wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 10:06 AM EDT

PDB ID	:	2J57
Title	:	X-ray reduced Paraccocus denitrificans methylamine dehydrogenase N- quinol in complex with amicyanin.
Authors	:	Pearson, A.R.; Pahl, R.; Davidson, V.L.; Wilmot, C.M.
Deposited on	:	2006-09-12
Resolution	:	2.25 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

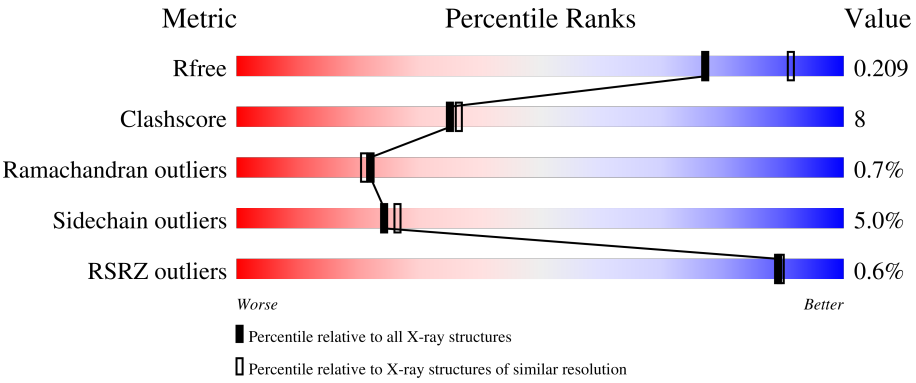
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	81% 18%
1	B	105	83% 16%
1	C	105	88% 10%
1	D	105	% 84% 15%
2	G	386	84% 14%

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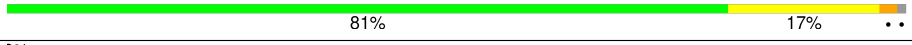
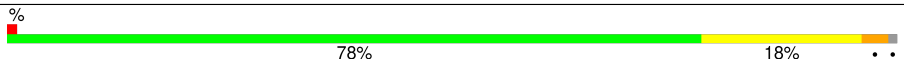
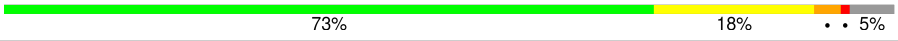
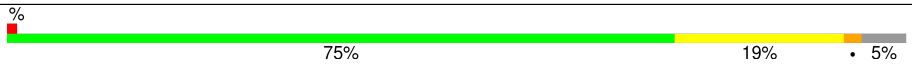
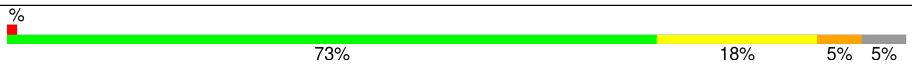
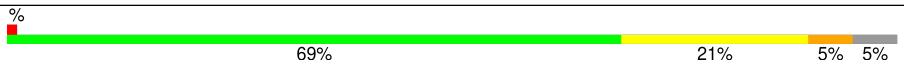
Mol	Chain	Length	Quality of chain
2	H	386	
2	I	386	
2	J	386	
3	K	131	
3	L	131	
3	M	131	
3	N	131	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20786 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			
1	C	105	Total	C	N	O	S	0	0	0
			806	516	132	152	6			
1	D	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	G	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
2	H	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
2	I	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
2	J	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	312	PHE	LEU	SEE REMARK 999	UNP P29894
G	313	VAL	LEU	SEE REMARK 999	UNP P29894
H	312	PHE	LEU	SEE REMARK 999	UNP P29894
H	313	VAL	LEU	SEE REMARK 999	UNP P29894
I	312	PHE	LEU	SEE REMARK 999	UNP P29894
I	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	K	125	Total	C	N	O	S	0	0	0
			956	590	162	191	13			
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	0
			956	590	162	191	13			
3	N	125	Total	C	N	O	S	0	0	0
			956	590	162	191	13			

