



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:45 AM GMT

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 full wwPDB 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/ValidationPDFNotes.html>

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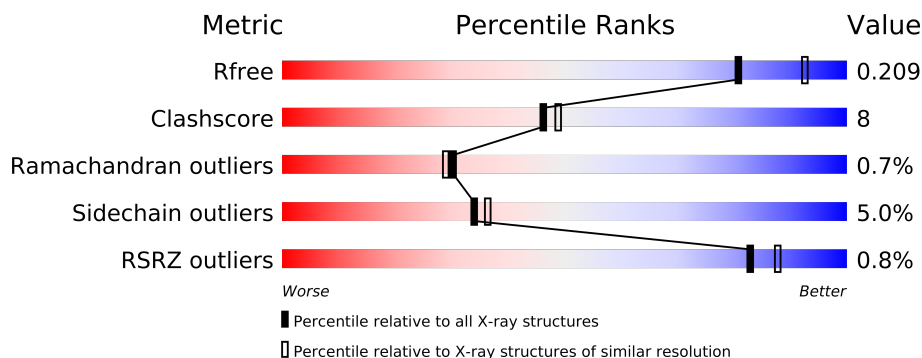
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	105	
1	B	105	
1	C	105	
1	D	105	
2	G	386	
2	H	386	
2	I	386	
2	J	386	
3	K	131	
3	L	131	
3	M	131	
3	N	131	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	CU	A	1106	-	X
4	CU	B	1106	-	X
4	CU	C	1106	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20786 atoms, of which 0 are hydrogen and 0 are deuterium.

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	B	1	Total	Cu	0	0
			1	1		
4	A	1	Total	Cu	0	0
			1	1		
4	D	1	Total	Cu	0	0
			1	1		
4	C	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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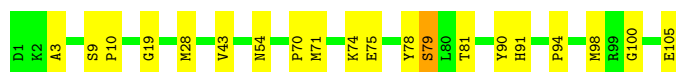
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	80	Total 80	O 80	0	0
5	M	90	Total 90	O 90	0	0
5	N	73	Total 73	O 73	0	0

### 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 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

Chain A: 



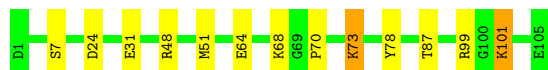
- Molecule 1: AMICYANIN

Chain B: 



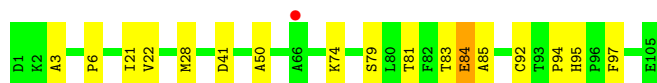
- Molecule 1: AMICYANIN

Chain C: 



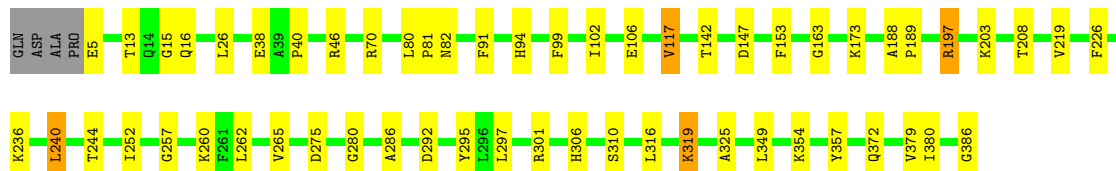
- Molecule 1: AMICYANIN

Chain D: 



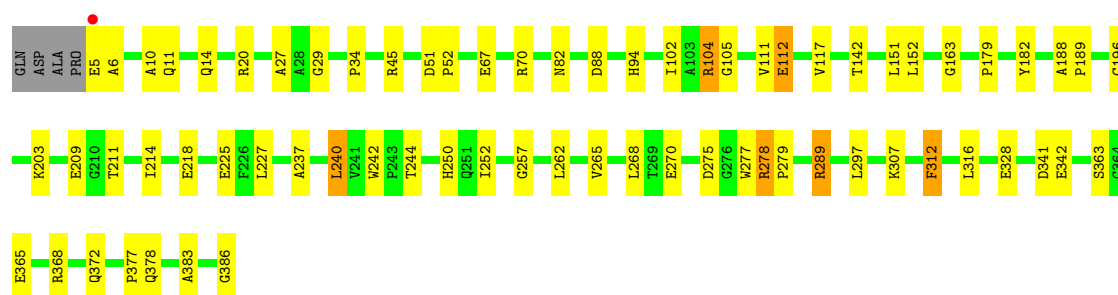
- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain G: 



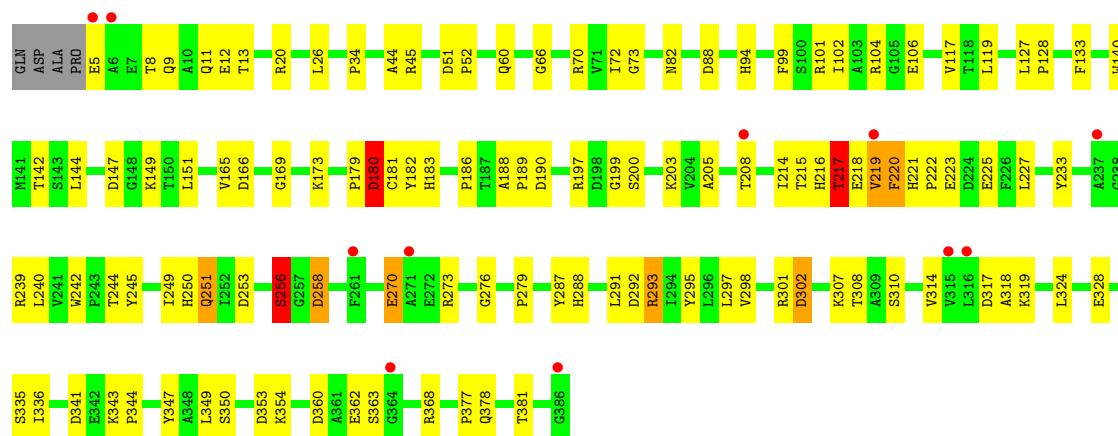
- Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain H: 



