



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:52 PM UTC

PDB ID : 2J56 / pdb_00002j56
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

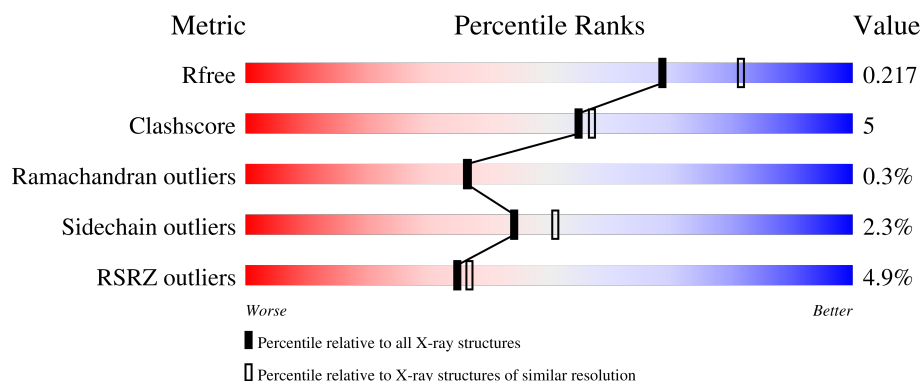
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	105	24% 89% 10% .
1	B	105	5% 91% 8% .
2	H	386	% 88% 7% ..
2	J	386	4% 87% 9% ..
3	L	131	3% 84% 10% 5%

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Mol	Chain	Length	Quality of chain
3	M	131	3% 83% 9% •• 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

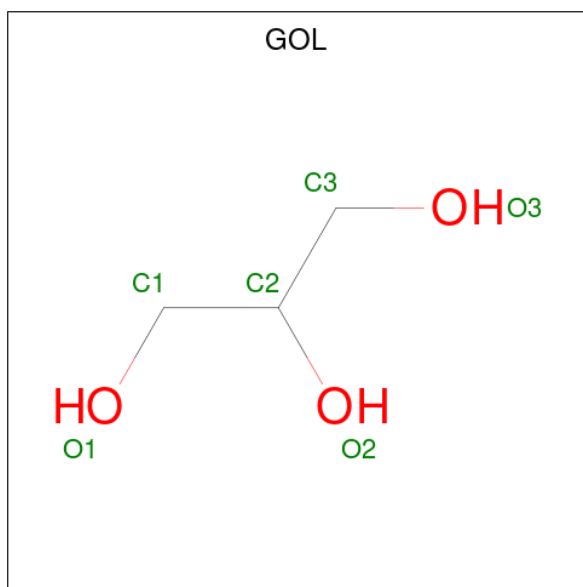
- Molecule 3 is a protein called METHYLAMINE DEHYDROGENASE LIGHT CHAIN.

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 (CCD ID: CU) (formula: Cu).

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

- Molecule 5 is GLYCEROL (CCD ID: 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 (CCD ID: 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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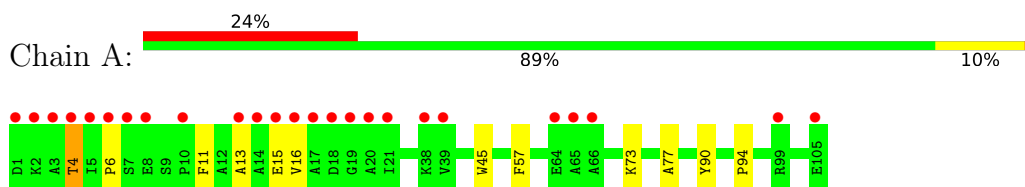
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	417	Total 417	O 417	0	0
7	J	278	Total 278	O 278	0	0
7	L	91	Total 91	O 91	0	0
7	M	99	Total 99	O 99	0	0

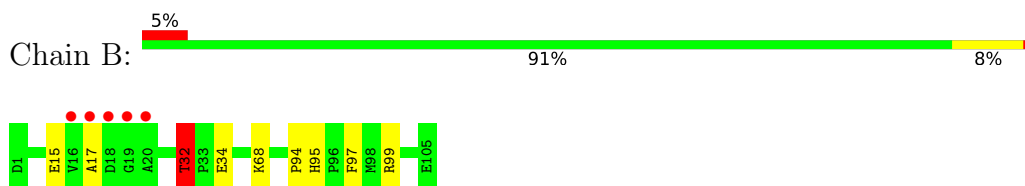
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

