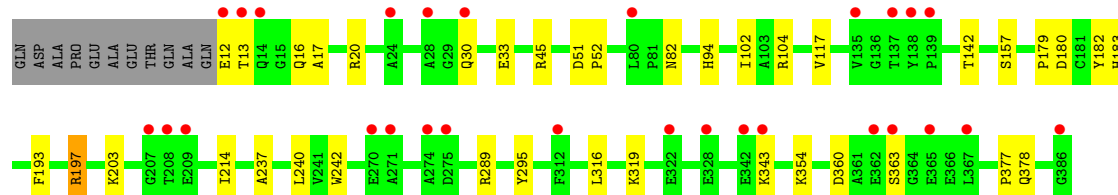
- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain H: 



- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain J: 



- Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain L: 



● Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.03Å 123.03Å 245.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.48 – 2.10 42.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (43.48-2.10) 97.3 (42.83-2.10)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.84 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.169 , 0.207 0.180 , 0.216	Depositor DCC
$R_{free}$ test set	5353 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 36.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 107151 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TQQ, CU, NA

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	0.65	0/827	0.68	0/1122
1	B	0.85	0/827	0.83	3/1122 (0.3%)
2	H	0.87	1/3009 (0.0%)	0.85	4/4100 (0.1%)
2	J	0.76	0/2987	0.80	5/4071 (0.1%)
3	L	0.84	0/964	0.76	0/1315
3	M	0.76	0/958	0.77	0/1309
All	All	0.81	1/9572 (0.0%)	0.80	12/13039 (0.1%)

