W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:53 AM GMT

PDB ID	:	2J55
Title	:	X-ray reduced Paraccocus denitrificans methylamine dehydrogenase O-quinone in complex with amicyanin.
Authors	:	Pearson, A.R.; Pahl, R.; Davidson, V.L.; Wilmot, C.M.
Deposited on	:	2006-09-12
Resolution	:	2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

http://wwpdb.org/validation/2016/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:

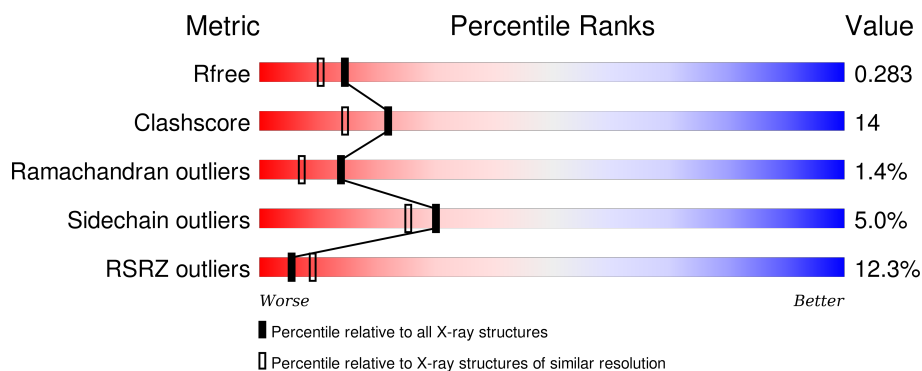|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.15 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		14
Ramachandran outliers		1.4%
Sidechain outliers		5.0%
RSRZ outliers		12.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	30% · 61% · 31% · 7% ·
1	B	105	9% · 78% · 21% ·
2	H	386	6% · 81% · 16% ··
2	J	386	20% · 71% · 24% · ·
3	L	131	5% · 60% · 32% · 5%

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Mol	Chain	Length	Quality of chain
3	M	131	3% ... 70% ... 20% ... 5% · 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TRQ	M	57	-	-	X	-
5	GOL	H	1387	-	-	-	X
5	GOL	H	1389	-	-	X	X
5	GOL	L	1132	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10411 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 806	C 516	N 132	O 152	S 6	0	0	0
1	B	105	Total 806	C 516	N 132	O 152	S 6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	382	Total 2988	C 1891	N 510	O 579	S 8	0	3	0
2	J	381	Total 2963	C 1876	N 508	O 571	S 8	0	1	0

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 956	C 590	N 161	O 192	S 13	0	0	0
3	M	125	Total 956	C 590	N 161	O 192	S 13	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cu 1	0	0
4	A	1	Total 1	Cu 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 6	C 3	O 3	0	0
5	H	1	Total 6	C 3	O 3	0	0
5	H	1	Total 6	C 3	O 3	0	0
5	L	1	Total 6	C 3	O 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total 29	O 29	0	0
6	B	109	Total 109	O 109	0	0
6	H	406	Total 406	O 406	0	0
6	J	205	Total 205	O 205	0	0

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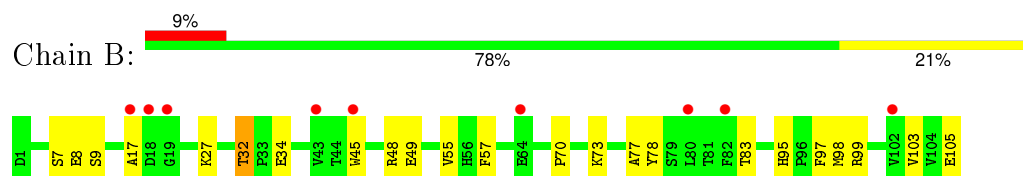| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	75	Total 75	O 75	0	0
6	M	86	Total 86	O 86	0	0