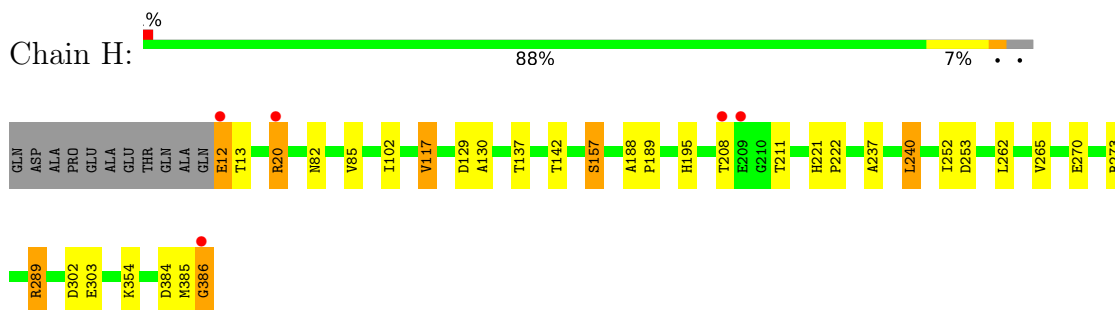
- Molecule 1: AMICYANIN



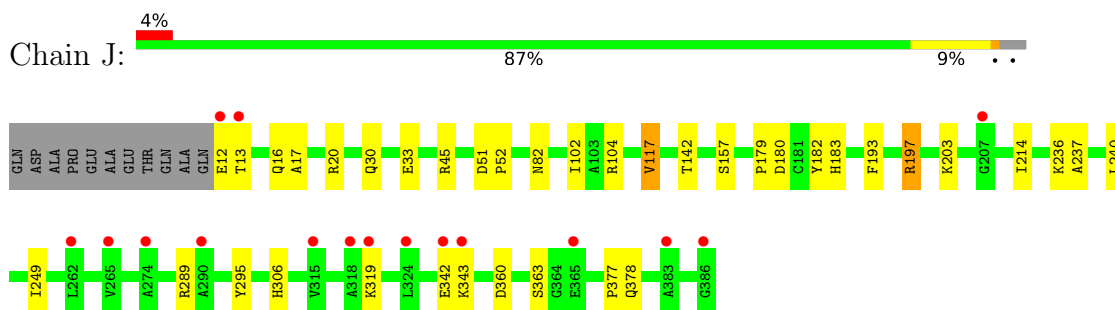
- Molecule 1: AMICYANIN



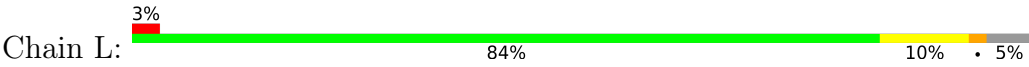
- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN



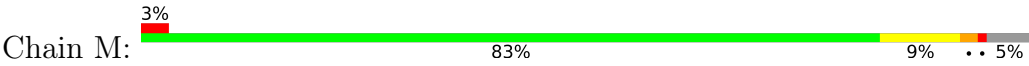
- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN



- Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN



● 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, α , β , γ	123.03Å 123.03Å 245.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.48 – 2.10 43.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (43.48-2.10) 97.3 (43.48-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.84 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.169 , 0.207 (Not available) , 0.217	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)	0.39 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, TQQ, 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	0.81	0/827	0.85	0/1122
1	B	1.00	0/827	0.95	1/1122 (0.1%)
2	H	1.01	1/3009 (0.0%)	1.02	7/4100 (0.2%)
2	J	0.92	1/2987 (0.0%)	0.94	6/4071 (0.1%)
3	L	1.00	1/964 (0.1%)	0.98	0/1315
3	M	0.96	1/958 (0.1%)	0.94	1/1309 (0.1%)
All	All	0.96	4/9572 (0.0%)	0.96	15/13039 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	130	ALA	C-N	-6.47	1.24	1.33
3	L	82	VAL	CA-CB	6.43	1.60	1.54
2	J	117	VAL	CA-CB	5.78	1.62	1.54
2	H	85	VAL	CA-CB	5.14	1.61	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	THR	CB-CA-C	-8.58	96.00	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	197	ARG	NE-CZ-NH1	-7.47	114.03	121.50
2	H	386	GLY	N-CA-C	-7.09	92.75	113.30
2	H	157	SER	CA-C-N	6.96	128.54	119.84
2	H	157	SER	C-N-CA	6.96	128.54	119.84
2	H	117	VAL	N-CA-C	6.46	117.14	111.90
3	M	104	ASN	N-CA-C	6.27	121.70	113.30
2	J	197	ARG	CG-CD-NE	-6.15	98.47	112.00
2	J	197	ARG	NE-CZ-NH2	5.82	124.44	119.20
2	J	306	HIS	N-CA-C	5.75	119.91	113.01
2	H	137	THR	N-CA-C	5.46	117.62	109.59
2	J	342	GLU	N-CA-C	5.36	116.80	111.07
2	H	385	MET	CA-C-N	5.20	131.06	121.70
2	H	385	MET	C-N-CA	5.20	131.06	121.70
2	J	104	ARG	CG-CD-NE	-5.12	100.73	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

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	7	0
1	B	806	0	790	9	0
2	H	2929	0	2811	17	0
2	J	2910	0	2796	32	0
3	L	956	0	858	13	0
3	M	950	0	853	16	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
7	L	91	0	0	1	0
7	M	99	0	0	2	0
All	All	10400	0	8906	87	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 5.