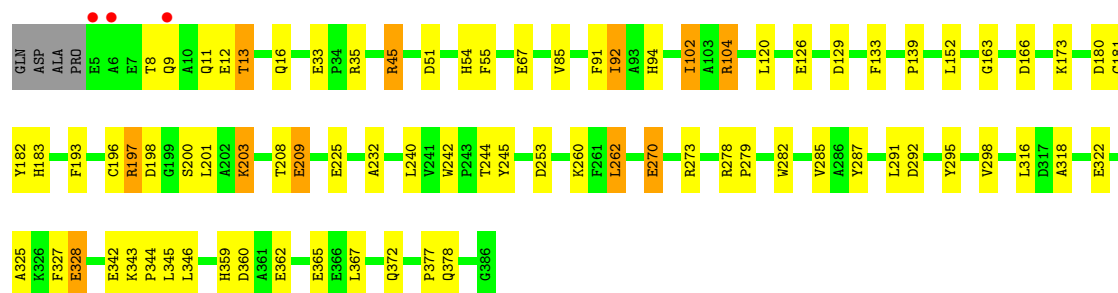
• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain I:



• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN

Chain J:



• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain K:



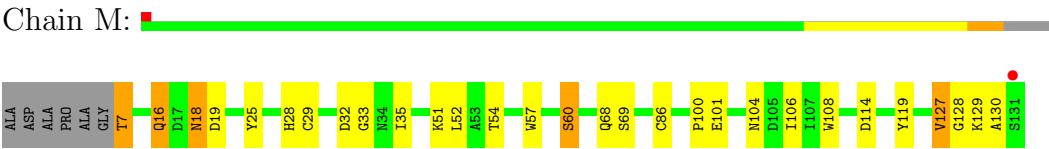
• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain L:

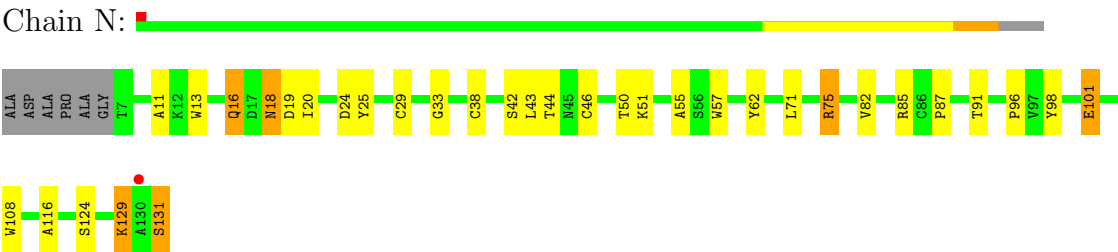




● Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN



● Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 30.6	EDS
Estimated twinning fraction	0.126 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 170983 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 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: TQQ, 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	0.92	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

