



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:53 pm 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

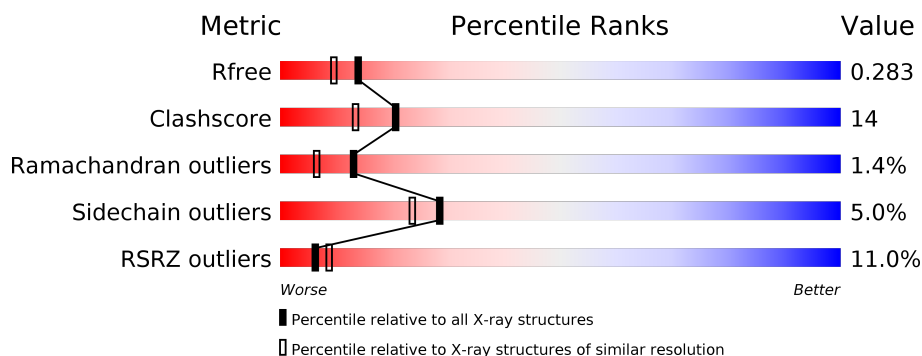
# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>28%</div> <div>61%</div> <div>31%</div> <div>7%</div> <div>•</div> </div>
1	B	105	<div> <div>8%</div> <div>78%</div> <div>21%</div> <div>•</div> </div>
2	H	386	<div> <div>4%</div> <div>81%</div> <div>16%</div> <div>••</div> </div>
2	J	386	<div> <div>18%</div> <div>71%</div> <div>24%</div> <div>••</div> </div>
3	L	131	<div> <div>5%</div> <div>60%</div> <div>32%</div> <div>• 5%</div> </div>
3	M	131	<div> <div>2%</div> <div>70%</div> <div>20%</div> <div>5% • 5%</div> </div>

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

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	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	382	Total	C	N	O	S	0	3	0
			2988	1891	510	579	8			
2	J	381	Total	C	N	O	S	0	1	0
			2963	1876	508	571	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	161	192	13			
3	M	125	Total	C	N	O	S	0	0	0
			956	590	161	192	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
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	L	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

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

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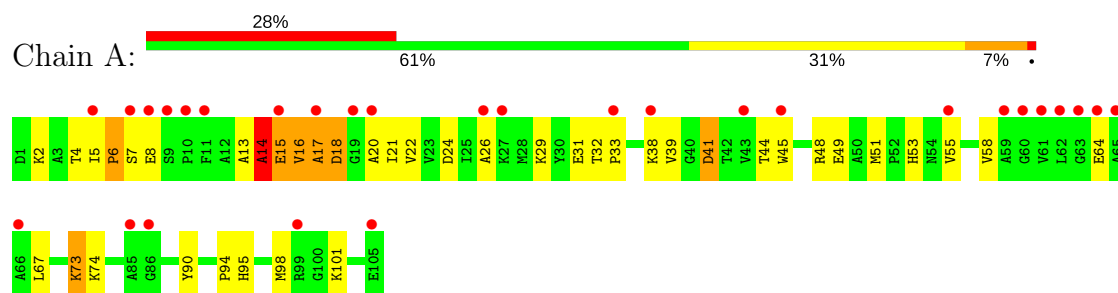
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	75	Total 75	O 75	0	0
6	M	86	Total 86	O 86	0	0

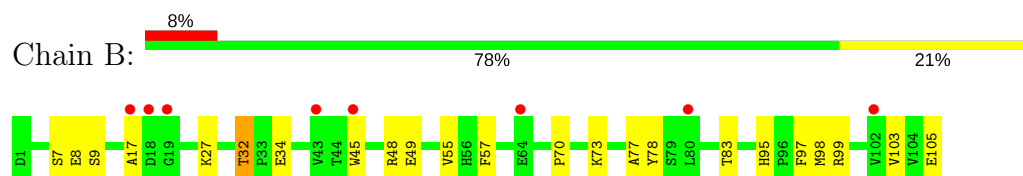
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