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	97	Total	O	0	0
			97	97		
5	C	101	Total	O	0	0
			101	101		
5	D	42	Total	O	0	0
			42	42		
5	G	408	Total	O	0	0
			408	408		
5	H	418	Total	O	0	0
			418	418		
5	I	175	Total	O	0	0
			175	175		
5	J	262	Total	O	0	0
			262	262		
5	K	72	Total	O	0	0
			72	72		

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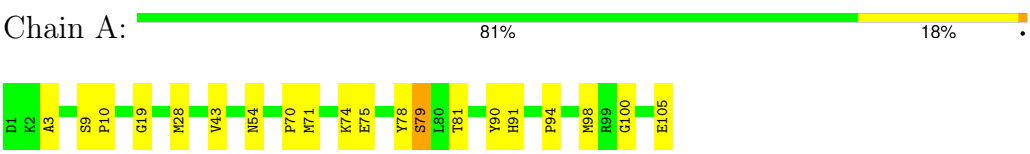
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	80	Total O 80 80	0	0
5	M	90	Total O 90 90	0	0
5	N	73	Total O 73 73	0	0

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.

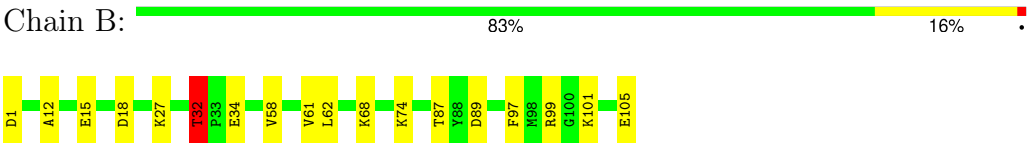
• Molecule 1: AMICYANIN

Chain A:



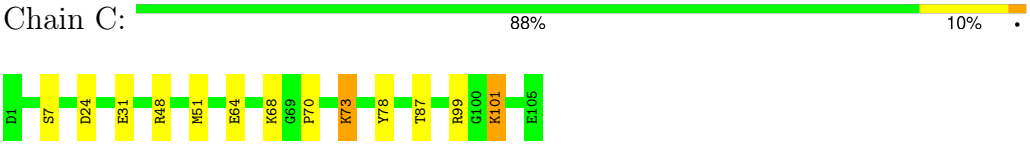
• Molecule 1: AMICYANIN

Chain B:



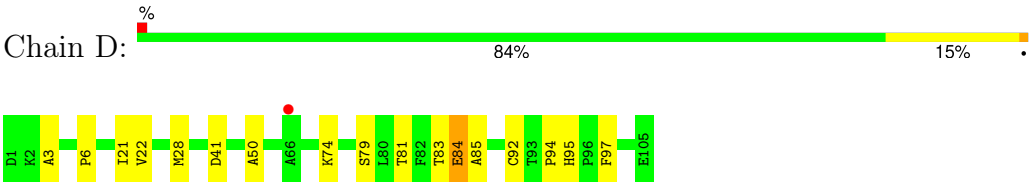
• Molecule 1: AMICYANIN

Chain C:



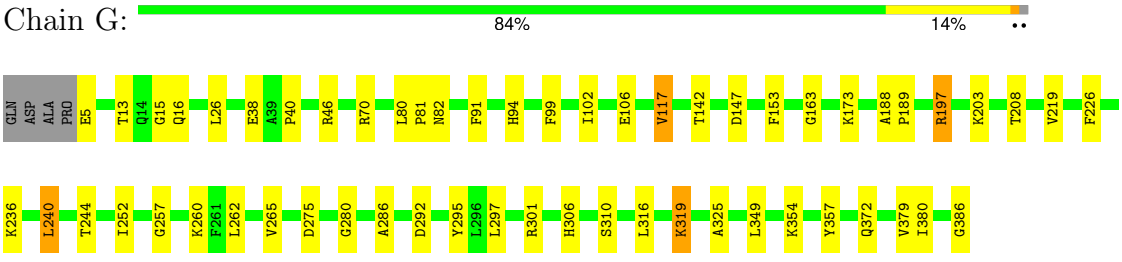
• Molecule 1: AMICYANIN

Chain D:



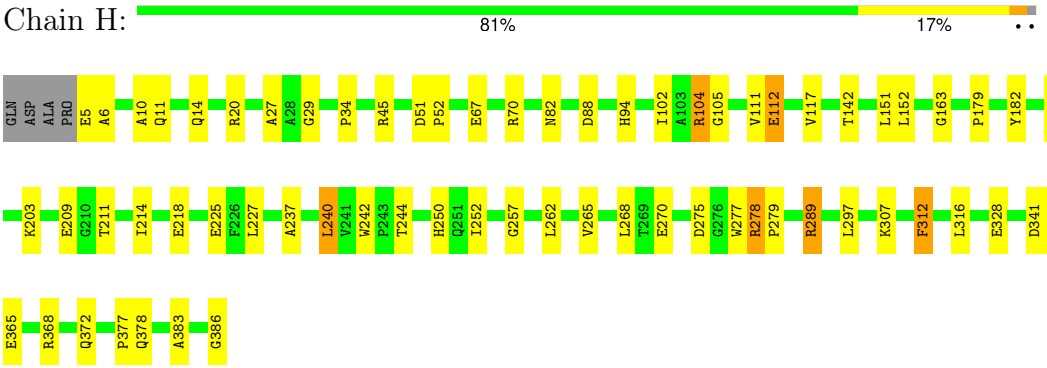
• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain G:



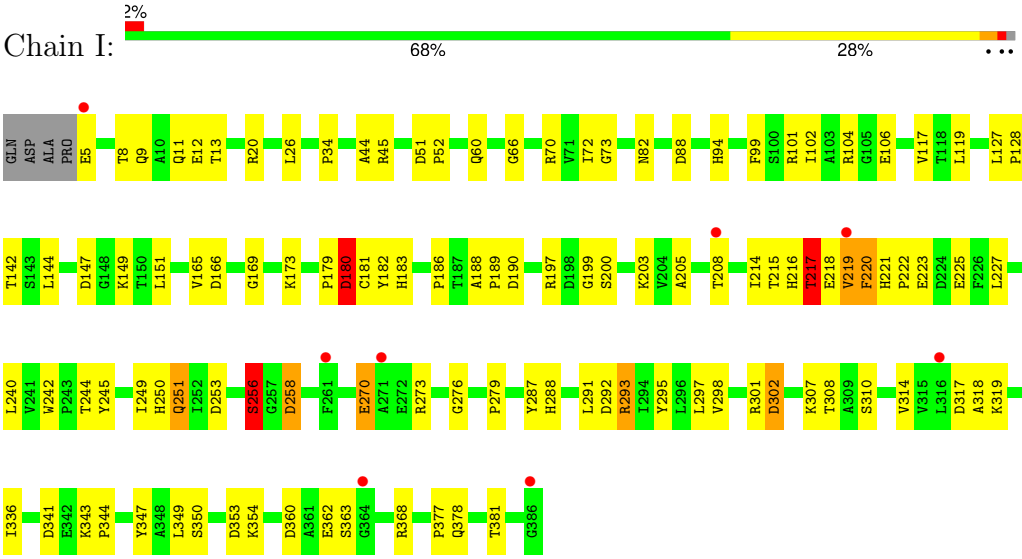
• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain H:



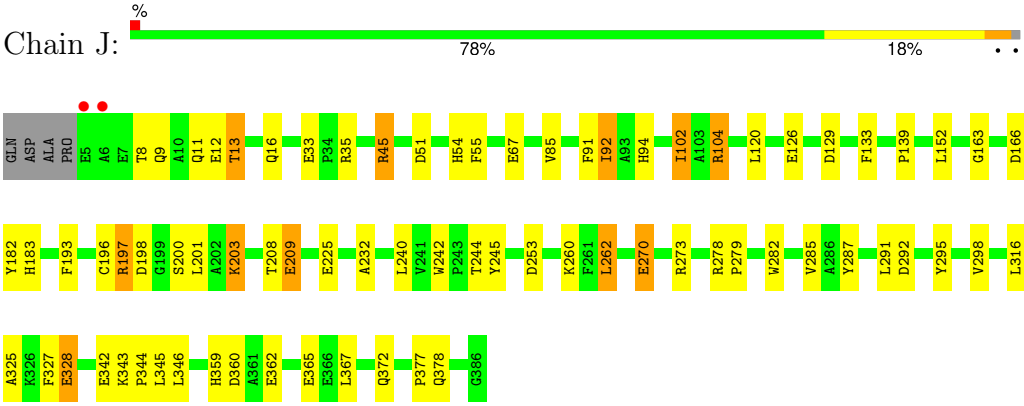
• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain I:



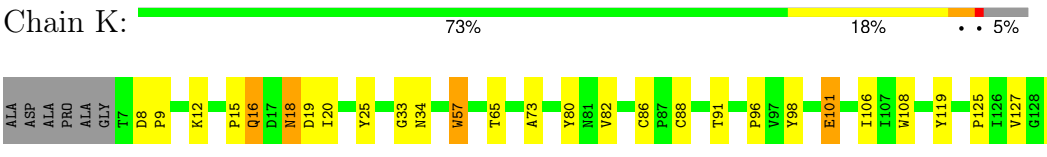
• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain J:



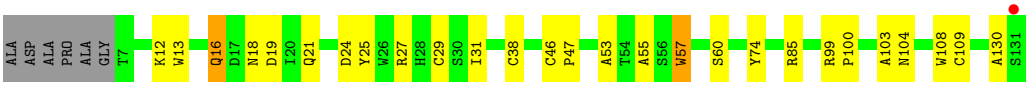
• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain K:



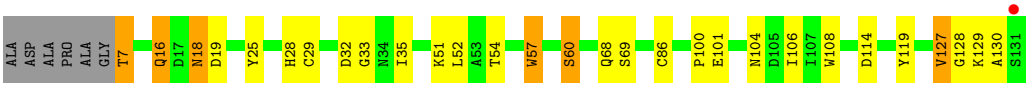
• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain L:



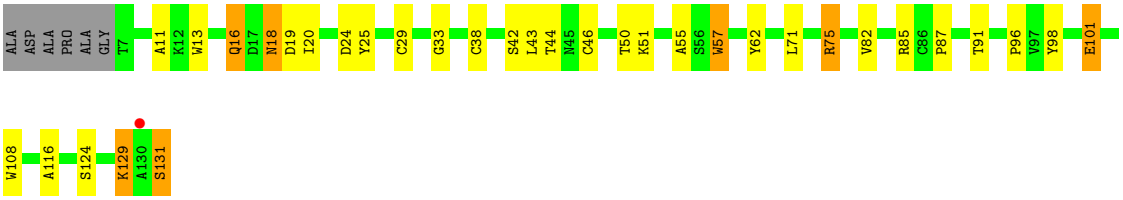
• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain M:



• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.13Å 123.44Å 246.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.25 45.85 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.39-2.25) 94.5 (45.85-2.25)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.179 , 0.241 0.182 , 0.209	Depositor DCC
R_{free} test set	8629 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 31.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.126 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20786	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: CU, TQQ

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	0.92	0/827	0.84	0/1122
1	B	1.12	0/827	0.91	1/1122 (0.1%)
1	C	1.03	0/827	0.92	0/1122
1	D	0.89	0/827	0.86	0/1122
2	G	1.15	6/3044 (0.2%)	1.01	4/4148 (0.1%)
2	H	1.17	7/3044 (0.2%)	1.04	10/4148 (0.2%)
2	I	0.91	2/3044 (0.1%)	0.90	3/4148 (0.1%)
2	J	1.02	2/3044 (0.1%)	0.95	5/4148 (0.1%)
3	K	1.09	3/964 (0.3%)	0.97	1/1315 (0.1%)
3	L	1.10	3/964 (0.3%)	0.98	3/1315 (0.2%)
3	M	1.11	0/964	0.94	0/1315
3	N	1.00	2/964 (0.2%)	0.98	3/1315 (0.2%)
All	All	1.06	25/19340 (0.1%)	0.96	30/26340 (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
3	K	0	1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	86	CYS	CB-SG	-7.53	1.69	1.82
2	H	218	GLU	CB-CG	6.83	1.65	1.52
3	K	88	CYS	CB-SG	-6.79	1.70	1.82
2	G	357	TYR	CD1-CE1	6.78	1.49	1.39
2	G	91	PHE	CE2-CZ	6.15	1.49	1.37