All (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
3	K	80	TYR	CD1-CE1	5.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	112	GLU	CD-OE2	-5.61	1.19	1.25
2	H	312	PHE	CG-CD2	5.57	1.47	1.38
2	G	325	ALA	CA-CB	5.55	1.64	1.52
3	N	38	CYS	CB-SG	-5.51	1.72	1.81
2	G	379	VAL	CB-CG2	5.49	1.64	1.52
2	J	196	CYS	CB-SG	5.49	1.91	1.82
2	J	91	PHE	CE2-CZ	5.46	1.47	1.37
3	N	11	ALA	CA-CB	5.45	1.63	1.52
2	I	133	PHE	CE1-CZ	5.44	1.47	1.37
2	G	286	ALA	CA-CB	5.39	1.63	1.52
2	H	111	VAL	CB-CG1	5.33	1.64	1.52
3	L	12	LYS	CE-NZ	5.31	1.62	1.49
2	G	219	VAL	CB-CG2	5.27	1.64	1.52
2	I	104	ARG	CB-CG	-5.25	1.38	1.52
3	L	38	CYS	CB-SG	-5.21	1.73	1.81
3	L	12	LYS	CD-CE	5.19	1.64	1.51
2	H	196	CYS	CB-SG	-5.06	1.73	1.81
2	H	383	ALA	CA-CB	5.06	1.63	1.52
2	H	312	PHE	CE1-CZ	5.06	1.47	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	N	85	ARG	NE-CZ-NH1	7.77	124.19	120.30
2	G	197	ARG	NE-CZ-NH1	-7.62	116.49	120.30
2	H	88	ASP	CB-CG-OD1	7.57	125.12	118.30
2	G	147	ASP	CB-CG-OD2	-7.49	111.56	118.30
2	H	278	ARG	NE-CZ-NH2	-7.31	116.64	120.30
2	H	341	ASP	CB-CG-OD1	7.19	124.77	118.30
2	H	70	ARG	NE-CZ-NH2	-6.97	116.81	120.30
3	N	75	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	I	219	VAL	C-N-CA	6.64	138.30	121.70
2	I	180	ASP	CB-CG-OD1	6.52	124.16	118.30
3	N	101	GLU	CB-CA-C	-6.29	97.82	110.40
2	H	289	ARG	NE-CZ-NH1	-6.26	117.17	120.30
2	J	129	ASP	CB-CG-OD2	-5.97	112.92	118.30
2	H	368	ARG	NE-CZ-NH1	5.96	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	240	LEU	CB-CG-CD2	5.80	120.86	111.00
2	J	104	ARG	CG-CD-NE	-5.72	99.78	111.80
2	G	70	ARG	NE-CZ-NH1	5.70	123.15	120.30
3	L	99	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	H	368	ARG	NE-CZ-NH2	-5.39	117.60	120.30
3	L	24	ASP	CB-CG-OD1	5.37	123.14	118.30
2	H	278	ARG	NE-CZ-NH1	5.25	122.93	120.30
3	L	85	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	J	120	LEU	CB-CG-CD2	-5.16	102.24	111.00
1	B	32	THR	CB-CA-C	-5.07	97.92	111.60
2	I	101	ARG	NE-CZ-NH2	-5.04	117.78	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (302) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
2:J:197:ARG:NH1	3:M:101:GLU:OE1	2.07	0.88
2:H:237:ALA:HB2	2:H:289:ARG:HG3	1.61	0.81
2:H:5:GLU:HB2	5:H:2007:HOH:O	1.81	0.80
2:G:5:GLU:HB3	5:G:2007:HOH:O	1.81	0.79
3:M:16:GLN:HE22	3:M:19:ASP:H	1.32	0.78
2:J:287:TYR:OH	5:J:2212:HOH:O	2.03	0.77
1:A:19:GLY:HA2	5:A:2009:HOH:O	1.85	0.75
2:G:372:GLN:OE1	5:G:2391:HOH:O	2.04	0.75
3:M:16:GLN:HE21	3:M:18:ASN:H	1.35	0.74
2:I:253:ASP:O	5:I:2135:HOH:O	2.06	0.74
2:H:372:GLN:OE1	5:H:2401:HOH:O	2.06	0.73
2:I:45:ARG:NH2	2:I:343:LYS:O	2.21	0.73
1:B:99:ARG:NH2	2:J:180:ASP:OD1	2.22	0.73
2:J:372:GLN:NE2	5:J:2251:HOH:O	2.21	0.72
3:L:16:GLN:HE21	3:L:16:GLN:C	1.93	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:K:16:GLN:HE22	3:K:19:ASP:H	1.38	0.71
2:I:188:ALA:HB1	2:I:189:PRO:HD2	1.74	0.69
3:L:25:TYR:CE2	3:L:27:ARG:HG3	2.27	0.69
2:I:297:LEU:HD22	2:I:310:SER:HB2	1.73	0.68
3:M:16:GLN:NE2	3:M:18:ASN:H	1.90	0.68
5:C:2099:HOH:O	2:I:180:ASP:HB2	1.93	0.68
2:G:5:GLU:HA	5:G:2006:HOH:O	1.94	0.68
3:N:57:TQQ:CZ3	3:N:108:TRP:CD1	2.56	0.67
3:N:16:GLN:NE2	3:N:18:ASN:H	1.93	0.67
1:D:22:VAL:O	5:D:2008:HOH:O	2.12	0.67
1:B:68:LYS:HE3	3:M:54:THR:OG1	1.95	0.66
2:I:293:ARG:HD3	2:I:324:LEU:CD1	2.22	0.66
2:I:239:ARG:HH12	2:I:318:ALA:HB1	1.62	0.65
2:I:292:ASP:OD2	2:I:318:ALA:HB3	1.96	0.65
2:H:179:PRO:HD3	2:H:214:ILE:HD13	1.79	0.65
2:I:291:LEU:HD11	2:I:344:PRO:HG3	1.78	0.64
3:K:57:TQQ:HB2	3:K:108:TRP:NE1	2.13	0.64
2:I:200:SER:HB2	5:I:2121:HOH:O	1.97	0.64
2:I:51:ASP:HA	2:I:377:PRO:HA	1.80	0.64
2:I:199:GLY:O	2:I:220:PHE:HB3	1.99	0.63
3:N:96:PRO:HB2	3:N:98:TYR:CE1	2.33	0.63
1:C:31:GLU:HB2	5:C:2033:HOH:O	1.99	0.63