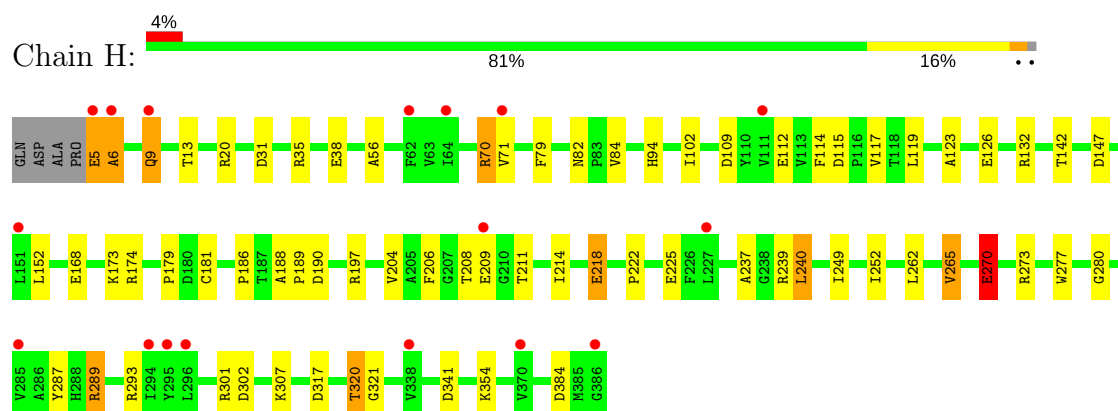
#### • Molecule 1: AMICYANIN



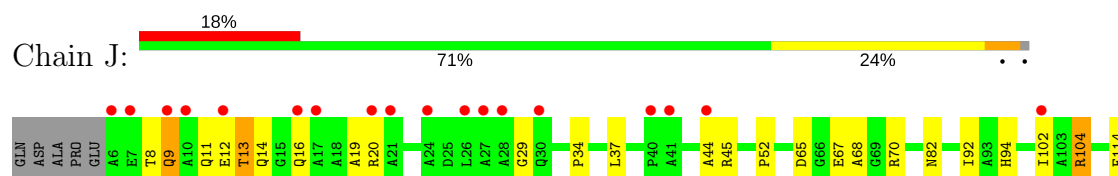
#### • Molecule 1: AMICYANIN

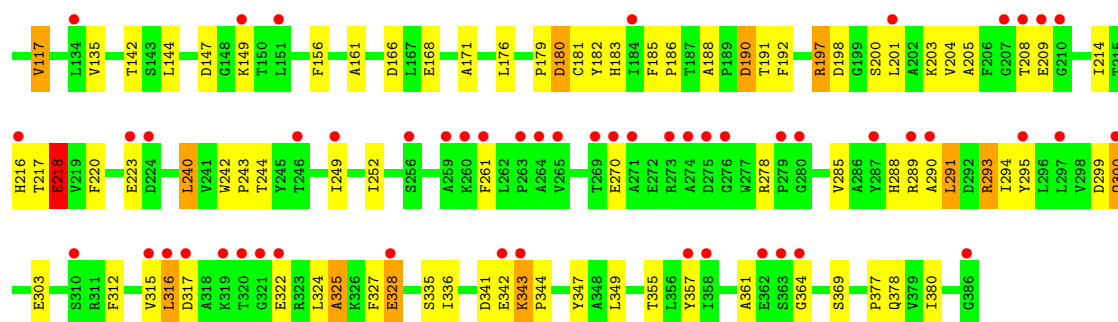


#### • Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

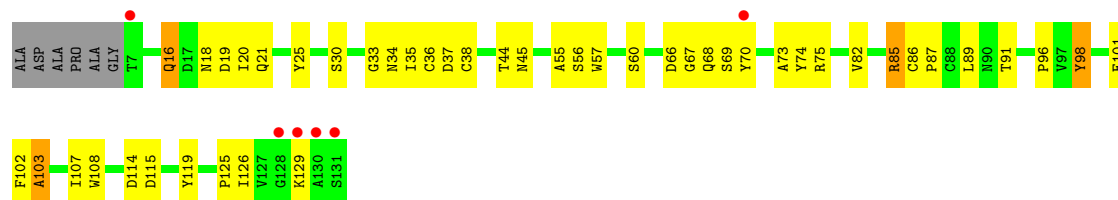


#### • Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

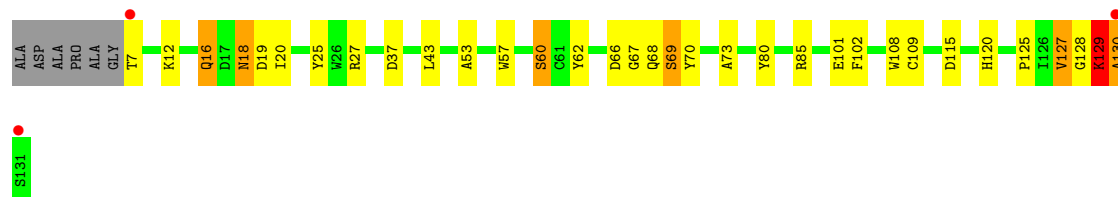




• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN



• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.33 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.189 , 0.245 0.233 , 0.283	Depositor DCC
$R_{free}$ test set	5085 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical 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: 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