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 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.
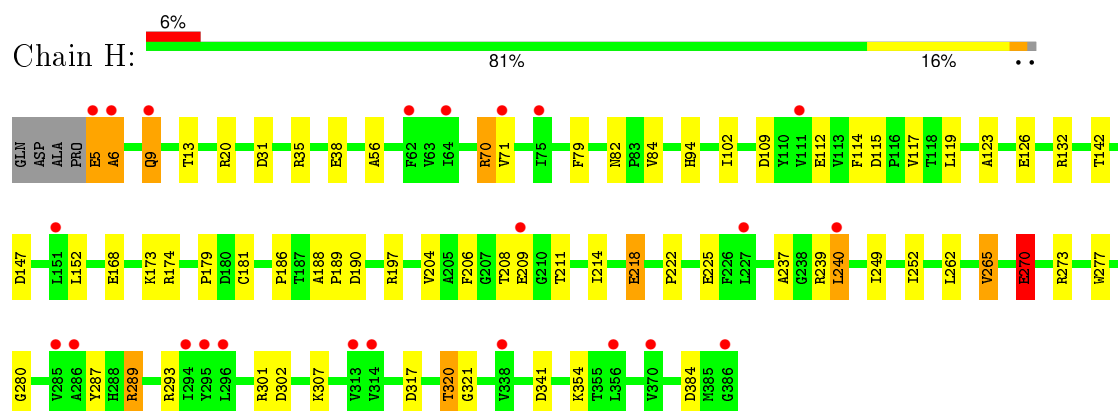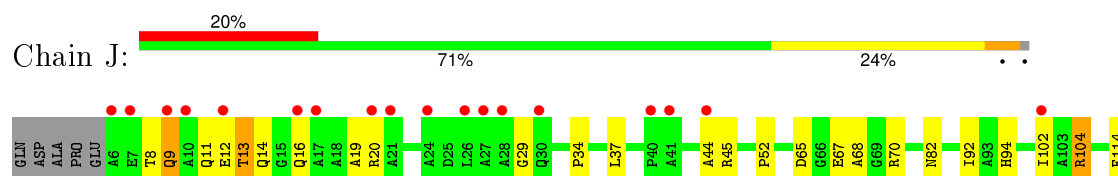
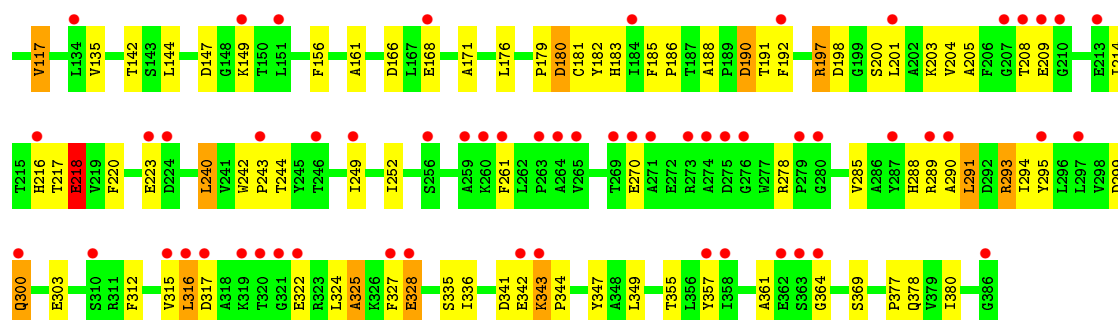- Molecule 1: AMICYANIN

- Molecule 1: AMICYANIN

- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN
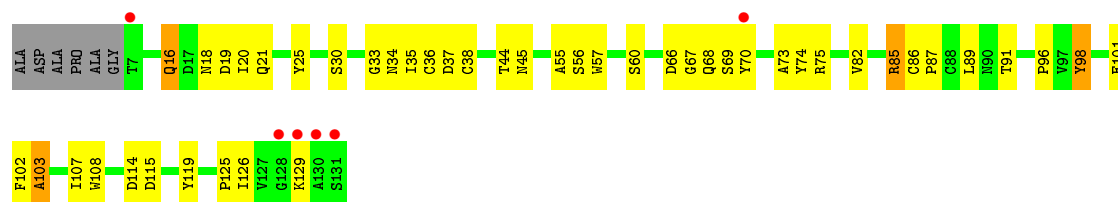

- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

V117 L134 V135 T142 S143 L144 D147 G148 K149 T150 L151 F156 A161 D166 L167 E168 A171 L176 P179 D180 C181 Y182 H183 I184 F185 P186 T187 A188 P189 D190 T191 F192 R197 D198 G199 S200 L201 A202 K203 V204 A205 P206 G207 T208 E209 G210 E213 I214

T215 H216 T217 E218 V219 F220 E223 D224 L240 V241 W242 P243 T244 Y245 T246 I249 I252 S256 A259 K260 F261 L262 P263 A264 V265 T269 E270 A271 E272 R273 A274 D275 G276 W277 R278 P279 G280 V285 A286 Y287 H288 R289 A290 L291 D292 R293 I294 Y295 L296 L297 V298 D299

Q300 E303 S310 R311 F312 V315 L316 D317 A318 K319 T320 G321 E322 R323 L324 A325 K326 F327 E328 S335 I336 D341 E342 K343 P344 Y347 A348 L349 T355 L356 Y357 I358 A361 E362 S363 G364 S369 P377 Q378 V379 I380 G386