2:G:236:LYS:NZ	5:G:2275:HOH:O	2.14	0.63
2:J:102:ILE:HD13	5:J:2102:HOH:O	1.99	0.63
2:J:35:ARG:NH1	5:J:2040:HOH:O	2.33	0.62
2:G:203:LYS:HE3	2:G:257:GLY:O	1.98	0.62
3:M:60:SER:HB2	3:M:130:ALA:CB	2.29	0.62
2:H:268:LEU:HD22	2:H:277:TRP:HB3	1.80	0.62
2:J:45:ARG:HD3	2:J:345:LEU:CD1	2.30	0.61
2:J:45:ARG:HD3	2:J:345:LEU:HD11	1.81	0.61
2:I:200:SER:CB	5:I:2121:HOH:O	2.48	0.61
2:J:197:ARG:HH12	3:M:101:GLU:CD	2.03	0.60
3:K:16:GLN:NE2	3:K:18:ASN:H	2.00	0.60
2:G:16:GLN:HA	3:K:18:ASN:O	2.01	0.60
3:N:16:GLN:HE21	3:N:18:ASN:H	1.50	0.60
2:I:314:VAL:C	5:I:2151:HOH:O	2.40	0.59
2:J:166:ASP:HB2	2:J:173:LYS:HD3	1.84	0.59
2:I:295:TYR:HA	5:I:2151:HOH:O	2.02	0.58
1:A:10:PRO:HD3	1:A:70:PRO:CB	2.34	0.58
2:I:291:LEU:CD1	2:I:344:PRO:HG3	2.33	0.57
2:J:360:ASP:OD1	2:J:362:GLU:HB3	2.05	0.56
3:N:16:GLN:HE22	3:N:19:ASP:H	1.51	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:199:GLY:HA3	2:I:219:VAL:HG13	1.85	0.56
1:A:10:PRO:HD3	1:A:70:PRO:HB2	1.86	0.56
2:H:188:ALA:HB1	2:H:189:PRO:HD2	1.86	0.56
2:I:188:ALA:HB1	2:I:189:PRO:CD	2.34	0.56
2:G:188:ALA:HB1	2:G:189:PRO:CD	2.36	0.56
1:D:94:PRO:HB3	3:N:55:ALA:HB1	1.86	0.56
1:B:32:THR:HG22	1:B:34:GLU:H	1.71	0.55
3:N:57:TQQ:HB2	3:N:108:TRP:NE1	2.21	0.55
5:H:2191:HOH:O	3:L:103:ALA:HB1	2.05	0.55
3:K:57:TQQ:HB2	3:K:108:TRP:HE1	1.71	0.55
2:I:52:PRO:HG2	2:I:378:GLN:HE21	1.72	0.55
2:J:16:GLN:HA	3:L:18:ASN:O	2.07	0.54
2:H:188:ALA:HB1	2:H:189:PRO:CD	2.37	0.54
2:I:219:VAL:HG12	2:I:221:HIS:O	2.08	0.54
2:I:221:HIS:CD2	2:I:227:LEU:HD22	2.43	0.54
2:J:45:ARG:NH2	2:J:343:LYS:O	2.41	0.54
1:A:43:VAL:O	1:A:79:SER:HA	2.07	0.54
3:M:32:ASP:OD2	3:M:104:ASN:O	2.26	0.54
2:J:126:GLU:OE2	5:J:2122:HOH:O	2.18	0.54
2:H:279:PRO:HA	2:H:297:LEU:O	2.07	0.54
2:H:386:GLY:HA3	5:H:2418:HOH:O	2.08	0.53
1:A:91:HIS:HA	1:A:98:MET:O	2.08	0.53
3:N:42:SER:O	3:N:43:LEU:C	2.45	0.53
3:L:13:TRP:HZ3	5:L:2046:HOH:O	1.92	0.53
2:I:288:HIS:CE1	2:I:291:LEU:HG	2.44	0.53
2:I:147:ASP:CG	2:I:149:LYS:HG3	2.29	0.53
2:G:188:ALA:HB1	2:G:189:PRO:HD2	1.91	0.52
3:K:73:ALA:O	3:K:125:PRO:HD2	2.10	0.52
2:I:180:ASP:OD2	2:I:197:ARG:HD2	2.09	0.52
2:I:218:GLU:O	2:I:220:PHE:HB2	2.10	0.52
2:G:306:HIS:CE1	3:N:91:THR:HB	2.45	0.52
3:K:16:GLN:HE21	3:K:18:ASN:H	1.56	0.52
2:H:112:GLU:OE2	2:J:104:ARG:NH2	2.34	0.52
2:J:360:ASP:HB2	2:J:367:LEU:HD21	1.92	0.51
2:I:256:SER:C	2:I:258:ASP:H	2.13	0.51
2:H:5:GLU:N	5:H:2004:HOH:O	2.42	0.51
1:B:58:VAL:O	1:B:61:VAL:HG23	2.09	0.51
2:I:151:LEU:HD23	2:I:151:LEU:C	2.31	0.51
2:J:152:LEU:HA	2:J:163:GLY:O	2.10	0.51
3:N:129:LYS:NZ	3:N:131:SER:HB2	2.26	0.51
1:C:70:PRO:HD2	1:C:78:TYR:CE1	2.45	0.51
2:I:381:THR:OG1	5:I:2172:HOH:O	2.19	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:104:ARG:HG3	2:H:105:GLY:N	2.26	0.51
3:M:127:VAL:HG22	3:M:128:GLY:N	2.26	0.50
2:J:346:LEU:HB3	2:J:359:HIS:HB2	1.92	0.50
2:I:335:SER:HB2	2:I:349:LEU:HB3	1.94	0.50
2:I:343:LYS:HA	5:I:2159:HOH:O	2.11	0.50
3:M:51:LYS:HE3	3:M:114:ASP:OD2	2.10	0.50
2:J:11:GLN:HG2	3:L:21:GLN:OE1	2.12	0.50
2:G:386:GLY:HA3	5:G:2407:HOH:O	2.10	0.50
2:I:140:TRP:CZ2	2:I:233:TYR:HB3	2.47	0.50
2:I:20:ARG:HG3	5:I:2011:HOH:O	2.11	0.50
2:I:360:ASP:OD1	2:I:362:GLU:HB2	2.12	0.50
2:G:297:LEU:HD22	2:G:310:SER:HB2	1.94	0.50
2:J:193:PHE:CE2	2:J:203:LYS:HB2	2.47	0.50
2:I:179:PRO:HD3	2:I:214:ILE:HD13	1.93	0.50
1:A:28:MET:O	1:A:98:MET:HG2	2.12	0.50
3:L:57:TQQ:HB2	3:L:108:TRP:HE1	1.77	0.50
2:J:139:PRO:HB3	5:J:2259:HOH:O	2.12	0.49
1:C:51:MET:CE	3:K:101:GLU:HB2	2.42	0.49
2:I:336:ILE:HA	2:I:347:TYR:O	2.12	0.49
2:I:190:ASP:O	2:I:205:ALA:HA	2.12	0.49
3:M:57:TQQ:HB2	3:M:108:TRP:NE1	2.27	0.49
2:J:85:VAL:HG13	2:J:92:ILE:HG22	1.94	0.49
3:N:51:LYS:HG3	3:N:116:ALA:HB2	1.94	0.49
1:A:9:SER:HA	1:A:70:PRO:HG3	1.95	0.49