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
2	H	0	2
2	J	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	35	ARG	CB-CG	-5.15	1.38	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	197	ARG	NE-CZ-NH1	-12.55	114.03	120.30
2	J	197	ARG	NE-CZ-NH2	8.27	124.44	120.30
2	H	386	GLY	N-CA-C	-8.14	92.75	113.10
1	B	99	ARG	NE-CZ-NH2	-7.83	116.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	147	ASP	CB-CG-OD1	6.70	124.33	118.30
2	J	104	ARG	NE-CZ-NH2	-6.60	117.00	120.30
2	J	197	ARG	CG-CD-NE	-6.35	98.47	111.80
1	B	99	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	32	THR	CB-CA-C	-5.78	96.00	111.60
2	J	104	ARG	CG-CD-NE	-5.27	100.73	111.80
2	H	88	ASP	CB-CG-OD1	5.17	122.95	118.30
2	H	197	ARG	NE-CZ-NH1	-5.16	117.72	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	157	SER	Mainchain,Peptide
2	J	157	SER	Mainchain,Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	806	0	790	6	0
1	B	806	0	790	9	0
2	H	2929	0	2811	14	0
2	J	2910	0	2796	31	0
3	L	956	0	858	13	0
3	M	950	0	853	15	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	H	6	0	8	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
7	A	49	0	0	1	0
7	B	99	0	0	2	0
7	H	417	0	0	2	0
7	J	278	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	91	0	0	1	0
7	M	99	0	0	2	0
All	All	10400	0	8906	81	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (81) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:57:TQQ:CE3	3:M:108:TRP:HD1	0.91	1.54
3:M:57:TQQ:CZ3	3:M:108:TRP:HD1	1.72	1.02
2:H:20:ARG:HH11	2:H:20:ARG:HG3	1.28	0.97
2:J:13:THR:HG22	2:J:16:GLN:HG2	1.47	0.96
1:B:99:ARG:NH2	2:J:180:ASP:OD1	2.02	0.92
1:A:73:LYS:HE3	7:A:2034:HOH:O	1.75	0.86
2:J:33:GLU:HG3	7:J:2022:HOH:O	1.76	0.86
2:J:13:THR:HG22	2:J:16:GLN:CG	2.09	0.82
2:J:12:GLU:OE2	2:J:20:ARG:NH1	2.18	0.76
2:J:12:GLU:HA	2:J:16:GLN:HE21	1.50	0.76
2:H:20:ARG:CG	2:H:20:ARG:HH11	2.02	0.73
1:B:17:ALA:HB1	7:B:2019:HOH:O	1.91	0.69
1:B:99:ARG:HH22	2:J:180:ASP:CG	1.95	0.69
2:J:13:THR:CG2	2:J:16:GLN:HG2	2.20	0.68
2:H:270[B]:GLU:OE1	7:H:2297:HOH:O	2.11	0.68
1:B:68:LYS:HE3	7:B:2067:HOH:O	1.92	0.68
3:L:16:GLN:NE2	3:L:18:ASN:H	1.93	0.67
3:M:57:TQQ:HB2	3:M:108:TRP:NE1	2.10	0.67
3:M:57:TQQ:CZ3	3:M:108:TRP:CD1	2.59	0.66
3:M:16:GLN:NE2	3:M:18:ASN:H	1.93	0.66
3:M:129:LYS:O	3:M:131:SER:N	2.31	0.63
2:J:13:THR:HG22	2:J:16:GLN:CD	2.19	0.63
3:L:57:TQQ:HB2	3:L:108:TRP:NE1	2.14	0.63
3:M:16:GLN:HE21	3:M:18:ASN:H	1.45	0.62
2:H:195:HIS:NE2	2:H:221:HIS:HE1	1.98	0.62
2:J:52:PRO:HG2	2:J:378:GLN:HE21	1.64	0.62
3:M:12:LYS:HE2	7:M:2008:HOH:O	1.99	0.62
2:H:237:ALA:HB2	2:H:289:ARG:HG3	1.81	0.62
3:L:16:GLN:HE21	3:L:18:ASN:H	1.47	0.61
3:L:16:GLN:HE22	3:L:19:ASP:H	1.48	0.61
2:J:13:THR:H	2:J:16:GLN:HE21	1.49	0.60
3:L:13:TRP:HZ3	7:L:2029:HOH:O	1.84	0.60
3:M:16:GLN:HE22	3:M:19:ASP:H	1.49	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:20:ARG:NH1	2:H:20:ARG:HG3	2.09	0.59
2:H:240:LEU:HD13	2:H:252:ILE:HD13	1.83	0.59
2:J:20:ARG:HB2	2:J:20:ARG:CZ	2.31	0.58
1:A:94:PRO:HB3	3:L:55:ALA:HB1	1.85	0.58
2:J:13:THR:H	2:J:16:GLN:NE2	2.02	0.58
2:H:384:ASP:OD1	2:H:386:GLY:OXT	2.23	0.57
2:J:45:ARG:NH2	2:J:343:LYS:O	2.38	0.56
1:B:95:HIS:HB3	1:B:97:PHE:CZ	2.40	0.55
2:H:273:ARG:NH2	7:H:2299:HOH:O	2.24	0.55
2:J:12:GLU:CD	2:J:20:ARG:HH12	2.09	0.55
3:L:57:TQQ:HB2	3:L:108:TRP:HE1	1.71	0.55
2:J:295:TYR:CD1	2:J:295:TYR:N	2.76	0.53
2:J:13:THR:HG23	2:J:16:GLN:H	1.73	0.53
2:J:12:GLU:OE2	2:J:20:ARG:CZ	2.58	0.51
2:J:197:ARG:NH1	3:M:101:GLU:OE1	2.39	0.51
3:M:57:TQQ:HB2	3:M:108:TRP:HE1	1.76	0.50
2:H:12:GLU:OE1	2:H:12:GLU:HA	2.11	0.50
3:M:129:LYS:C	3:M:131:SER:N	2.65	0.49
2:H:289:ARG:NH1	2:H:384:ASP:OD1	2.45	0.49
2:J:82:ASN:HB3	2:J:142:THR:HB	1.94	0.49
1:A:11:PHE:HE2	1:A:16:VAL:HG22	1.77	0.49
3:M:130:ALA:HB1	7:M:2099:HOH:O	2.13	0.49
2:J:179:PRO:HD3	2:J:214:ILE:HD13	1.95	0.48
1:B:32:THR:HG22	1:B:34:GLU:H	1.79	0.47
2:J:51:ASP:HA	2:J:377:PRO:HA	1.96	0.47
2:J:17:ALA:HA	2:J:20:ARG:NH1	2.30	0.46
2:H:221:HIS:HD2	2:H:222:PRO:O	1.98	0.46
2:H:82:ASN:HB3	2:H:142:THR:HB	1.98	0.45
2:J:12:GLU:CD	2:J:20:ARG:NH1	2.68	0.45
1:B:68:LYS:HE2	1:B:68:LYS:HB3	1.77	0.44
2:J:193:PHE:CE2	2:J:203:LYS:HB2	2.52	0.44
3:L:25:TYR:HB3	3:L:28:HIS:CD2	2.51	0.44
1:A:4:THR:O	1:A:6:PRO:HD3	2.18	0.43
1:A:45:TRP:O	1:A:77:ALA:HA	2.19	0.43
3:L:20:ILE:HG22	3:L:25:TYR:CZ	2.54	0.43
2:J:360:ASP:OD1	2:J:363:SER:OG	2.31	0.42
3:L:56:SER:HA	3:L:108:TRP:HB3	2.01	0.42
1:B:94:PRO:HB3	3:M:55:ALA:HB1	2.01	0.42
3:L:16:GLN:C	3:L:16:GLN:HE21	2.23	0.42
3:L:96:PRO:HB2	3:L:98:TYR:CE1	2.55	0.42
2:J:12:GLU:OE2	2:J:20:ARG:NH2	2.53	0.42
2:J:237:ALA:HB2	2:J:289:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:53:ALA:HB2	3:M:109:CYS:HA	2.01	0.42
2:J:182:TYR:O	2:J:183:HIS:HB2	2.21	0.41
1:A:57:PHE:CE2	1:A:90:TYR:HB3	2.55	0.41
2:J:16:GLN:HA	3:L:18:ASN:O	2.21	0.40
2:H:188:ALA:HB1	2:H:189:PRO:HD2	2.04	0.40
1:B:97:PHE:CZ	2:J:197:ARG:NH1	2.89	0.40