All (87) 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:HG3	2:H:20:ARG:HH11	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
1:B:99:ARG:HH22	2:J:180:ASP:CG	1.95	0.73
2:H:20:ARG:HH11	2:H:20:ARG:CG	2.02	0.73
1:B:17:ALA:HB1	7:B:2019:HOH:O	1.91	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
2:J:13:THR:HG22	2:J:16:GLN:CD	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:12:GLU:CD	2:J:20:ARG:HH12	2.09	0.60
3:M:16:GLN:HE22	3:M:19:ASP:H	1.49	0.59
2:H:20:ARG:HG3	2:H:20:ARG:NH1	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
3:L:57:TQQ:HB2	3:L:108:TRP:HE1	1.71	0.55
3:M:129:LYS:C	3:M:131:SER:N	2.65	0.54
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:HA	2:H:12:GLU:OE1	2.11	0.50
2:H:289:ARG:NH1	2:H:384:ASP:OD1	2.45	0.49
2:J:12:GLU:CD	2:J:20:ARG:NH1	2.68	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
3:L:16:GLN:HE21	3:L:16:GLN:C	2.23	0.47
2:J:51:ASP:HA	2:J:377:PRO:HA	1.96	0.47
2:J:360:ASP:OD1	2:J:363:SER:OG	2.31	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
3:M:98:TYR:C	3:M:100:PRO:HD3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:236:LYS:NZ	7:J:2188:HOH:O	2.49	0.44
1:A:13:ALA:C	1:A:15:GLU:H	2.25	0.43
2:H:302:ASP:CG	2:H:303:GLU:N	2.76	0.43
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
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: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
3:M:53:ALA:HB2	3:M:109:CYS:HA	2.01	0.42
1:A:57:PHE:CE2	1:A:90:TYR:HB3	2.55	0.41
2:H:129:ASP:O	2:H:130:ALA:C	2.63	0.41
2:J:182:TYR:O	2:J:183:HIS:HB2	2.21	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
2:H:253:ASP:OD1	2:H:253:ASP:C	2.64	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%)	36	36
2	J	373/386 (97%)	362 (97%)	10 (3%)	1 (0%)	36	36
3	L	122/131 (93%)	119 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	122/131 (93%)	119 (98%)	2 (2%)	1 (1%)	16	12
All	All	1198/1244 (96%)	1158 (97%)	37 (3%)	3 (0%)	36	36

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%)	63	72
1	B	84/85 (99%)	82 (98%)	2 (2%)	43	49
2	H	305/311 (98%)	294 (96%)	11 (4%)	31	34
2	J	302/311 (97%)	297 (98%)	5 (2%)	53	62
3	L	104/106 (98%)	102 (98%)	2 (2%)	50	58
3	M	103/106 (97%)	101 (98%)	2 (2%)	50	58
All	All	982/1004 (98%)	959 (98%)	23 (2%)	44	51

All (23) 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	117	VAL
2	H	208	THR

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Mol	Chain	Res	Type
2	H	211	THR
2	H	240	LEU
2	H	262	LEU
2	H	265	VAL
2	H	289	ARG
2	H	354	LYS
2	J	30	GLN
2	J	117	VAL
2	J	240	LEU
2	J	249	ILE
2	J	319	LYS
3	L	16	GLN
3	L	60	SER
3	M	16	GLN
3	M	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
2	H	16	GLN
2	H	50	ASN
2	H	61	GLN
2	H	221	HIS
2	H	378	GLN
2	J	16	GLN
2	J	50	ASN
2	J	61	GLN
2	J	378	GLN
3	L	16	GLN
3	L	34	ASN
3	L	68	GLN
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	16,17,18	2.16	5 (31%)	14,24,26	2.15	4 (28%)
3	TQQ	L	57	3	16,17,18	2.26	6 (37%)	14,24,26	1.96	4 (28%)