2:G:82:ASN:HB3	2:G:142:THR:HB	1.95	0.49
3:M:25:TYR:HB3	3:M:28:HIS:CD2	2.47	0.49
2:I:307:LYS:HD2	3:K:91:THR:HG21	1.94	0.49
3:L:19:ASP:O	3:L:25:TYR:HB2	2.12	0.49
2:J:54:HIS:O	2:J:55:PHE:HB2	2.13	0.49
1:A:70:PRO:HD2	1:A:78:TYR:CE1	2.48	0.48
1:D:3:ALA:HA	1:D:81:THR:O	2.12	0.48
2:J:328:GLU:HB2	5:J:2226:HOH:O	2.13	0.48
2:I:70:ARG:NH1	5:I:2050:HOH:O	2.46	0.48
3:K:16:GLN:C	3:K:16:GLN:HE21	2.16	0.48
1:B:101:LYS:HE3	5:B:2040:HOH:O	2.13	0.48
3:M:60:SER:HB2	3:M:130:ALA:HB2	1.95	0.48
2:H:363:SER:OG	2:H:365:GLU:HG2	2.12	0.48
2:H:227:LEU:HD12	2:H:244:THR:HG22	1.96	0.48
2:H:52:PRO:HG2	2:H:378:GLN:HE21	1.77	0.48
2:J:193:PHE:CZ	2:J:203:LYS:HB2	2.48	0.48
2:H:11:GLN:HG2	5:M:2020:HOH:O	2.12	0.48
2:J:208:THR:HG23	2:J:209:GLU:H	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:166:ASP:OD2	2:I:169:GLY:HA3	2.14	0.48
3:N:33:GLY:O	3:N:87:PRO:HA	2.14	0.48
2:G:240:LEU:HD13	2:G:252:ILE:HD13	1.96	0.48
2:H:82:ASN:HB3	2:H:142:THR:HB	1.96	0.48
3:M:7:THR:O	3:M:7:THR:HG22	2.14	0.47
3:L:57:TQQ:HB2	3:L:108:TRP:NE1	2.28	0.47
2:J:208:THR:HG23	2:J:209:GLU:N	2.29	0.47
2:J:133:PHE:CZ	3:M:106:ILE:HG12	2.49	0.47
2:I:222:PRO:HD2	2:I:225:GLU:HB3	1.96	0.47
2:G:5:GLU:HG2	2:G:372:GLN:HE21	1.79	0.47
2:I:140:TRP:CE2	2:I:233:TYR:HB3	2.48	0.47
3:L:53:ALA:HB2	3:L:109:CYS:HA	1.95	0.47
1:A:3:ALA:HA	1:A:81:THR:O	2.14	0.47
3:L:60:SER:HB3	3:L:130:ALA:CB	2.44	0.47
2:J:181:CYS:C	2:J:182:TYR:CD1	2.88	0.47
1:B:99:ARG:HH22	2:J:180:ASP:CG	2.17	0.47
3:N:57:TQQ:HB2	3:N:108:TRP:HE1	1.80	0.46
1:B:105:GLU:HB3	5:B:2097:HOH:O	2.16	0.46
2:I:225:GLU:OE1	2:I:250:HIS:NE2	2.35	0.46
1:A:54:ASN:HB3	1:A:71:MET:SD	2.56	0.46
2:H:203:LYS:HE3	2:H:257:GLY:O	2.15	0.46
2:H:342:GLU:HA	5:H:2368:HOH:O	2.14	0.46
2:J:9:GLN:O	2:J:13:THR:HG22	2.16	0.46
3:K:96:PRO:HB2	3:K:98:TYR:CE1	2.51	0.46
2:G:197:ARG:HH12	3:N:101:GLU:CD	2.18	0.46
1:A:94:PRO:HB3	3:L:55:ALA:HB1	1.98	0.46
2:G:15:GLY:HA3	3:K:19:ASP:OD1	2.15	0.46
1:C:73:LYS:HG2	3:K:127:VAL:HG13	1.98	0.46
2:I:179:PRO:O	2:I:181:CYS:N	2.49	0.46
2:H:278:ARG:HD3	5:H:2326:HOH:O	2.16	0.46
2:I:44:ALA:HB1	2:I:341:ASP:HB3	1.98	0.46
2:I:144:LEU:O	2:I:186:PRO:HG2	2.16	0.46
2:G:280:GLY:HA3	2:G:301:ARG:CZ	2.45	0.46
2:H:237:ALA:HB2	2:H:289:ARG:CG	2.38	0.45
2:I:34:PRO:HB3	3:N:44:THR:O	2.16	0.45
2:J:197:ARG:HH11	3:M:100:PRO:HD2	1.82	0.45
3:M:57:TQQ:CE2	3:M:104:ASN:HB2	2.46	0.45
1:B:74:LYS:HE2	5:M:2090:HOH:O	2.15	0.45
2:I:314:VAL:O	5:I:2151:HOH:O	2.21	0.45
2:H:45:ARG:NH1	2:H:67:GLU:OE1	2.41	0.45
2:I:253:ASP:N	5:I:2135:HOH:O	2.47	0.45
2:J:262:LEU:HB3	5:J:2194:HOH:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:226:PHE:O	2:G:244:THR:HA	2.16	0.45
2:I:11:GLN:HG2	5:N:2016:HOH:O	2.17	0.45
2:I:34:PRO:HG2	3:N:75:ARG:NH1	2.32	0.45
2:H:27:ALA:C	2:H:29:GLY:H	2.20	0.45
3:M:57:TQQ:HB2	3:M:108:TRP:HE1	1.82	0.45
2:I:8:THR:O	2:I:12:GLU:HB2	2.17	0.44
2:I:270:GLU:HG2	2:I:273:ARG:HH12	1.82	0.44
2:G:173:LYS:NZ	5:G:2219:HOH:O	2.45	0.44
2:H:252:ILE:HD12	2:H:252:ILE:N	2.33	0.44
2:G:5:GLU:HG2	2:G:372:GLN:NE2	2.33	0.44
3:M:33:GLY:HA3	3:M:119:TYR:OH	2.17	0.44
2:J:292:ASP:OD1	2:J:318:ALA:HB3	2.17	0.44
1:D:21:ILE:HD12	1:D:41:ASP:HB3	1.98	0.44
3:N:19:ASP:O	3:N:25:TYR:HB2	2.17	0.44
2:H:152:LEU:HA	2:H:163:GLY:O	2.17	0.44
2:G:80:LEU:N	2:G:81:PRO:HD3	2.33	0.44
3:K:20:ILE:HG22	3:K:25:TYR:CZ	2.53	0.44
2:I:227:LEU:HB3	2:I:242:TRP:NE1	2.32	0.44
2:H:10:ALA:O	2:H:14:GLN:HG3	2.17	0.44
2:G:319:LYS:H	2:G:319:LYS:HG3	1.49	0.44
2:J:344:PRO:HD2	5:J:2237:HOH:O	2.18	0.44
2:J:279:PRO:HA	2:J:298:VAL:HA	1.99	0.44
1:C:99:ARG:NH2	5:C:2099:HOH:O	2.49	0.44
2:G:197:ARG:NH1	3:N:101:GLU:OE2	2.47	0.44
3:N:71:LEU:HA	3:N:71:LEU:HD12	1.85	0.44
1:C:24:ASP:OD1	1:C:48:ARG:NE	2.44	0.44
2:H:312:PHE:CE2	2:H:328:GLU:HG3	2.53	0.44