All (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
2	H	84	VAL	CB-CG1	6.62	1.66	1.52
2	J	156	PHE	CE2-CZ	6.62	1.50	1.37
3	L	36	CYS	CB-SG	-6.22	1.71	1.82
2	H	126[A]	GLU	CG-CD	6.09	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	126[B]	GLU	CG-CD	6.09	1.61	1.51
2	J	117	VAL	CA-CB	6.01	1.67	1.54
2	H	270[A]	GLU	CG-CD	5.99	1.60	1.51
2	H	270[B]	GLU	CG-CD	5.99	1.60	1.51
2	H	126[A]	GLU	CB-CG	5.96	1.63	1.52
2	H	126[B]	GLU	CB-CG	5.96	1.63	1.52
3	M	102	PHE	CE1-CZ	5.94	1.48	1.37
2	J	65	ASP	CB-CG	5.87	1.64	1.51
2	H	114	PHE	CE1-CZ	5.84	1.48	1.37
2	H	123	ALA	CA-CB	5.83	1.64	1.52
2	J	171	ALA	CA-CB	5.63	1.64	1.52
2	J	185	PHE	CE2-CZ	5.58	1.48	1.37
2	H	209	GLU	CG-CD	5.58	1.60	1.51
3	L	98	TYR	CG-CD1	5.53	1.46	1.39
2	H	79	PHE	CE2-CZ	5.47	1.47	1.37
2	H	277	TRP	CE3-CZ3	5.41	1.47	1.38
2	H	239	ARG	CG-CD	5.37	1.65	1.51
2	J	135	VAL	CA-CB	5.29	1.65	1.54
1	B	103	VAL	CB-CG1	5.25	1.63	1.52
2	H	38	GLU	CB-CG	5.25	1.62	1.52
2	J	218	GLU	CG-CD	5.19	1.59	1.51
2	H	31	ASP	CB-CG	5.18	1.62	1.51
2	H	287	TYR	CE2-CZ	5.11	1.45	1.38
3	L	103	ALA	N-CA	5.07	1.56	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	H	70	ARG	CD-NE-CZ	10.61	138.46	123.60
2	J	104	ARG	NE-CZ-NH2	-10.26	115.17	120.30
2	J	197	ARG	NE-CZ-NH2	9.55	125.08	120.30
2	H	293	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	H	197	ARG	NE-CZ-NH1	-7.91	116.34	120.30
2	H	302	ASP	CB-CG-OD1	-7.86	111.23	118.30
1	A	14	ALA	N-CA-C	-7.80	89.94	111.00
1	B	48	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	J	104	ARG	CG-CD-NE	-7.02	97.05	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	35	ARG	NE-CZ-NH1	-6.93	116.83	120.30
2	J	190	ASP	CB-CG-OD1	6.89	124.50	118.30
2	J	240	LEU	CB-CG-CD1	-6.80	99.44	111.00
3	M	66	ASP	CB-CG-OD1	6.24	123.91	118.30
2	H	147	ASP	CB-CG-OD1	6.10	123.79	118.30
2	H	341	ASP	CB-CG-OD1	6.04	123.74	118.30
3	M	60	SER	N-CA-CB	5.98	119.47	110.50
2	H	320	THR	N-CA-C	5.97	127.11	111.00
2	H	20	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	J	104	ARG	NE-CZ-NH1	5.77	123.18	120.30
2	H	239	ARG	NE-CZ-NH1	5.69	123.15	120.30
3	L	85	ARG	NE-CZ-NH2	-5.68	117.46	120.30
3	M	85	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	J	293	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	J	197	ARG	CG-CD-NE	-5.45	100.35	111.80
2	H	132	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	H	289	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	A	16	VAL	CB-CA-C	-5.13	101.64	111.40
1	B	98	MET	CG-SD-CE	5.12	108.39	100.20
2	H	320	THR	CA-C-N	5.08	126.37	116.20
2	H	109	ASP	CB-CG-OD1	5.08	122.87	118.30
3	L	85	ARG	NE-CZ-NH1	5.06	122.83	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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
3:L:68:GLN:HB2	6:L:2038:HOH:O	1.58	1.01
2:J:217:THR:HG21	2:J:261:PHE:CZ	1.97	0.99
5:H:1389:GOL:H12	6:H:2012:HOH:O	1.62	0.97
2:J:8:THR:HA	2:J:9:GLN:HG3	1.44	0.96
2:H:289:ARG:HH12	2:H:384:ASP:CG	1.68	0.95
3:M:57:TRQ:CZ3	3:M:108:TRP:HD1	1.79	0.95
3:M:127:VAL:HG22	3:M:128:GLY:H	1.31	0.93
1:A:16:VAL:HG13	1:A:17:ALA:N	1.87	0.89
1:A:21:ILE:HD11	1:A:41:ASP:OD1	1.72	0.88
2:J:34:PRO:HG2	3:L:75:ARG:NH1	1.88	0.88
2:J:217:THR:HG21	2:J:261:PHE:HZ	1.39	0.88
1:A:20:ALA:CB	6:A:2006:HOH:O	2.23	0.86
1:A:16:VAL:HB	6:A:2003:HOH:O	1.75	0.85
2:H:174:ARG:NH1	6:H:2216:HOH:O	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:127:VAL:HG22	3:M:128:GLY:N	1.93	0.84