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	-	1/5/19/21	0/2/2/2
3	TQQ	L	57	3	-	0/5/19/21	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	57	TQQ	CH2-N2	5.90	1.37	1.28
3	M	57	TQQ	CH2-N2	5.87	1.37	1.28
3	M	57	TQQ	CD2-CG	3.62	1.49	1.42
3	L	57	TQQ	CD2-CG	3.30	1.48	1.42
3	L	57	TQQ	CZ3-CE3	2.72	1.41	1.35
3	M	57	TQQ	CZ3-CH2	-2.67	1.40	1.44
3	L	57	TQQ	CZ3-CH2	-2.55	1.40	1.44
3	M	57	TQQ	CZ3-CE3	2.36	1.41	1.35
3	L	57	TQQ	CE3-CD2	2.20	1.45	1.40
3	L	57	TQQ	CE2-NE1	-2.16	1.34	1.38
3	M	57	TQQ	CE3-CD2	2.09	1.45	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	57	TQQ	CD1-CG-CD2	-4.96	101.48	105.95
3	L	57	TQQ	CD1-CG-CD2	-4.54	101.85	105.95
3	M	57	TQQ	CZ2-CE2-NE1	4.50	138.20	127.25
3	L	57	TQQ	CG-CD1-NE1	3.55	113.80	109.22
3	M	57	TQQ	CG-CD1-NE1	3.03	113.13	109.22
3	L	57	TQQ	CZ2-CE2-NE1	2.99	134.54	127.25
3	L	57	TQQ	CB-CG-CD2	2.96	133.63	127.63
3	M	57	TQQ	CB-CG-CD2	2.23	132.15	127.63

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	57	TQQ	C-CA-CB-CG

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 oligosaccharides 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	0.59	0	5,5,5	1.21	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(°)	Ideal(°)
5	H	1387	GOL	O2-C2-C3	2.16	118.12	109.18

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	105/105 (100%)	1.26	25 (23%) 2 2	28, 41, 57, 60	1 (0%)
1	B	105/105 (100%)	0.03	5 (4%) 35 38	20, 25, 38, 48	1 (0%)
2	H	375/386 (97%)	-0.39	5 (1%) 75 77	14, 21, 35, 52	2 (0%)
2	J	375/386 (97%)	0.46	16 (4%) 40 41	17, 32, 47, 55	0
3	L	124/131 (94%)	0.06	4 (3%) 50 53	20, 27, 38, 53	0
3	M	124/131 (94%)	-0.24	4 (3%) 50 53	14, 23, 42, 57	0
All	All	1208/1244 (97%)	0.12	59 (4%) 35 37	14, 27, 47, 60	4 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	386	GLY	5.7
2	H	12	GLU	5.6
1	A	14	ALA	4.7
3	M	130	ALA	4.5
1	B	18	ASP	3.7
2	J	13	THR	3.7
3	M	131	SER	3.7
1	A	7	SER	3.6
1	A	39	VAL	3.3
1	B	16	VAL	3.3
3	L	131	SER	3.2
3	L	13	TRP	3.1
1	B	17	ALA	3.1
1	A	18	ASP	3.1
1	B	19	GLY	3.1
1	B	20	ALA	3.1
2	J	290	ALA	3.0
1	A	66	ALA	3.0
2	J	343	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	16	VAL	2.9
1	A	5	ILE	2.9
1	A	64	GLU	2.9
2	H	209	GLU	2.9
2	J	386	GLY	2.8
1	A	17	ALA	2.8
1	A	38	LYS	2.7
2	J	342	GLU	2.7
1	A	1	ASP	2.7
2	J	274	ALA	2.6
2	H	20	ARG	2.6
2	J	12	GLU	2.6
1	A	15	GLU	2.5
1	A	19	GLY	2.5
1	A	20	ALA	2.5
3	M	129	LYS	2.4
2	J	207	GLY	2.4
1	A	8	GLU	2.4
1	A	105	GLU	2.4
1	A	6	PRO	2.4
2	J	324	LEU	2.4
3	L	68	GLN	2.4
2	J	319	LYS	2.4
1	A	10	PRO	2.3
1	A	13	ALA	2.3
1	A	65	ALA	2.3
1	A	4	THR	2.3
1	A	3	ALA	2.3
2	J	315	VAL	2.2
2	J	262	LEU	2.2
3	M	13	TRP	2.2
3	L	130	ALA	2.2
2	J	318	ALA	2.2
1	A	21	ILE	2.1
2	J	265	VAL	2.1
2	J	383	ALA	2.1
2	H	208	THR	2.1
1	A	2	LYS	2.1
2	J	365	GLU	2.0
1	A	99	ARG	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TQQ	L	57	16/17	0.96	0.06	22,24,26,27	0
3	TQQ	M	57	16/17	0.97	0.06	23,24,25,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CU	A	1106	1/1	0.98	0.04	32,32,32,32	0
5	GOL	H	1387	6/6	0.98	0.06	21,23,27,27	0
6	NA	M	1131	1/1	0.98	0.04	23,23,23,23	0
6	NA	L	1132	1/1	0.99	0.03	18,18,18,18	0
4	CU	B	1106	1/1	0.99	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.