3:N:46:CYS:HB3	3:N:50:THR:OG1	2.18	0.44
2:I:302:ASP:OD1	3:K:12:LYS:HG3	2.18	0.44
2:I:66:GLY:O	2:I:368:ARG:HD2	2.18	0.43
3:L:16:GLN:NE2	3:L:16:GLN:C	2.67	0.43
2:J:245:TYR:O	2:J:279:PRO:HD2	2.17	0.43
2:I:245:TYR:O	2:I:279:PRO:HD2	2.18	0.43
2:I:279:PRO:HA	2:I:298:VAL:HA	2.01	0.43
2:I:179:PRO:HG2	2:I:181:CYS:SG	2.58	0.43
1:B:89:ASP:OD1	1:B:101:LYS:HG3	2.17	0.43
1:D:95:HIS:HB3	1:D:97:PHE:CZ	2.53	0.43
1:C:68:LYS:HE3	5:C:2077:HOH:O	2.18	0.43
3:N:16:GLN:C	3:N:16:GLN:HE21	2.21	0.43
3:L:100:PRO:HA	3:L:103:ALA:HB3	1.99	0.43
2:J:45:ARG:NH1	2:J:67:GLU:OE1	2.44	0.43
2:H:182:TYR:CD1	2:H:182:TYR:N	2.87	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:260:LYS:O	2:J:262:LEU:HD13	2.18	0.43
2:G:173:LYS:HD2	2:G:173:LYS:HA	1.85	0.43
2:I:308:THR:HG21	3:K:9:PRO:O	2.19	0.43
2:I:360:ASP:OD1	2:I:363:SER:N	2.45	0.43
2:H:34:PRO:HB2	3:M:52:LEU:HD21	2.00	0.43
2:I:73:GLY:HA3	2:I:119:LEU:HD11	2.00	0.43
2:H:225:GLU:OE1	2:H:250:HIS:NE2	2.52	0.43
2:I:82:ASN:HB3	2:I:142:THR:HB	2.00	0.43
1:A:90:TYR:CZ	1:A:100:GLY:HA3	2.54	0.42
3:N:62:TYR:HD1	5:N:2043:HOH:O	2.01	0.42
2:J:295:TYR:CD1	2:J:295:TYR:N	2.87	0.42
3:M:35:ILE:HD12	3:M:86:CYS:HB3	2.02	0.42
1:B:97:PHE:CZ	2:J:197:ARG:NH1	2.87	0.42
3:K:106:ILE:HD12	3:K:108:TRP:CZ2	2.55	0.42
2:J:325:ALA:HB1	2:J:327:PHE:CE1	2.54	0.42
2:G:349:LEU:HB2	2:G:380:ILE:HD11	2.01	0.42
1:D:83:THR:O	1:D:84:GLU:HB2	2.18	0.42
1:D:92:CYS:SG	1:D:94:PRO:HD2	2.59	0.42
1:B:12:ALA:O	1:B:15:GLU:HB2	2.19	0.42
3:K:129:LYS:O	3:K:130:ALA:HB2	2.20	0.42
1:B:1:ASP:HB2	1:B:62:LEU:O	2.20	0.42
2:G:295:TYR:CD1	2:G:295:TYR:N	2.87	0.42
1:D:50:ALA:HA	1:D:74:LYS:HB2	2.02	0.42
2:I:319:LYS:O	5:I:2152:HOH:O	2.21	0.42
2:I:239:ARG:HH11	2:I:251:GLN:HG2	1.84	0.42
3:L:16:GLN:HE22	3:L:19:ASP:H	1.68	0.42
2:I:222:PRO:HD2	2:I:225:GLU:CB	2.48	0.42
2:J:225:GLU:HG2	2:J:244:THR:HG21	2.01	0.42
2:G:99:PHE:HA	2:G:106:GLU:O	2.19	0.42
3:K:34:ASN:ND2	3:K:82:VAL:CG2	2.83	0.42
2:I:216:HIS:C	2:I:217:THR:O	2.57	0.41
1:B:87:THR:HG21	5:B:2093:HOH:O	2.19	0.41
2:G:38:GLU:HB3	2:G:117:VAL:HG23	2.03	0.41
2:G:153:PHE:CE1	2:G:163:GLY:HA3	2.55	0.41
2:G:40:PRO:O	2:G:46:ARG:NH2	2.53	0.41
2:H:51:ASP:HA	2:H:377:PRO:HA	2.01	0.41
2:I:203:LYS:O	2:I:214:ILE:HA	2.20	0.41
3:N:20:ILE:HG22	3:N:25:TYR:CZ	2.56	0.41
2:J:8:THR:O	2:J:12:GLU:HG3	2.20	0.41
2:I:99:PHE:HA	2:I:106:GLU:O	2.21	0.41
2:I:291:LEU:HD13	2:I:293:ARG:HH12	1.86	0.41
1:C:51:MET:HE1	3:K:101:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:292:ASP:OD2	2:G:319:LYS:HG2	2.21	0.41
1:C:87:THR:CG2	1:C:101:LYS:HD3	2.51	0.41
3:M:16:GLN:NE2	3:M:19:ASP:H	2.10	0.41
2:I:295:TYR:N	2:I:295:TYR:CD1	2.89	0.41
1:A:10:PRO:HD3	1:A:70:PRO:CG	2.51	0.41
2:I:52:PRO:HG2	2:I:378:GLN:NE2	2.34	0.41
1:D:28:MET:CE	3:N:101:GLU:HG2	2.51	0.41
2:I:350:SER:HB3	2:I:353:ASP:HB2	2.03	0.41
2:J:51:ASP:HA	2:J:377:PRO:HA	2.02	0.41
2:J:200:SER:O	2:J:201:LEU:HD23	2.21	0.41
2:H:20:ARG:HD2	5:H:2005:HOH:O	2.21	0.41
1:A:74:LYS:HG2	1:A:75:GLU:HG2	2.03	0.41
2:I:70:ARG:O	2:I:72:ILE:HG23	2.21	0.41
2:J:182:TYR:O	2:J:183:HIS:HB2	2.21	0.41
2:H:307:LYS:NZ	3:L:104:ASN:OD1	2.54	0.40
3:L:60:SER:HB3	3:L:130:ALA:HB3	2.02	0.40
2:J:282:TRP:CD1	2:J:378:GLN:HB3	2.56	0.40
2:I:127:LEU:HA	2:I:128:PRO:HD3	1.95	0.40
3:L:46:CYS:HA	3:L:47:PRO:HD3	1.84	0.40
3:K:33:GLY:HA3	3:K:119:TYR:OH	2.22	0.40
3:K:129:LYS:HG2	3:K:129:LYS:O	2.20	0.40
3:N:13:TRP:CZ3	3:N:24:ASP:HA	2.57	0.40
2:I:182:TYR:O	2:I:183:HIS:HB2	2.20	0.40
2:H:151:LEU:HD23	2:H:151:LEU:C	2.42	0.40
2:J:270:GLU:HA	2:J:273:ARG:NH1	2.36	0.40
2:I:60:GLN:NE2	3:N:82:VAL:O	2.54	0.40
2:I:151:LEU:HB3	2:I:165:VAL:HB	2.04	0.40
3:L:57:TQQ:CE2	3:L:74:TYR:HB2	2.52	0.40
1:D:6:PRO:HD2	1:D:79:SER:O	2.22	0.40
2:J:232:ALA:HB2	2:J:285:VAL:HG13	2.04	0.40