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	197	ARG	NE-CZ-NH1	-10.78	114.91	120.30
2	G	147	ASP	CB-CG-OD1	9.81	127.13	118.30
2	H	70	ARG	NE-CZ-NH1	9.42	125.01	120.30
3	K	8	ASP	CB-CG-OD1	8.49	125.94	118.30
2	J	197	ARG	NE-CZ-NH2	8.21	124.41	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	130	ALA	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	14	0
1	B	806	0	790	13	0
1	C	806	0	790	9	0
1	D	806	0	790	10	0
2	G	2967	0	2845	31	0
2	H	2967	0	2845	34	0
2	I	2967	0	2845	80	0
2	J	2967	0	2845	50	0
3	K	956	0	858	22	0
3	L	956	0	858	19	0
3	M	956	0	858	22	0
3	N	956	0	858	28	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	48	0	0	1	0
5	B	97	0	0	3	0
5	C	101	0	0	4	1
5	D	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	408	0	0	6	0
5	H	418	0	0	8	1
5	I	175	0	0	13	0
5	J	262	0	0	9	0
5	K	72	0	0	0	0
5	L	80	0	0	1	0
5	M	90	0	0	2	0
5	N	73	0	0	2	0
All	All	20786	0	17972	302	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 302 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:N:57:TQQ:CE3	3:N:108:TRP:HD1	0.94	1.56
2:I:179:PRO:HB2	5:I:2117:HOH:O	1.49	1.13
3:N:57:TQQ:CZ3	3:N:108:TRP:HD1	1.68	1.07
2:I:293:ARG:HD3	2:I:324:LEU:HD13	1.48	0.95
2:I:287:TYR:OH	2:I:292:ASP:OD1	1.90	0.90

All (1) 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)
5:C:2017:HOH:O	5:H:2282:HOH:O[3_655]	2.04	0.16

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%)	98 (95%)	5 (5%)	0	100 100
1	B	103/105 (98%)	96 (93%)	7 (7%)	0	100 100
1	C	103/105 (98%)	103 (100%)	0	0	100 100
1	D	103/105 (98%)	99 (96%)	2 (2%)	2 (2%)	8 4
2	G	380/386 (98%)	366 (96%)	13 (3%)	1 (0%)	41 46
2	H	380/386 (98%)	359 (94%)	19 (5%)	2 (0%)	29 29
2	I	380/386 (98%)	352 (93%)	21 (6%)	7 (2%)	8 4
2	J	380/386 (98%)	359 (94%)	19 (5%)	2 (0%)	29 29
3	K	122/131 (93%)	114 (93%)	6 (5%)	2 (2%)	9 5
3	L	122/131 (93%)	119 (98%)	3 (2%)	0	100 100
3	M	122/131 (93%)	118 (97%)	4 (3%)	0	100 100
3	N	122/131 (93%)	118 (97%)	4 (3%)	0	100 100
All	All	2420/2488 (97%)	2301 (95%)	103 (4%)	16 (1%)	22 21

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	180	ASP
2	I	220	PHE
2	I	249	ILE
2	I	217	THR
3	K	101	GLU

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%)	82 (98%)	2 (2%)	49 58
1	B	84/85 (99%)	81 (96%)	3 (4%)	35 42
1	C	84/85 (99%)	80 (95%)	4 (5%)	25 28
1	D	84/85 (99%)	84 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	308/311 (99%)	295 (96%)	13 (4%)	30 34
2	H	308/311 (99%)	296 (96%)	12 (4%)	32 38
2	I	308/311 (99%)	284 (92%)	24 (8%)	12 11
2	J	308/311 (99%)	289 (94%)	19 (6%)	18 17
3	K	104/106 (98%)	100 (96%)	4 (4%)	33 39
3	L	104/106 (98%)	101 (97%)	3 (3%)	42 51
3	M	104/106 (98%)	95 (91%)	9 (9%)	10 8
3	N	104/106 (98%)	98 (94%)	6 (6%)	20 20
All	All	1984/2008 (99%)	1885 (95%)	99 (5%)	24 26