● **Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN**

Chain L:

5%

60%32%5%

ALA ASP ALA PRO ALA GLY T7 Q16 D17 N18 D19 I20 Q21 Y25 S30 G33 N34 I35 C36 D37 C38 T44 N45 A55 S56 W57 S60 D66 G67 Q68 S69 Y70 A73 Y74 R75 V82 R85 C86 P87 C88 L89 N90 T91 P96 V97 Y98 E101

F102 A103 I107 W108 D114 D115 Y119 P125 I126 V127 G128 K129 A130 S131

● **Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN**

Chain M:

3%

70%20%5%5%

ALA ASP ALA PRO ALA GLY T7 K12 Q16 D17 N18 D19 I20 Y25 W26 R27 D37 L43 A53 W57 S60 C61 Y62 D66 G67 Q68 S69 Y70 A73 Y80 R85 E101 F102 W108 C109 D115 T118 Y119 H120 P125 I126 V127 G128

K129 A130 S131

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	122.73Å 122.73Å 246.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.70 – 2.15 21.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (21.70-2.15) 98.9 (21.70-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.33 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.245 0.231 , 0.283	Depositor DCC
R_{free} test set	5081 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.31$	Xtriage
Outliers	1 of 101510 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10411	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	1.05	0/827	1.04	2/1122 (0.2%)
1	B	1.30	2/827 (0.2%)	1.02	2/1122 (0.2%)
2	H	1.50	20/3071 (0.7%)	1.38	18/4184 (0.4%)
2	J	1.16	7/3043 (0.2%)	1.06	9/4147 (0.2%)
3	L	1.31	3/964 (0.3%)	1.03	2/1315 (0.2%)
3	M	1.26	1/964 (0.1%)	1.04	3/1315 (0.2%)
All	All	1.31	33/9696 (0.3%)	1.16	36/13205 (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	A	0	1
2	H	0	1
3	M	0	1
All	All	0	3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	70	ARG	CZ-NH1	9.95	1.46	1.33
2	H	270[A]	GLU	CB-CG	9.65	1.70	1.52
2	H	270[B]	GLU	CB-CG	9.65	1.70	1.52
2	H	71	VAL	CB-CG1	8.91	1.71	1.52
1	B	9	SER	CB-OG	7.71	1.52	1.42

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	70	ARG	NE-CZ-NH1	34.49	137.55	120.30
2	H	70	ARG	NE-CZ-NH2	-32.05	104.28	120.30
2	H	289	ARG	NE-CZ-NH1	-13.92	113.34	120.30
2	J	197	ARG	NE-CZ-NH1	-12.22	114.19	120.30
2	H	197	ARG	NE-CZ-NH2	11.45	126.02	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ALA	Peptide
2	H	320	THR	Peptide
3	M	129	LYS	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	806	0	790	37	0
1	B	806	0	790	19	0
2	H	2988	0	2862	40	0
2	J	2963	0	2843	98	0
3	L	956	0	857	44	0
3	M	956	0	857	31	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	H	18	0	24	12	0
5	L	6	0	8	2	0
6	A	29	0	0	9	0
6	B	109	0	0	4	2
6	H	406	0	0	13	2
6	J	205	0	0	14	0
6	L	75	0	0	2	0
6	M	86	0	0	8	0
All	All	10411	0	9031	255	2

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.

The worst 5 of 255 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:TRQ:CE3	3:M:108:TRP:HD1	0.86	1.49
2:H:70:ARG:NH2	5:H:1389:GOL:H2	1.27	1.43
1:A:14:ALA:O	1:A:16:VAL:N	1.70	1.20
2:H:289:ARG:NH1	2:H:384:ASP:OD2	1.81	1.13
2:H:70:ARG:CZ	5:H:1389:GOL:H2	1.88	1.03

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2028:HOH:O	6:H:2034:HOH:O[8_665]	1.99	0.21
6:B:2011:HOH:O	6:H:2272:HOH:O[8_665]	2.10	0.10

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%)	90 (87%)	6 (6%)	7 (7%)	1	0
1	B	103/105 (98%)	100 (97%)	2 (2%)	1 (1%)	19	11
2	H	383/386 (99%)	369 (96%)	12 (3%)	2 (0%)	34	26
2	J	380/386 (98%)	350 (92%)	25 (7%)	5 (1%)	15	8
3	L	122/131 (93%)	115 (94%)	6 (5%)	1 (1%)	24	15
3	M	122/131 (93%)	113 (93%)	7 (6%)	2 (2%)	12	5
All	All	1213/1244 (98%)	1137 (94%)	58 (5%)	18 (2%)	14	6