2:H:218:GLU:HG3	6:H:2246:HOH:O	1.79	0.83
3:L:16:GLN:NE2	3:L:18:ASN:H	1.78	0.82
2:J:270:GLU:HB2	6:J:2166:HOH:O	1.78	0.82
1:B:105:GLU:HG2	6:B:2107:HOH:O	1.80	0.81
2:H:70:ARG:HH21	5:H:1389:GOL:H2	1.39	0.81
1:A:16:VAL:HG13	1:A:17:ALA:H	1.46	0.81
3:M:68:GLN:HE21	3:M:129:LYS:NZ	1.78	0.81
2:J:197:ARG:NH1	3:M:101:GLU:OE1	2.13	0.80
2:J:291:LEU:HB3	2:J:293:ARG:HE	1.47	0.80
2:J:8:THR:HB	2:J:9:GLN:HB2	1.64	0.80
2:J:270:GLU:CB	6:J:2166:HOH:O	2.31	0.78
5:H:1389:GOL:H31	3:M:37:ASP:OD1	1.85	0.77
1:A:33:PRO:HD2	6:A:2009:HOH:O	1.83	0.77
1:B:73:LYS:HE2	6:M:2085:HOH:O	1.84	0.76
2:H:70:ARG:HH22	5:H:1389:GOL:C2	1.98	0.76
1:B:73:LYS:HD3	6:M:2085:HOH:O	1.87	0.75
3:M:127:VAL:CG2	3:M:128:GLY:N	2.49	0.75
2:J:8:THR:O	2:J:11:GLN:HB3	1.86	0.75
5:H:1389:GOL:C3	3:M:37:ASP:OD1	2.34	0.75
1:A:20:ALA:HB1	6:A:2006:HOH:O	1.85	0.74
2:J:217:THR:HG21	2:J:261:PHE:CE2	2.22	0.74
2:J:369:SER:O	6:J:2197:HOH:O	2.06	0.73
1:B:49:GLU:OE1	6:B:2052:HOH:O	2.06	0.73
3:L:57:TRQ:HB2	3:L:108:TRP:NE1	2.04	0.73
2:H:179:PRO:HD3	2:H:214:ILE:HD12	1.71	0.72
2:J:312:PHE:CE1	2:J:328:GLU:HG3	2.25	0.71
2:J:317:ASP:HB2	2:J:324:LEU:HD21	1.72	0.71
2:H:317:ASP:O	2:H:321:GLY:HA2	1.90	0.71
2:J:344:PRO:O	2:J:361:ALA:CB	2.39	0.70
3:L:16:GLN:HE22	3:L:19:ASP:H	1.40	0.69
2:H:70:ARG:NH2	5:H:1389:GOL:O2	2.25	0.69
2:J:166:ASP:OD2	6:J:2126:HOH:O	2.09	0.69
3:M:57:TRQ:HB2	3:M:108:TRP:NE1	2.08	0.68
3:L:19:ASP:O	3:L:25:TYR:HB2	1.94	0.68
1:A:20:ALA:HB2	6:A:2006:HOH:O	1.92	0.68
1:A:17:ALA:HB3	1:A:20:ALA:HB2	1.75	0.67
3:M:68:GLN:HE21	3:M:129:LYS:HZ2	1.40	0.67
2:J:344:PRO:O	2:J:361:ALA:HB2	1.95	0.67
2:H:70:ARG:HH21	5:H:1389:GOL:C2	1.98	0.67
3:M:57:TRQ:CZ3	3:M:108:TRP:CD1	2.65	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:HIS:HD1	1:A:98:MET:CE	2.08	0.66
3:M:16:GLN:HE22	3:M:19:ASP:H	1.42	0.66
1:B:83:THR:O	6:B:2083:HOH:O	2.12	0.66
3:M:16:GLN:HE21	3:M:18:ASN:H	1.43	0.66
1:A:90:TYR:O	6:A:2026:HOH:O	2.15	0.65
5:L:1132:GOL:H31	6:L:2075:HOH:O	1.96	0.64
2:J:52:PRO:HG2	2:J:378:GLN:HE21	1.62	0.64
2:J:14:GLN:NE2	2:J:68:ALA:O	2.31	0.64
2:J:45:ARG:NH2	2:J:343:LYS:O	2.30	0.63
1:A:17:ALA:O	1:A:18:ASP:HB2	1.97	0.63
3:M:57:TRQ:HB2	3:M:108:TRP:HE1	1.63	0.63
5:H:1389:GOL:O1	6:H:2406:HOH:O	2.15	0.63
2:J:288:HIS:CE1	2:J:291:LEU:HD13	2.34	0.63
2:J:336:ILE:HA	2:J:347:TYR:O	1.99	0.62
3:L:16:GLN:HE21	3:L:18:ASN:H	1.46	0.62
2:J:182:TYR:O	2:J:183:HIS:HB2	1.97	0.62
3:L:20:ILE:HG22	3:L:25:TYR:CZ	2.34	0.62
2:J:11:GLN:HG2	3:L:21:GLN:OE1	1.99	0.62
1:A:53:HIS:ND1	1:A:98:MET:CE	2.62	0.61
2:J:315:VAL:HB	2:J:325:ALA:HB3	1.83	0.61
3:M:68:GLN:NE2	3:M:129:LYS:NZ	2.48	0.61
3:L:68:GLN:HG2	3:L:69:SER:N	2.16	0.61
2:H:273:ARG:HG2	6:H:2293:HOH:O	2.01	0.61
2:J:44:ALA:HB1	2:J:341:ASP:HB3	1.83	0.61
3:L:89:LEU:H	5:L:1132:GOL:H11	1.66	0.60
3:M:115:ASP:HB2	6:M:2077:HOH:O	2.01	0.60
2:J:16:GLN:HG3	2:J:20:ARG:NH2	2.17	0.60
1:B:99:ARG:NH2	2:J:180[B]:ASP:OD2	2.35	0.59
2:J:19:ALA:HB2	3:L:20:ILE:HG23	1.83	0.59
3:M:68:GLN:NE2	3:M:129:LYS:HZ1	2.01	0.59
2:H:5:GLU:O	2:H:6:ALA:CB	2.51	0.58
2:H:211:THR:HG23	6:H:2237:HOH:O	2.03	0.58
2:J:8:THR:HA	2:J:9:GLN:CG	2.26	0.58
3:L:56:SER:HB2	3:L:74:TYR:O	2.03	0.58
3:M:16:GLN:NE2	3:M:18:ASN:H	2.00	0.58
2:J:144:LEU:O	2:J:186:PRO:HG2	2.04	0.57
1:B:95:HIS:HB3	1:B:97:PHE:CE2	2.39	0.57
2:J:217:THR:CG2	2:J:261:PHE:CE2	2.87	0.57