There are no symmetry-related clashes.

## 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	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
1	B	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
2	H	375/386 (97%)	361 (96%)	13 (4%)	1 (0%)	50	49
2	J	373/386 (97%)	362 (97%)	10 (3%)	1 (0%)	50	49
3	L	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
3	M	122/131 (93%)	119 (98%)	2 (2%)	1 (1%)	27	20
All	All	1198/1244 (96%)	1158 (97%)	37 (3%)	3 (0%)	50	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	130	ALA
2	H	102	ILE
2	J	102	ILE

### 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	84/85 (99%)	83 (99%)	1 (1%)	82	87
1	B	84/85 (99%)	82 (98%)	2 (2%)	61	65
2	H	305/311 (98%)	294 (96%)	11 (4%)	47	46
2	J	302/311 (97%)	294 (97%)	8 (3%)	59	62
3	L	104/106 (98%)	101 (97%)	3 (3%)	55	57
3	M	103/106 (97%)	101 (98%)	2 (2%)	69	73
All	All	982/1004 (98%)	955 (97%)	27 (3%)	56	60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	B	15	GLU
1	B	32	THR
2	H	12	GLU
2	H	13	THR
2	H	20	ARG
2	H	94	HIS
2	H	211	THR
2	H	240	LEU
2	H	262	LEU
2	H	265	VAL
2	H	289	ARG
2	H	316	LEU
2	H	354	LYS
2	J	30	GLN
2	J	94	HIS
2	J	117	VAL
2	J	240	LEU
2	J	242	TRP
2	J	316	LEU
2	J	319	LYS
2	J	354	LYS
3	L	16	GLN
3	L	60	SER
3	L	131	SER
3	M	16	GLN
3	M	18	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	16	GLN
2	H	221	HIS
2	H	378	GLN
2	J	16	GLN
2	J	378	GLN
3	L	16	GLN
3	L	34	ASN
3	M	16	GLN
3	M	18	ASN
3	M	34	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z  > 2$
3	TQQ	L	57	3	17,17,18	5.37	7 (41%)	19,24,26	2.53	4 (21%)
3	TQQ	M	57	3	17,17,18	5.26	6 (35%)	19,24,26	2.53	4 (21%)