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	Distance(Å)	Clash(Å)
5:C:2017:HOH:O	5:H:2282:HOH:O[3_655]	2.04	0.16

## 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%)	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%)	12	6
2	G	380/386 (98%)	366 (96%)	13 (3%)	1 (0%)	50	54
2	H	380/386 (98%)	359 (94%)	19 (5%)	2 (0%)	38	38
2	I	380/386 (98%)	352 (93%)	21 (6%)	7 (2%)	13	6
2	J	380/386 (98%)	359 (94%)	19 (5%)	2 (0%)	38	38
3	K	122/131 (93%)	114 (93%)	6 (5%)	2 (2%)	14	8
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%)	30	29

All (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
3	K	130	ALA
1	D	84	GLU
1	D	85	ALA
2	I	102	ILE
2	I	256	SER
2	J	198	ASP
2	H	6	ALA
2	I	276	GLY

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Mol	Chain	Res	Type
2	J	102	ILE
2	G	102	ILE
2	H	102	ILE

### 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%)	82 (98%)	2 (2%)	61	71
1	B	84/85 (99%)	81 (96%)	3 (4%)	47	54
1	C	84/85 (99%)	80 (95%)	4 (5%)	35	39
1	D	84/85 (99%)	84 (100%)	0	100	100
2	G	308/311 (99%)	295 (96%)	13 (4%)	40	46
2	H	308/311 (99%)	296 (96%)	12 (4%)	43	51
2	I	308/311 (99%)	284 (92%)	24 (8%)	18	15
2	J	308/311 (99%)	289 (94%)	19 (6%)	26	24
3	K	104/106 (98%)	100 (96%)	4 (4%)	44	52
3	L	104/106 (98%)	101 (97%)	3 (3%)	55	64
3	M	104/106 (98%)	95 (91%)	9 (9%)	15	12
3	N	104/106 (98%)	98 (94%)	6 (6%)	28	28
All	All	1984/2008 (99%)	1885 (95%)	99 (5%)	34	36

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	SER
1	A	105	GLU
1	B	18	ASP
1	B	27	LYS
1	B	32	THR
1	C	7	SER
1	C	64	GLU
1	C	73	LYS

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Mol	Chain	Res	Type
1	C	101	LYS
2	G	13	THR
2	G	26	LEU
2	G	94	HIS
2	G	117	VAL
2	G	208	THR
2	G	240	LEU
2	G	260	LYS
2	G	262	LEU
2	G	265	VAL
2	G	275	ASP
2	G	316	LEU
2	G	319	LYS
2	G	354	LYS
2	H	94	HIS
2	H	104	ARG
2	H	117	VAL
2	H	209	GLU
2	H	211	THR
2	H	240	LEU
2	H	242	TRP
2	H	262	LEU
2	H	265	VAL
2	H	270	GLU
2	H	275	ASP
2	H	316	LEU
2	I	5	GLU
2	I	9	GLN
2	I	13	THR
2	I	26	LEU
2	I	88	ASP
2	I	94	HIS
2	I	117	VAL
2	I	173	LYS
2	I	208	THR
2	I	215	THR
2	I	217	THR
2	I	223	GLU
2	I	240	LEU
2	I	244	THR
2	I	251	GLN
2	I	256	SER

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Mol	Chain	Res	Type
2	I	258	ASP
2	I	270	GLU
2	I	293	ARG
2	I	301	ARG
2	I	302	ASP
2	I	317	ASP
2	I	328	GLU
2	I	354	LYS
2	J	13	THR
2	J	33	GLU
2	J	45	ARG
2	J	92	ILE
2	J	94	HIS
2	J	203	LYS
2	J	209	GLU
2	J	240	LEU
2	J	242	TRP
2	J	253	ASP
2	J	262	LEU
2	J	270	GLU
2	J	278	ARG
2	J	291	LEU
2	J	316	LEU
2	J	322	GLU
2	J	328	GLU
2	J	342	GLU
2	J	365	GLU
3	K	15	PRO
3	K	16	GLN
3	K	18	ASN
3	K	65	THR
3	L	16	GLN
3	L	29	CYS
3	L	31	ILE
3	M	7	THR
3	M	16	GLN
3	M	18	ASN
3	M	29	CYS
3	M	60	SER
3	M	68	GLN
3	M	69	SER
3	M	127	VAL

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Mol	Chain	Res	Type
3	M	129	LYS
3	N	16	GLN
3	N	18	ASN
3	N	29	CYS
3	N	124	SER
3	N	129	LYS
3	N	131	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	91	HIS
2	G	16	GLN
2	G	372	GLN
2	G	378	GLN
2	H	378	GLN
2	I	9	GLN
2	I	14	GLN
2	I	94	HIS
2	I	378	GLN
2	J	331	HIS
2	J	378	GLN
3	K	16	GLN
3	K	34	ASN
3	L	16	GLN
3	L	34	ASN
3	M	16	GLN
3	M	18	ASN
3	M	34	ASN
3	M	68	GLN
3	N	16	GLN
3	N	34	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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	K	57	3	17,17,18	5.64	8 (47%)	19,24,26	2.49	4 (21%)
3	TQQ	L	57	3	17,17,18	5.31	9 (52%)	19,24,26	2.60	5 (26%)
3	TQQ	M	57	3	17,17,18	5.38	9 (52%)	19,24,26	2.80	5 (26%)
3	TQQ	N	57	3	17,17,18	5.55	10 (58%)	19,24,26	2.34	4 (21%)