2:J:179:PRO:O	2:J:181:CYS:N	2.35	0.57
2:J:217:THR:CG2	2:J:261:PHE:CZ	2.81	0.57
5:H:1389:GOL:H32	3:M:37:ASP:OD1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:CD1	1:A:41:ASP:OD1	2.51	0.57
2:J:82:ASN:HB3	2:J:142:THR:HB	1.86	0.56
2:J:70:ARG:HG3	2:J:70:ARG:HH11	1.70	0.56
3:L:20:ILE:HG22	3:L:25:TYR:CE1	2.40	0.56
2:J:34:PRO:HB3	3:L:44:THR:O	2.05	0.56
3:L:57:TRQ:HB2	3:L:108:TRP:HE1	1.68	0.56
2:J:349:LEU:HB2	2:J:380:ILE:HD11	1.87	0.56
2:J:216:HIS:CD2	6:J:2139:HOH:O	2.59	0.56
2:J:249:ILE:HD12	2:J:294:ILE:HG21	1.88	0.55
3:L:16:GLN:HE21	3:L:16:GLN:C	2.10	0.55
2:J:188:ALA:HB3	2:J:191:THR:HB	1.89	0.55
1:B:73:LYS:CD	6:M:2085:HOH:O	2.46	0.55
2:J:316:LEU:HA	2:J:324:LEU:HG	1.89	0.55
3:M:73:ALA:O	3:M:125:PRO:HD2	2.07	0.55
2:J:290:ALA:HB3	2:J:291:LEU:HD13	1.89	0.54
3:L:21:GLN:NE2	3:L:37:ASP:OD2	2.38	0.54
2:H:179:PRO:HD3	2:H:214:ILE:CD1	2.36	0.54
2:H:179:PRO:HB2	2:H:181:CYS:SG	2.48	0.54
3:L:38:CYS:HB3	3:L:85:ARG:NH1	2.22	0.54
2:H:222:PRO:HG2	2:H:225:GLU:HB2	1.88	0.54
1:A:16:VAL:O	1:A:17:ALA:CB	2.56	0.53
5:H:1387:GOL:H31	6:H:2277:HOH:O	2.07	0.53
2:J:92:ILE:HG13	2:J:114:PHE:HB2	1.89	0.53
2:J:217:THR:HG22	2:J:218:GLU:N	2.24	0.53
2:H:173:LYS:HE3	6:H:2214:HOH:O	2.08	0.53
3:L:68:GLN:HE22	3:L:129:LYS:HE2	1.74	0.53
6:H:2187:HOH:O	3:L:103:ALA:HB1	2.07	0.53
1:A:16:VAL:CG1	1:A:17:ALA:N	2.60	0.53
1:B:32:THR:HG22	1:B:34:GLU:H	1.73	0.53
2:H:9:GLN:HG2	6:H:2006:HOH:O	2.08	0.53
2:J:349:LEU:HD11	2:J:377:PRO:HB2	1.91	0.52
2:J:37:LEU:HD21	3:L:45:ASN:CB	2.39	0.52
2:J:249:ILE:CD1	2:J:294:ILE:HG21	2.39	0.52
1:B:73:LYS:CE	6:M:2085:HOH:O	2.47	0.52
2:H:240:LEU:HD13	2:H:252:ILE:HD13	1.91	0.52
2:J:147:ASP:OD2	2:J:149:LYS:HD2	2.09	0.52
2:J:344:PRO:O	2:J:361:ALA:HB3	2.10	0.52
1:A:8:GLU:HB3	6:A:2002:HOH:O	2.10	0.51
2:H:173:LYS:CE	6:H:2214:HOH:O	2.58	0.51
2:H:82:ASN:HB3	2:H:142:THR:HB	1.93	0.51
3:L:55:ALA:O	3:L:56:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ALA:CB	1:A:20:ALA:HB2	2.41	0.51
2:H:5:GLU:O	2:H:6:ALA:HB2	2.10	0.51
2:J:34:PRO:HG2	3:L:75:ARG:HH12	1.71	0.51
1:A:8:GLU:O	6:A:2001:HOH:O	2.18	0.50
2:J:312:PHE:HE1	2:J:328:GLU:HG3	1.71	0.50
2:J:149:LYS:HD3	2:J:168:GLU:OE1	2.12	0.50
2:J:244:THR:HB	6:J:2146:HOH:O	2.12	0.50
1:A:51:MET:O	1:A:53:HIS:CD2	2.65	0.49
1:A:16:VAL:O	1:A:17:ALA:HB2	2.12	0.49
1:A:38:LYS:O	1:A:41:ASP:HB2	2.12	0.49
2:J:52:PRO:CG	2:J:378:GLN:HE21	2.25	0.49
2:H:112:GLU:OE2	2:J:104:ARG:NH2	2.37	0.49
2:J:243:PRO:HG3	2:J:285:VAL:HB	1.94	0.49
2:J:70:ARG:NH1	6:J:2058:HOH:O	2.46	0.48
3:L:96:PRO:HB2	3:L:98:TYR:CE1	2.48	0.48
2:H:56:ALA:HA	3:L:82:VAL:HG12	1.96	0.48
2:H:307:LYS:HD2	3:L:91:THR:HG21	1.95	0.48
1:A:18:ASP:C	1:A:20:ALA:H	2.16	0.48
2:J:37:LEU:HD21	3:L:45:ASN:HB2	1.95	0.48
2:J:45:ARG:NH1	2:J:67:GLU:OE1	2.45	0.48
2:H:204:VAL:HG22	2:H:214:ILE:HD13	1.95	0.48
2:J:13:THR:HG21	6:J:2006:HOH:O	2.13	0.48
3:M:53:ALA:HB2	3:M:109:CYS:HA	1.94	0.48
2:J:13:THR:CG2	6:J:2007:HOH:O	2.61	0.48
1:B:45:TRP:CE2	1:B:55:VAL:HG11	2.49	0.48
2:J:8:THR:CA	2:J:9:GLN:HG3	2.31	0.48
2:J:8:THR:CB	2:J:9:GLN:HB2	2.39	0.48
2:J:278:ARG:HD2	2:J:303:GLU:HA	1.97	0.47
3:M:62:TYR:OH	3:M:67:GLY:HA2	2.14	0.47
3:L:35:ILE:HD12	3:L:86:CYS:HB3	1.97	0.47
1:B:97:PHE:HA	2:J:180[B]:ASP:OD2	2.14	0.47
2:J:70:ARG:HG3	2:J:70:ARG:NH1	2.29	0.46
1:A:17:ALA:O	1:A:18:ASP:CB	2.62	0.46
2:J:29:GLY:O	6:J:2021:HOH:O	2.20	0.46
3:L:57:TRQ:HZ3	3:L:108:TRP:HB2	1.98	0.46
