Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:17 am BST

PDB ID	:	2J56
Title	:	X-ray reduced Paraccocus denitrificans methylamine dehydrogenase N-semiquinone in complex with amicyanin.
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 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 following versions of software and data (see references ①) were used in the production of this report:

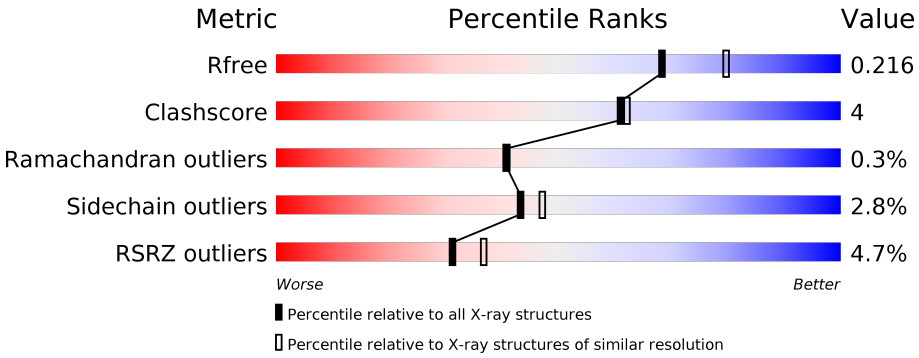
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 >=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	105	13% 90% 9% •
1	B	105	4% 91% 7% ••
2	H	386	% 89% 6% • •
2	J	386	7% 87% 10% •
3	L	131	2% 84% 11% • 5%
3	M	131	5% 85% 8% • 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10400 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 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

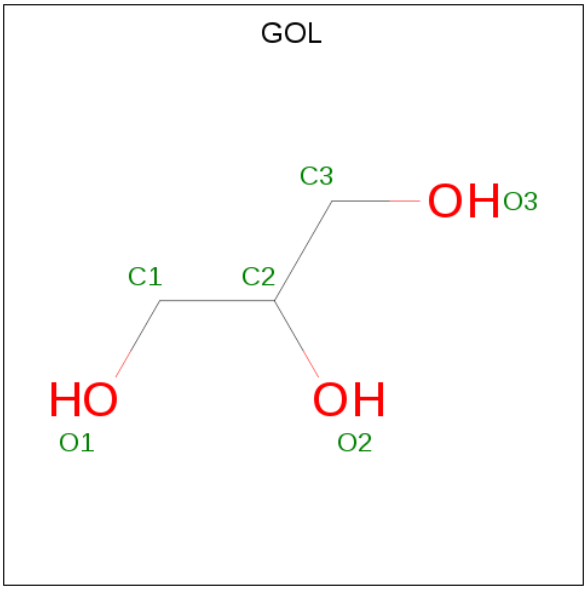
- Molecule 3 is a protein called METHYLAMINE DEHYDROGENASE LIGHT CHAIN.

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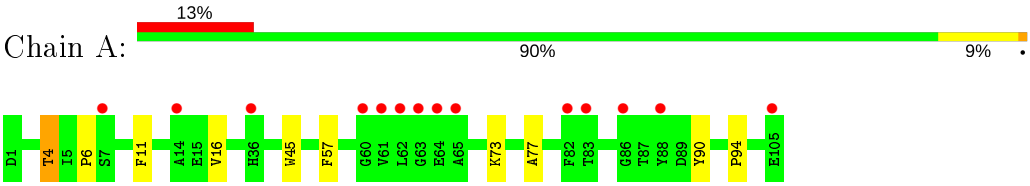
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	417	Total O 417 417	0	0
7	J	278	Total O 278 278	0	0
7	L	91	Total O 91 91	0	0
7	M	99	Total O 99 99	0	0

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.

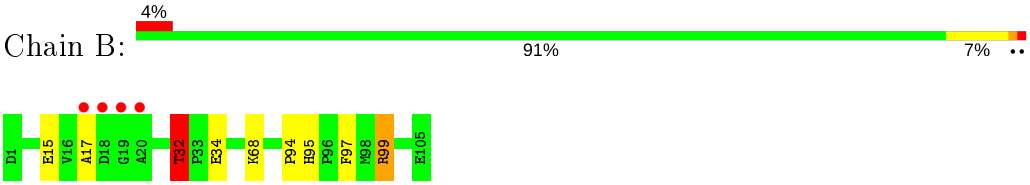
- Molecule 1: AMICYANIN

Chain A:



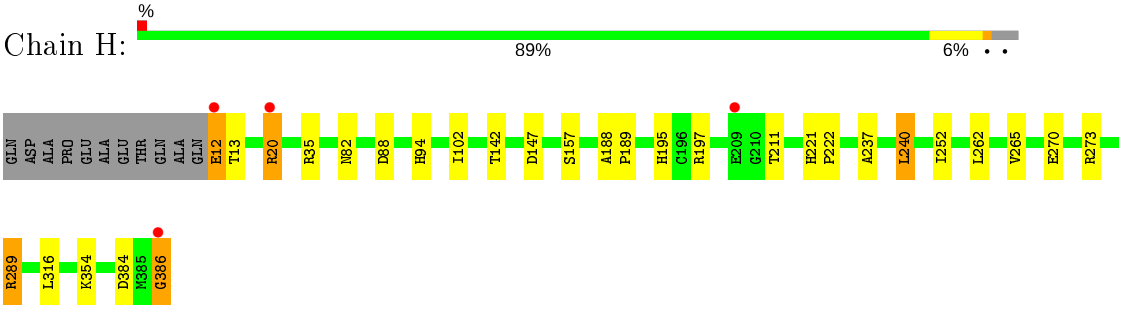
- Molecule 1: AMICYANIN

Chain B:



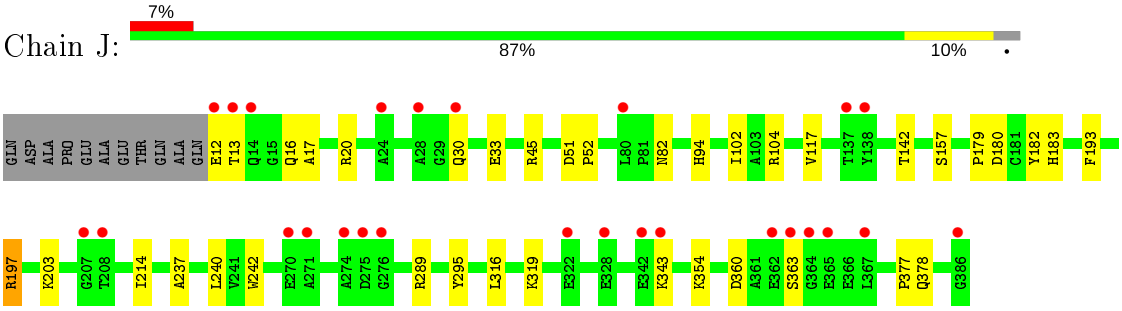
- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain H:



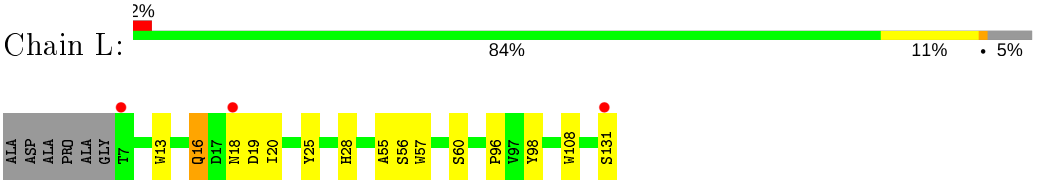
- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain J:



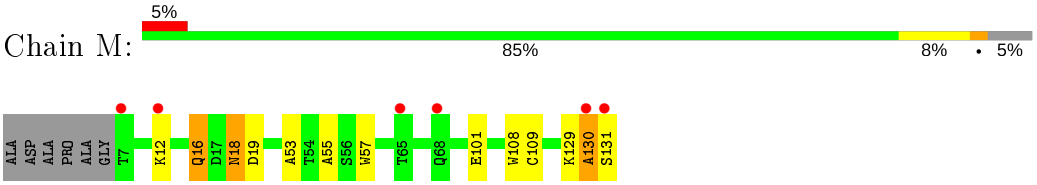
- Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain L:



• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 49.6	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	0.95	EDS
Total number of atoms	10400	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[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: 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 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	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
7	L	91	0	0	1	0
7	M	99	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10400	0	8906	81	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 4.

All (81) 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)
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
1:B:68:LYS:HE3	7:B:2067:HOH:O	1.92	0.68
2:H:270[B]:GLU:OE1	7:H:2297:HOH:O	2.11	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
2:H:237:ALA:HB2	2:H:289:ARG:HG3	1.81	0.62
3:M:12:LYS:HE2	7:M:2008:HOH:O	1.99	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	Interatomic distance (Å)	Clash overlap (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:CZ	2:J:20:ARG:HB2	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:N	2:J:295:TYR:CD1	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
2:H:289:ARG:NH1	2:H:384:ASP:OD1	2.45	0.49
3:M:129:LYS:C	3:M:131:SER:N	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:237:ALA:HB2	2:J:289:ARG:HG3	2.01	0.42
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 (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	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%)	41	41
2	J	373/386 (97%)	362 (97%)	10 (3%)	1 (0%)	41	41
3	L	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
3	M	122/131 (93%)	119 (98%)	2 (2%)	1 (1%)	19	15
All	All	1198/1244 (96%)	1158 (97%)	37 (3%)	3 (0%)	41	41

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 (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	84/85 (99%)	83 (99%)	1 (1%)	71	77
1	B	84/85 (99%)	82 (98%)	2 (2%)	49	53
2	H	305/311 (98%)	294 (96%)	11 (4%)	35	36
2	J	302/311 (97%)	294 (97%)	8 (3%)	46	50
3	L	104/106 (98%)	101 (97%)	3 (3%)	42	46
3	M	103/106 (97%)	101 (98%)	2 (2%)	57	63
All	All	982/1004 (98%)	955 (97%)	27 (3%)	43	48