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
3	TQQ	L	57	3	-	0/4/19/21	0/0/2/2
3	TQQ	M	57	3	-	0/4/19/21	0/0/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	57	TQQ	O-C	20.08	1.25	1.11
3	L	57	TQQ	O-C	19.96	1.25	1.11
3	M	57	TQQ	CD2-CG	4.60	1.49	1.41
3	L	57	TQQ	CE2-CZ2	-4.39	1.46	1.50
3	L	57	TQQ	CZ3-CE3	4.34	1.41	1.34
3	L	57	TQQ	CD2-CG	4.25	1.48	1.41
3	M	57	TQQ	CZ3-CE3	3.86	1.41	1.34
3	M	57	TQQ	CD2-CE2	3.19	1.45	1.40
3	L	57	TQQ	CD2-CE2	2.92	1.44	1.40
3	L	57	TQQ	CA-C	2.90	1.53	1.48
3	L	57	TQQ	CH2-N2	2.46	1.37	1.25
3	M	57	TQQ	CH2-N2	2.45	1.37	1.25
3	M	57	TQQ	CA-C	2.33	1.52	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	57	TQQ	CD1-CG-CD2	-7.32	101.48	104.97
3	L	57	TQQ	C-CA-N	-7.16	106.67	113.83
3	L	57	TQQ	CD1-CG-CD2	-6.53	101.85	104.97
3	M	57	TQQ	C-CA-N	-6.40	107.44	113.83
3	L	57	TQQ	CG-CD1-NE1	3.46	113.80	107.94
3	M	57	TQQ	CG-CD1-NE1	3.07	113.13	107.94
3	L	57	TQQ	CB-CG-CD1	-2.12	124.49	128.12
3	M	57	TQQ	CE2-CD2-CG	2.01	109.44	107.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
5	GOL	H	1387	-	5,5,5	0.49	0	5,5,5	1.18	1 (20%)

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
5	GOL	H	1387	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1387	GOL	O2-C2-C3	2.17	118.12	108.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	105/105 (100%)	0.69	12 (11%) 6 6	28, 42, 57, 60	1 (0%)
1	B	105/105 (100%)	-0.13	4 (3%) 38 43	20, 25, 38, 52	1 (0%)
2	H	375/386 (97%)	-0.17	5 (1%) 74 78	14, 21, 35, 52	0
2	J	375/386 (97%)	0.51	28 (7%) 14 16	17, 32, 47, 55	0
3	L	125/131 (95%)	-0.06	2 (1%) 68 72	20, 27, 38, 53	0
3	M	125/131 (95%)	-0.00	5 (4%) 36 41	14, 23, 42, 57	0
All	All	1210/1244 (97%)	0.15	56 (4%) 31 34	14, 27, 47, 60	2 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	ASP	5.7
2	J	208	THR	5.7
2	J	274	ALA	4.9
2	J	207	GLY	4.8
2	H	12	GLU	4.5
2	J	271	ALA	4.2
2	J	386	GLY	4.2
1	A	64	GLU	4.1
2	J	24	ALA	4.0
2	J	270	GLU	3.8
1	A	105	GLU	3.7
2	J	30	GLN	3.6
1	B	19	GLY	3.5
3	M	130	ALA	3.5
2	J	28	ALA	3.5
2	J	12	GLU	3.3
3	L	7	THR	3.3
3	M	7	THR	3.3
2	J	342	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	J	363	SER	3.3
1	B	17	ALA	3.2
2	J	365	GLU	3.2
2	J	343	LYS	3.1
1	A	65	ALA	3.1
2	H	20	ARG	3.0
2	H	209	GLU	3.0
2	J	13	THR	3.0
1	A	86	GLY	2.8
2	J	275	ASP	2.7
3	M	12	LYS	2.7
2	J	14	GLN	2.7
3	M	131	SER	2.5
2	J	138	TYR	2.5
1	A	36	HIS	2.5
1	A	88	TYR	2.4
2	H	386	GLY	2.4
2	J	137	THR	2.4
2	J	328	GLU	2.4
1	B	20	ALA	2.3
3	L	18	ASN	2.3
1	A	60	GLY	2.3
2	J	322	GLU	2.3
1	A	82	PHE	2.3
1	A	8	GLU	2.3
2	J	135	VAL	2.2
1	A	7	SER	2.2
2	J	209	GLU	2.2
2	J	362	GLU	2.1
2	J	367	LEU	2.1
1	A	63	GLY	2.1
2	J	312	PHE	2.1
2	H	208	THR	2.1
2	J	80	LEU	2.1
2	J	139	PRO	2.1
3	M	68	GLN	2.1
1	A	62	LEU	2.0

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

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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	TQQ	M	57	16/17	0.14	0.87	23,24,25,26	0
3	TQQ	L	57	16/17	0.13	0.39	22,24,26,27	0

### 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NA	L	1132	1/1	0.15	0.45	18,18,18,18	0
6	NA	M	1131	1/1	0.15	-0.39	23,23,23,23	0
5	GOL	H	1387	6/6	0.12	-0.54	21,23,27,27	0
4	CU	B	1106	1/1	0.07	-1.96	28,28,28,28	0
4	CU	A	1106	1/1	0.08	-2.44	32,32,32,32	0

### 6.5 Other polymers

There are no such residues in this entry.