2:J:299:ASP:OD1	2:J:300:GLN:N	2.48	0.45
2:J:355:THR:HG21	2:J:357:TYR:CE1	2.51	0.45
3:L:57:TRQ:CZ3	3:L:108:TRP:HB2	2.45	0.45
1:A:26:ALA:HB3	1:A:31:GLU:OE2	2.16	0.45
1:A:95:HIS:HB2	1:A:98:MET:SD	2.56	0.45
2:J:328:GLU:O	6:J:2180:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:57:TRQ:CD2	3:M:108:TRP:CD1	2.78	0.45
2:J:223:GLU:HG3	6:J:2141:HOH:O	2.16	0.45
2:H:190:ASP:HB2	2:H:206:PHE:O	2.16	0.45
1:A:49:GLU:HA	1:A:74:LYS:HE2	1.99	0.45
2:H:270[A]:GLU:OE1	6:H:2286:HOH:O	2.21	0.45
2:J:217:THR:CG2	2:J:218:GLU:N	2.80	0.45
2:J:190:ASP:O	2:J:205:ALA:HA	2.16	0.45
2:J:270:GLU:HB3	6:J:2166:HOH:O	2.07	0.44
3:L:73:ALA:O	3:L:125:PRO:HD2	2.17	0.44
2:J:181:CYS:C	2:J:182:TYR:CD1	2.91	0.44
2:J:203:LYS:O	2:J:214:ILE:HA	2.17	0.44
2:J:204:VAL:HG22	2:J:214:ILE:HG12	2.00	0.44
1:A:22:VAL:HG22	1:A:44:THR:HB	1.99	0.44
1:A:2:LYS:HE2	6:A:2020:HOH:O	2.17	0.44
2:H:218:GLU:HG3	2:H:218:GLU:H	1.69	0.44
1:B:97:PHE:CZ	2:J:197:ARG:NH1	2.86	0.44
2:H:237:ALA:HB2	2:H:289:ARG:HG3	1.98	0.44
2:J:288:HIS:HE1	2:J:290:ALA:HB3	1.82	0.44
2:J:16:GLN:HB3	3:L:18:ASN:O	2.18	0.44
2:J:200:SER:O	2:J:201:LEU:HD23	2.18	0.43
1:A:94:PRO:HB3	3:L:55:ALA:HB1	2.00	0.43
1:B:70:PRO:HD2	1:B:78:TYR:CE1	2.53	0.43
3:M:69:SER:O	3:M:130:ALA:N	2.51	0.43
1:A:14:ALA:O	1:A:15:GLU:C	2.44	0.43
2:J:355:THR:HG21	2:J:357:TYR:CZ	2.53	0.43
3:L:101:GLU:HG2	3:L:102:PHE:CD2	2.53	0.43
1:A:24:ASP:OD1	1:A:48:ARG:NE	2.48	0.43
1:A:45:TRP:CD2	1:A:55:VAL:HG11	2.53	0.43
1:A:16:VAL:HG22	1:A:18:ASP:H	1.83	0.43
3:L:114:ASP:O	3:L:115:ASP:HB2	2.19	0.43
3:M:69:SER:HB2	6:M:2051:HOH:O	2.19	0.43
1:B:95:HIS:HB3	1:B:97:PHE:CZ	2.53	0.43
3:L:20:ILE:HA	3:L:25:TYR:CG	2.54	0.43
2:J:197:ARG:HB2	6:M:2068:HOH:O	2.19	0.43
2:H:188:ALA:HB1	2:H:189:PRO:CD	2.49	0.43
2:H:188:ALA:HB1	2:H:189:PRO:HD2	2.01	0.43
2:J:290:ALA:HB3	2:J:291:LEU:CD1	2.48	0.43
1:B:105:GLU:OXT	6:B:2109:HOH:O	2.21	0.43
2:J:327:PHE:CG	2:J:364:GLY:HA3	2.53	0.42
2:J:161:ALA:HA	2:J:176:LEU:O	2.20	0.42
2:J:186:PRO:HA	2:J:192:PHE:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:152:LEU:HD12	2:H:186:PRO:HG3	2.02	0.42
1:B:99:ARG:HH22	2:J:180[B]:ASP:CG	2.23	0.42
2:J:198:ASP:C	2:J:198:ASP:OD1	2.58	0.42
2:J:201:LEU:HD21	2:J:220:PHE:CE1	2.54	0.42
2:J:295:TYR:CD1	2:J:295:TYR:N	2.87	0.42
3:M:80:TYR:HB2	3:M:120:HIS:HB2	2.01	0.42
2:H:249:ILE:HB	2:H:265:VAL:HG12	2.02	0.41
2:H:270[A]:GLU:H	2:H:270[A]:GLU:CD	2.21	0.41
3:L:66:ASP:OD2	3:L:70:TYR:OH	2.30	0.41
3:L:33:GLY:O	3:L:87:PRO:HA	2.20	0.41
3:M:20:ILE:HG22	3:M:25:TYR:CZ	2.55	0.41
3:M:68:GLN:HB2	3:M:70:TYR:CE1	2.55	0.41
1:A:73:LYS:HB2	1:A:73:LYS:HE3	1.98	0.41
3:M:7:THR:CG2	6:M:2002:HOH:O	2.68	0.41
2:H:115:ASP:O	2:H:119:LEU:HA	2.20	0.41
3:L:70:TYR:HB3	3:L:126:ILE:HG23	2.02	0.41
3:L:107:ILE:HD12	3:L:119:TYR:HB2	2.02	0.41
1:B:45:TRP:O	1:B:77:ALA:HA	2.20	0.41
2:J:13:THR:HA	2:J:16:GLN:HG2	2.02	0.41
3:L:34:ASN:ND2	3:L:82:VAL:CG2	2.84	0.41
2:H:280:GLY:HA3	2:H:301:ARG:CZ	2.51	0.41
2:J:343:LYS:HA	2:J:344:PRO:HD3	1.90	0.41
1:B:57:PHE:N	1:B:57:PHE:CD1	2.89	0.40
2:J:16:GLN:CB	3:L:18:ASN:O	2.70	0.40
2:J:289:ARG:HB3	6:J:2187:HOH:O	2.20	0.40
2:H:168:GLU:HG3	6:H:2091:HOH:O	2.21	0.40
2:J:9:GLN:H	2:J:12:GLU:HG3	1.87	0.40
3:L:35:ILE:HG22	3:L:37:ASP:H	1.87	0.40
3:M:27:ARG:HD2	3:M:43:LEU:HD21	2.04	0.40
1:A:6:PRO:HB2	1:A:7:SER:H	1.71	0.40
2:J:335:SER:HB2	2:J:349:LEU:HB3	2.04	0.40