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

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Mol	Chain	Res	Type
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 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	$\#\|Z\| > 2$
3	TQQ	M	57	3	12,17,18	1.54	2 (16%)	11,24,26	3.72	3 (27%)
3	TQQ	L	57	3	12,17,18	1.84	3 (25%)	11,24,26	3.27	5 (45%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	57	TQQ	CZ3-CE3	4.21	1.41	1.34
3	M	57	TQQ	CZ3-CE3	3.74	1.41	1.34
3	M	57	TQQ	CZ3-CH2	-2.73	1.40	1.44
3	L	57	TQQ	CE2-CZ2	-2.65	1.46	1.50
3	L	57	TQQ	CZ3-CH2	-2.62	1.40	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	57	TQQ	CZ2-CE2-NE1	11.44	138.20	119.94
3	L	57	TQQ	CZ2-CE2-NE1	9.14	134.54	119.94
3	L	57	TQQ	O2-CZ2-CE2	-3.01	118.65	121.84
3	L	57	TQQ	CB-CG-CD2	3.01	133.63	127.09
3	L	57	TQQ	CB-CG-CD1	-2.81	124.49	127.97
3	M	57	TQQ	CD2-CE2-NE1	-2.73	105.23	109.64
3	M	57	TQQ	CB-CG-CD2	2.33	132.15	127.09
3	L	57	TQQ	CB-CA-C	2.02	115.25	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	57	TQQ	5	0
3	L	57	TQQ	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	0.57	0	5,5,5	1.14	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	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	1387	GOL	O2-C2-C3	2.04	118.12	109.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	1387	GOL	O2-C2-C3-O3
5	H	1387	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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^{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	105/105 (100%)	0.76	14 (13%) 3 4	28, 42, 57, 60	1 (0%)
1	B	105/105 (100%)	-0.15	4 (3%) 40 46	20, 25, 38, 52	1 (0%)
2	H	375/386 (97%)	-0.21	4 (1%) 80 84	14, 21, 35, 52	0
2	J	375/386 (97%)	0.44	26 (6%) 16 21	17, 32, 47, 55	0
3	L	124/131 (94%)	-0.18	3 (2%) 59 64	20, 27, 38, 53	0
3	M	124/131 (94%)	0.01	6 (4%) 30 36	14, 23, 42, 57	0
All	All	1208/1244 (97%)	0.11	57 (4%) 31 37	14, 27, 47, 60	2 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	ASP	6.2
2	J	274	ALA	5.1
2	J	208	THR	5.1
2	J	386	GLY	4.8
2	J	271	ALA	4.7
2	H	12	GLU	4.7
2	J	207	GLY	4.7
1	A	64	GLU	4.3
3	M	130	ALA	4.0
1	A	105	GLU	3.9
2	J	24	ALA	3.9
1	B	19	GLY	3.8
2	J	270	GLU	3.8
2	J	363	SER	3.6
2	J	342	GLU	3.5
2	J	30	GLN	3.5
1	A	65	ALA	3.4
2	J	343	LYS	3.4
2	J	12	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	17	ALA	3.3
2	J	28	ALA	3.2
2	J	13	THR	3.2
2	J	275	ASP	3.2
2	H	20	ARG	3.1
2	J	365	GLU	3.1
2	H	209	GLU	3.1
1	A	86	GLY	3.0
1	A	63	GLY	2.9
1	A	88	TYR	2.8
3	M	7	THR	2.7
1	A	60	GLY	2.7
3	M	68	GLN	2.7
2	H	386	GLY	2.7
3	M	131	SER	2.6
1	B	20	ALA	2.6
2	J	328	GLU	2.6
2	J	137	THR	2.5
1	A	36	HIS	2.5
1	A	7	SER	2.5
2	J	14	GLN	2.4
3	L	18	ASN	2.4
2	J	276	GLY	2.3
1	A	62	LEU	2.3
1	A	82	PHE	2.3
3	L	7	THR	2.3
1	A	61	VAL	2.3
3	M	65	THR	2.3
2	J	138	TYR	2.2
3	M	12	LYS	2.2
2	J	362	GLU	2.2
1	A	83	THR	2.2
2	J	322	GLU	2.2
1	A	14	ALA	2.1
2	J	364	GLY	2.1
2	J	80	LEU	2.1
3	L	131	SER	2.0
2	J	367	LEU	2.0

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^{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	TQQ	M	57	16/17	0.97	0.14	23,24,25,26	0
3	TQQ	L	57	16/17	0.97	0.11	22,24,26,27	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^{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
4	CU	A	1106	1/1	0.98	0.07	32,32,32,32	0
5	GOL	H	1387	6/6	0.98	0.13	21,23,27,27	0
4	CU	B	1106	1/1	0.99	0.06	28,28,28,28	0
6	NA	L	1132	1/1	0.99	0.14	18,18,18,18	0
6	NA	M	1131	1/1	0.99	0.18	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.