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ALA
1	A	15	GLU
1	A	17	ALA
2	H	6	ALA
2	J	9	GLN

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%)	75 (89%)	9 (11%)	8	4
1	B	84/85 (99%)	80 (95%)	4 (5%)	31	27
2	H	311/311 (100%)	298 (96%)	13 (4%)	36	34
2	J	308/311 (99%)	292 (95%)	16 (5%)	29	23
3	L	104/106 (98%)	101 (97%)	3 (3%)	50	49
3	M	104/106 (98%)	98 (94%)	6 (6%)	25	19
All	All	995/1004 (99%)	944 (95%)	51 (5%)	30	24

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	270[A]	GLU
2	J	117	VAL
3	M	18	ASN
2	H	354	LYS
2	J	208	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	34	ASN
3	M	68	GLN
3	M	18	ASN
3	L	16	GLN

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Mol	Chain	Res	Type
3	M	16	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)

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	TRQ	L	57	3	14,17,18	2.71	5 (35%)	8,24,26	1.94	2 (25%)
3	TRQ	M	57	3	14,17,18	3.31	5 (35%)	8,24,26	2.20	4 (50%)

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	TRQ	L	57	3	-	0/3/19/21	0/2/2/2
3	TRQ	M	57	3	-	0/3/19/21	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	57	TRQ	CZ3-CH2	-3.32	1.36	1.45
3	M	57	TRQ	CZ3-CH2	-2.09	1.40	1.45
3	L	57	TRQ	CB-CA	2.04	1.58	1.53
3	M	57	TRQ	O7-CZ2	3.17	1.30	1.23
3	L	57	TRQ	CZ3-CE3	3.72	1.40	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	57	TRQ	CB-CG-CD1	-3.27	123.93	127.97
3	M	57	TRQ	CB-CG-CD1	-2.40	125.00	127.97
3	M	57	TRQ	CD2-CE3-CZ3	2.37	123.82	121.16
3	M	57	TRQ	CB-CG-CD2	2.43	130.12	124.40
3	M	57	TRQ	CD1-NE1-CE2	3.42	113.18	104.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	57	TRQ	4	0
3	M	57	TRQ	6	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	0.55	0	5,5,5	0.90	0
5	GOL	H	1388	-	5,5,5	0.71	0	5,5,5	1.05	0
5	GOL	H	1389	2	5,5,5	0.59	0	5,5,5	1.39	1 (20%)
5	GOL	L	1132	3	5,5,5	0.55	0	5,5,5	0.94	0

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
5	GOL	H	1388	-	-	0/4/4/4	0/0/0/0
5	GOL	H	1389	2	-	0/4/4/4	0/0/0/0
5	GOL	L	1132	3	-	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(^{o})	Ideal(^{o})
5	H	1389	GOL	O3-C3-C2	3.03	124.88	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1387	GOL	1	0
5	H	1389	GOL	11	0
5	L	1132	GOL	2	0

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, 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	105/105 (100%)	1.64	32 (30%)	1	1	62, 79, 91, 97	0
1	B	105/105 (100%)	0.50	9 (8%)	13	19	48, 56, 68, 81	0
2	H	382/386 (98%)	0.31	23 (6%)	25	34	38, 48, 64, 86	0
2	J	381/386 (98%)	1.15	76 (19%)	1	2	46, 71, 89, 97	0
3	L	124/131 (94%)	0.55	6 (4%)	34	45	48, 61, 74, 104	0
3	M	124/131 (94%)	0.49	4 (3%)	51	61	40, 54, 72, 102	0
All	All	1221/1244 (98%)	0.75	150 (12%)	5	9	38, 59, 87, 104	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	274	ALA	7.9
2	J	28	ALA	7.5
2	J	386	GLY	7.1
3	M	131	SER	6.9
2	J	6	ALA	6.8

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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	TRQ	L	57	16/17	0.95	0.15	-	54,57,60,61	0
3	TRQ	M	57	16/17	0.97	0.17	-	54,57,59,59	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	GOL	H	1387	6/6	0.84	0.26	10.26	66,71,74,75	0
5	GOL	L	1132	6/6	0.82	0.31	7.95	75,76,77,77	0
5	GOL	H	1389	6/6	0.90	0.25	3.47	39,46,54,58	0
5	GOL	H	1388	6/6	0.95	0.11	-0.06	27,42,45,51	0
4	CU	B	1106	1/1	0.98	0.10	-1.85	65,65,65,65	0
4	CU	A	1106	1/1	0.91	0.07	-3.68	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.