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

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/105 (98%)	90 (87%)	6 (6%)	7 (7%)	1	0
1	B	103/105 (98%)	100 (97%)	2 (2%)	1 (1%)	18	11
2	H	383/386 (99%)	369 (96%)	12 (3%)	2 (0%)	32	25
2	J	380/386 (98%)	350 (92%)	25 (7%)	5 (1%)	14	7
3	L	122/131 (93%)	115 (94%)	6 (5%)	1 (1%)	22	14
3	M	122/131 (93%)	113 (93%)	7 (6%)	2 (2%)	11	4
All	All	1213/1244 (98%)	1137 (94%)	58 (5%)	18 (2%)	13	5

All (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
2	J	180[A]	ASP
2	J	180[B]	ASP
3	L	67	GLY
3	M	130	ALA
1	A	6	PRO
1	B	17	ALA
1	A	18	ASP
2	H	102	ILE
2	J	102	ILE
2	J	325	ALA
1	A	58	VAL
1	A	39	VAL
3	M	127	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/85 (99%)	75 (89%)	9 (11%)	8	4
1	B	84/85 (99%)	80 (95%)	4 (5%)	30	25
2	H	311/311 (100%)	298 (96%)	13 (4%)	34	32
2	J	308/311 (99%)	292 (95%)	16 (5%)	27	22
3	L	104/106 (98%)	101 (97%)	3 (3%)	48	46
3	M	104/106 (98%)	98 (94%)	6 (6%)	23	18
All	All	995/1004 (99%)	944 (95%)	51 (5%)	28	22

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	ILE
1	A	29	LYS
1	A	32	THR
1	A	41	ASP
1	A	64	GLU
1	A	67	LEU
1	A	73	LYS
1	A	101	LYS
1	B	7	SER
1	B	8	GLU
1	B	27	LYS
1	B	32	THR
2	H	5	GLU
2	H	9	GLN
2	H	13	THR
2	H	94	HIS
2	H	117	VAL
2	H	208	THR
2	H	218	GLU
2	H	240	LEU
2	H	262	LEU

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Mol	Chain	Res	Type
2	H	265	VAL
2	H	270[A]	GLU
2	H	270[B]	GLU
2	H	354	LYS
2	J	13	THR
2	J	94	HIS
2	J	117	VAL
2	J	208	THR
2	J	209	GLU
2	J	218	GLU
2	J	240	LEU
2	J	242	TRP
2	J	252	ILE
2	J	291	LEU
2	J	300	GLN
2	J	316	LEU
2	J	322	GLU
2	J	328	GLU
2	J	342	GLU
2	J	343	LYS
3	L	16	GLN
3	L	30	SER
3	L	60	SER
3	M	12	LYS
3	M	16	GLN
3	M	18	ASN
3	M	60	SER
3	M	69	SER
3	M	129	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	378	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
3	M	68	GLN

### 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	TRQ	L	57	3	16,17,18	2.79	5 (31%)	15,24,26	1.45	3 (20%)
3	TRQ	M	57	3	16,17,18	3.19	6 (37%)	15,24,26	1.85	6 (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	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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	57	TRQ	CH2-CZ2	-4.54	1.48	1.53
3	L	57	TRQ	CZ3-CH2	-3.36	1.36	1.45
3	M	57	TRQ	CH2-CZ2	-3.13	1.50	1.53
3	M	57	TRQ	CZ3-CH2	-2.13	1.40	1.45
3	M	57	TRQ	O7-CZ2	3.11	1.30	1.23
3	L	57	TRQ	CZ3-CE3	3.43	1.40	1.34
3	M	57	TRQ	CZ3-CE3	4.22	1.41	1.34
3	L	57	TRQ	CD2-CE2	4.43	1.46	1.40
3	M	57	TRQ	CD2-CE2	5.96	1.48	1.40
3	L	57	TRQ	CD2-CG	7.06	1.49	1.40
3	M	57	TRQ	CD2-CG	8.76	1.52	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	57	TRQ	CB-CG-CD1	-3.27	123.93	127.97
3	M	57	TRQ	CD2-CE2-NE1	-2.69	105.30	109.64
3	M	57	TRQ	CB-CG-CD1	-2.40	125.00	127.97
3	M	57	TRQ	O6-CH2-CZ2	-2.26	117.03	118.72
3	M	57	TRQ	CZ3-CH2-CZ2	2.16	121.90	118.73
3	M	57	TRQ	CD2-CE3-CZ3	2.17	123.82	121.09
3	L	57	TRQ	CB-CG-CD2	2.68	132.92	127.09
3	L	57	TRQ	CB-CA-C	2.80	116.81	111.41
3	M	57	TRQ	CB-CA-C	3.40	117.96	111.41