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

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	57	TQQ	O-C	20.71	1.25	1.11
3	N	57	TQQ	O-C	20.54	1.25	1.11
3	M	57	TQQ	O-C	19.76	1.25	1.11
3	L	57	TQQ	O-C	18.95	1.24	1.11
3	L	57	TQQ	O2-CZ2	5.07	1.34	1.23
3	K	57	TQQ	CE2-NE1	-4.80	1.31	1.36
3	N	57	TQQ	O2-CZ2	4.75	1.33	1.23
3	M	57	TQQ	CZ3-CE3	4.68	1.42	1.34
3	M	57	TQQ	O2-CZ2	4.24	1.32	1.23
3	L	57	TQQ	CD2-CG	4.23	1.48	1.41
3	N	57	TQQ	CE2-NE1	-4.20	1.32	1.36
3	M	57	TQQ	CD2-CG	4.10	1.48	1.41
3	K	57	TQQ	O2-CZ2	4.08	1.32	1.23
3	L	57	TQQ	CD2-CE2	3.95	1.46	1.40
3	K	57	TQQ	CD2-CG	3.95	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	57	TQQ	CA-C	3.81	1.55	1.48
3	N	57	TQQ	CE2-CZ2	-3.67	1.47	1.50
3	K	57	TQQ	CE2-CZ2	-3.55	1.47	1.50
3	N	57	TQQ	CD2-CG	3.53	1.47	1.41
3	L	57	TQQ	CA-C	3.51	1.55	1.48
3	K	57	TQQ	CZ3-CE3	3.44	1.40	1.34
3	M	57	TQQ	CE2-NE1	-3.30	1.33	1.36
3	L	57	TQQ	CD1-CG	3.26	1.43	1.38
3	L	57	TQQ	CH2-N2	3.18	1.41	1.25
3	N	57	TQQ	CA-C	3.15	1.54	1.48
3	M	57	TQQ	CA-C	3.01	1.54	1.48
3	K	57	TQQ	CD2-CE2	2.96	1.44	1.40
3	L	57	TQQ	CZ3-CE3	2.96	1.39	1.34
3	M	57	TQQ	CD2-CE2	2.85	1.44	1.40
3	L	57	TQQ	CE2-NE1	-2.71	1.34	1.36
3	M	57	TQQ	CE2-CZ2	-2.56	1.48	1.50
3	M	57	TQQ	CH2-N2	2.52	1.38	1.25
3	N	57	TQQ	CZ3-CE3	2.33	1.38	1.34
3	N	57	TQQ	CH2-N2	2.31	1.37	1.25
3	N	57	TQQ	CD2-CE2	2.08	1.43	1.40
3	N	57	TQQ	CB-CA	2.05	1.58	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	57	TQQ	C-CA-N	-7.77	106.06	113.83
3	L	57	TQQ	CD1-CG-CD2	-7.30	101.48	104.97
3	M	57	TQQ	CD1-CG-CD2	-7.05	101.60	104.97
3	N	57	TQQ	CD1-CG-CD2	-6.77	101.74	104.97
3	K	57	TQQ	CD1-CG-CD2	-6.56	101.84	104.97
3	K	57	TQQ	C-CA-N	-6.24	107.59	113.83
3	N	57	TQQ	C-CA-N	-5.76	108.08	113.83
3	L	57	TQQ	C-CA-N	-4.70	109.13	113.83
3	K	57	TQQ	CG-CD1-NE1	3.75	114.28	107.94
3	M	57	TQQ	CG-CD1-NE1	3.73	114.25	107.94
3	L	57	TQQ	O2-CZ2-CE2	3.68	125.07	118.29
3	L	57	TQQ	CG-CD1-NE1	3.28	113.48	107.94
3	N	57	TQQ	O2-CZ2-CE2	3.08	123.97	118.29
3	L	57	TQQ	CE3-CZ3-CH2	2.94	126.46	121.82
3	N	57	TQQ	CG-CD1-NE1	2.86	112.78	107.94
3	K	57	TQQ	CG-CD2-CE3	2.24	135.55	127.38
3	M	57	TQQ	O2-CZ2-CE2	2.18	122.32	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	57	TQQ	CG-CD2-CE3	2.17	135.29	127.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	-0.04	0 100 100	29, 42, 52, 58	0
1	B	105/105 (100%)	-0.26	0 100 100	22, 27, 37, 48	0
1	C	105/105 (100%)	-0.32	0 100 100	21, 29, 39, 51	0
1	D	105/105 (100%)	-0.12	1 (0%) 79 84	30, 40, 50, 57	0
2	G	382/386 (98%)	-0.28	0 100 100	15, 23, 38, 62	0
2	H	382/386 (98%)	-0.24	1 (0%) 91 95	14, 22, 37, 58	0
2	I	382/386 (98%)	0.19	11 (2%) 49 56	25, 43, 61, 76	0
2	J	382/386 (98%)	-0.13	3 (0%) 83 88	19, 37, 53, 81	0
3	K	125/131 (95%)	-0.14	0 100 100	18, 29, 44, 67	0
3	L	125/131 (95%)	-0.17	1 (0%) 83 88	20, 29, 39, 56	0
3	M	125/131 (95%)	-0.19	1 (0%) 83 88	15, 25, 42, 64	0
3	N	125/131 (95%)	-0.08	1 (0%) 83 88	21, 32, 44, 69	0
All	All	2448/2488 (98%)	-0.13	19 (0%) 83 88	14, 31, 53, 81	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	386	GLY	3.8
2	J	5	GLU	3.8
3	M	131	SER	3.2
2	I	364	GLY	3.0
2	J	6	ALA	3.0
2	I	271	ALA	2.9
2	I	316	LEU	2.6
1	D	66	ALA	2.5
3	N	130	ALA	2.4
2	I	5	GLU	2.4
2	I	208	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	237	ALA	2.3
2	I	219	VAL	2.2
2	I	261	PHE	2.1
2	J	9	GLN	2.1
3	L	131	SER	2.1
2	I	6	ALA	2.0
2	H	5	GLU	2.0
2	I	315	VAL	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	TQQ	M	57	16/17	0.12	0.41	26,29,31,32	0
3	TQQ	N	57	16/17	0.12	-0.39	23,25,27,28	0
3	TQQ	L	57	16/17	0.11	-0.73	22,24,26,28	0
3	TQQ	K	57	16/17	0.10	-0.94	25,30,33,34	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CU	B	1106	1/1	0.15	2.91	32,32,32,32	0
4	CU	A	1106	1/1	0.16	2.57	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CU	C	1106	1/1	0.13	2.24	34,34,34,34	0
4	CU	D	1106	1/1	0.12	0.56	38,38,38,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.