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	354	LYS
2	J	291	LEU
2	J	33	GLU
2	J	240	LEU
2	J	342	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	N	57	3	13,17,18	2.68	6 (46%)	10,24,26	3.02	2 (20%)
3	TQQ	L	57	3	13,17,18	3.08	5 (38%)	10,24,26	3.17	5 (50%)
3	TQQ	M	57	3	13,17,18	2.68	4 (30%)	10,24,26	2.94	3 (30%)
3	TQQ	K	57	3	13,17,18	2.34	5 (38%)	10,24,26	2.86	4 (40%)

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	N	57	3	-	0/4/19/21	0/2/2/2
3	TQQ	L	57	3	-	0/4/19/21	0/2/2/2
3	TQQ	M	57	3	-	0/4/19/21	0/2/2/2
3	TQQ	K	57	3	-	1/4/19/21	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	57	TQQ	CH2-N2	8.11	1.41	1.28
3	M	57	TQQ	CH2-N2	6.07	1.38	1.28
3	N	57	TQQ	CH2-N2	5.45	1.37	1.28
3	L	57	TQQ	O2-CZ2	5.36	1.34	1.23
3	N	57	TQQ	O2-CZ2	5.02	1.33	1.23

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	57	TQQ	CZ2-CE2-NE1	7.34	131.66	119.94
3	M	57	TQQ	CZ2-CE2-NE1	6.38	130.13	119.94
3	K	57	TQQ	CZ2-CE2-NE1	6.33	130.05	119.94
3	L	57	TQQ	CZ2-CE2-NE1	6.25	129.92	119.94
3	L	57	TQQ	CD1-CG-CD2	-5.77	101.48	104.79

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 13 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.18	0 100 100	29, 42, 52, 58	0
1	B	105/105 (100%)	-0.40	0 100 100	22, 27, 37, 48	0
1	C	105/105 (100%)	-0.45	0 100 100	21, 29, 39, 51	0
1	D	105/105 (100%)	-0.24	1 (0%) 82 84	30, 40, 50, 57	0
2	G	382/386 (98%)	-0.42	0 100 100	15, 23, 38, 62	0
2	H	382/386 (98%)	-0.38	0 100 100	14, 22, 37, 58	0
2	I	382/386 (98%)	0.05	9 (2%) 59 62	25, 43, 61, 76	0
2	J	382/386 (98%)	-0.26	2 (0%) 91 91	19, 37, 53, 81	0
3	K	124/131 (94%)	-0.28	0 100 100	18, 29, 44, 67	0
3	L	124/131 (94%)	-0.32	1 (0%) 86 87	20, 29, 39, 56	0
3	M	124/131 (94%)	-0.35	1 (0%) 86 87	15, 25, 42, 64	0
3	N	124/131 (94%)	-0.23	1 (0%) 86 87	21, 32, 44, 69	0
All	All	2444/2488 (98%)	-0.27	15 (0%) 89 89	14, 31, 53, 81	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	5	GLU	3.7
2	I	386	GLY	3.5
3	M	131	SER	3.1
2	J	6	ALA	2.9
2	I	364	GLY	2.8

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. 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	K	57	16/17	0.97	0.10	25,30,33,34	0
3	TQQ	M	57	16/17	0.97	0.12	26,29,31,32	0
3	TQQ	N	57	16/17	0.97	0.11	23,25,27,28	0
3	TQQ	L	57	16/17	0.98	0.10	22,24,26,28	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	D	1106	1/1	0.96	0.12	38,38,38,38	0
4	CU	A	1106	1/1	0.98	0.16	34,34,34,34	0
4	CU	C	1106	1/1	0.99	0.13	34,34,34,34	0
4	CU	B	1106	1/1	1.00	0.14	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.