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	1.00	0
5	GOL	H	1389	2	5,5,5	0.61	0	5,5,5	1.34	1 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	L	1132	3	5,5,5	0.55	0	5,5,5	0.95	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(°)	Ideal(°)
5	H	1389	GOL	O3-C3-C2	2.94	124.88	110.07

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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	105/105 (100%)	1.53	29 (27%) <b>1</b> <b>1</b>	62, 79, 91, 97	0
1	B	105/105 (100%)	0.43	8 (7%) <b>15</b> <b>19</b>	48, 56, 68, 81	0
2	H	382/386 (98%)	0.25	17 (4%) <b>34</b> <b>42</b>	38, 48, 64, 86	0
2	J	381/386 (98%)	1.06	71 (18%) <b>1</b> <b>2</b>	46, 71, 89, 97	0
3	L	124/131 (94%)	0.48	6 (4%) <b>31</b> <b>39</b>	48, 61, 74, 104	0
3	M	124/131 (94%)	0.42	3 (2%) <b>59</b> <b>67</b>	40, 54, 72, 102	0
All	All	1221/1244 (98%)	0.67	134 (10%) <b>6</b> <b>9</b>	38, 59, 87, 104	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	274	ALA	7.5
2	J	28	ALA	7.1
2	J	386	GLY	6.8
3	M	131	SER	6.6
2	J	6	ALA	6.5
2	J	342	GLU	5.8
1	A	9	SER	5.8
1	A	17	ALA	5.7
3	M	130	ALA	5.5
1	A	85	ALA	5.3
1	A	59	ALA	5.0
1	A	65	ALA	4.9
1	A	64	GLU	4.8
2	J	27	ALA	4.8
3	L	131	SER	4.8
2	J	276	GLY	4.7
1	A	43	VAL	4.6
1	A	5	ILE	4.5
1	B	18	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	19	GLY	4.4
2	J	24	ALA	4.4
2	J	271	ALA	4.4
3	L	130	ALA	4.3
1	A	8	GLU	4.3
2	J	321	GLY	4.3
2	J	264	ALA	4.2
2	J	259	ALA	4.2
1	A	60	GLY	4.2
2	J	297	LEU	4.1
2	J	275	ASP	4.0
2	J	209	GLU	3.9
2	H	5	GLU	3.9
3	L	7	THR	3.8
2	H	6	ALA	3.7
2	J	270	GLU	3.7
2	J	320	THR	3.7
2	J	261	PHE	3.6
2	J	322	GLU	3.6
2	J	362	GLU	3.6
2	J	319	LYS	3.6
2	J	364	GLY	3.6
1	A	19	GLY	3.5
1	A	38	LYS	3.4
1	A	63	GLY	3.4
1	A	105	GLU	3.4
2	J	30	GLN	3.3
1	A	86	GLY	3.3
2	H	9	GLN	3.3
2	H	209	GLU	3.2
2	H	386	GLY	3.2
2	J	201	LEU	3.1
2	J	208	THR	3.1
2	J	224	ASP	3.1
2	J	260	LYS	3.1
2	J	263	PRO	3.1
1	B	80	LEU	3.1
2	J	44	ALA	3.0
2	J	287	TYR	3.0
1	A	33	PRO	3.0
2	J	10	ALA	3.0
1	A	45	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	17	ALA	2.9
2	J	256	SER	2.9
3	M	7	THR	2.9
2	J	20	ARG	2.9
1	A	7	SER	2.9
3	L	128	GLY	2.8
1	A	15	GLU	2.8
2	J	151	LEU	2.8
2	J	316	LEU	2.8
2	J	343	LYS	2.8
2	J	9	GLN	2.8
1	A	61	VAL	2.7
2	J	328	GLU	2.7
1	B	45	TRP	2.7
1	A	66	ALA	2.7
2	J	16	GLN	2.6
2	J	246	THR	2.6
2	J	295	TYR	2.6
2	J	102	ILE	2.6
2	J	269	THR	2.6
2	J	290	ALA	2.5
2	H	64	ILE	2.5
2	J	300	GLN	2.5
2	J	17	ALA	2.5
1	A	27	LYS	2.5
2	J	273	ARG	2.5
2	J	289	ARG	2.5
1	A	11	PHE	2.5
2	J	21	ALA	2.5
1	A	55	VAL	2.5
2	J	315	VAL	2.5
3	L	129	LYS	2.5
2	H	370	VAL	2.4
2	J	363	SER	2.4
2	J	317	ASP	2.4
2	J	7	GLU	2.4
2	J	249	ILE	2.4
2	J	207	GLY	2.4
1	B	102	VAL	2.4
2	J	265	VAL	2.4
2	J	279	PRO	2.4
2	H	296	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	151	LEU	2.3
2	J	134	LEU	2.3
2	J	41	ALA	2.3
2	J	184	ILE	2.3
2	J	149	LYS	2.3
2	H	71	VAL	2.3
2	H	111	VAL	2.3
2	J	210	GLY	2.3
2	J	358	ILE	2.3
1	A	62	LEU	2.3
1	A	26	ALA	2.2
1	B	43	VAL	2.2
2	J	216	HIS	2.2
2	H	285	VAL	2.2
2	H	295	TYR	2.2
2	J	280	GLY	2.2
2	J	310	SER	2.2
3	L	70	TYR	2.2
1	B	64	GLU	2.2
2	J	40	PRO	2.1
2	H	227	LEU	2.1
2	H	338	VAL	2.1
1	A	99	ARG	2.1
2	J	12	GLU	2.1
2	H	294	ILE	2.1
1	A	10	PRO	2.1
2	H	62	PHE	2.1
2	J	223	GLU	2.0
2	J	357	TYR	2.0
1	A	20	ALA	2.0
2	J	26	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	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.