



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:44 AM GMT

PDB ID : 2J55
Title : X-RAY REDUCED PARACCOCUS DENITRIFICANS METHYLAMINE
DEHYDROGENASE O-QUINONE IN COMPLEX WITH AMICYANIN.
Authors : Pearson, A.R.; Pahl, R.; Davidson, V.L.; Wilmot, C.M.
Deposited on : 2006-09-12
Resolution : 2.15 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

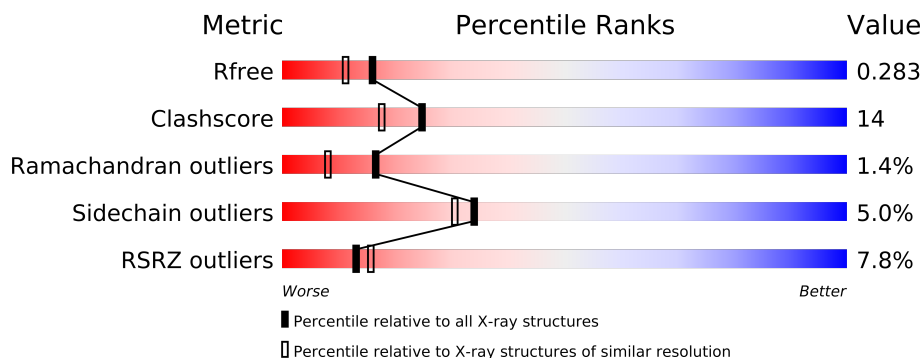
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.15 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}	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
2	H	386	
2	J	386	
3	L	131	
3	M	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
5	GOL	H	1387	-	X
5	GOL	H	1389	-	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 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			

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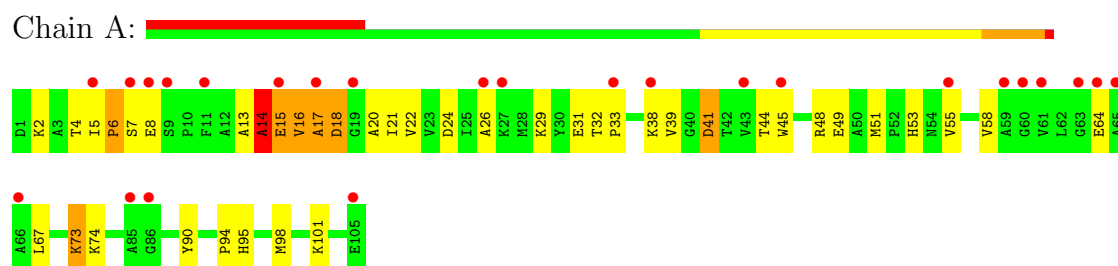
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	75	Total 75	O 75	0	0
6	M	86	Total 86	O 86	0	0

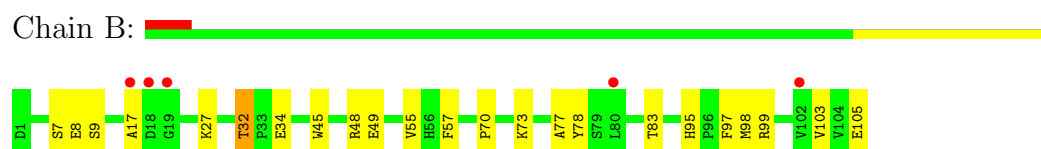
3 Residue-property plots

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

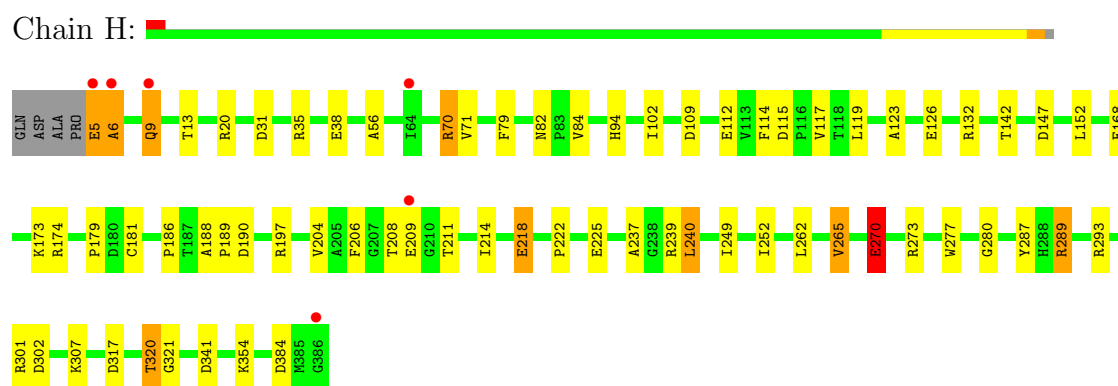
• Molecule 1: AMICYANIN



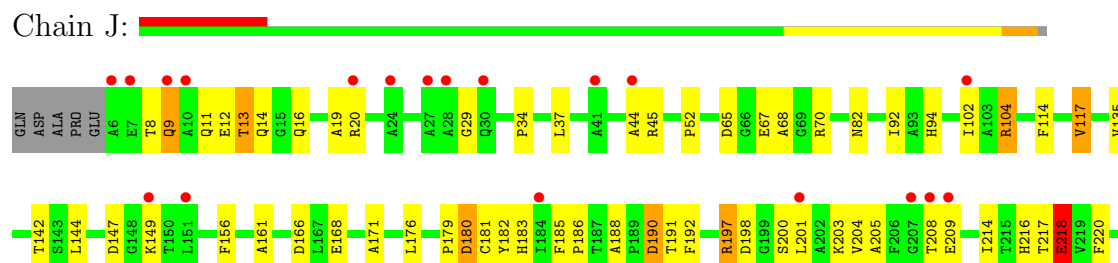
• Molecule 1: AMICYANIN

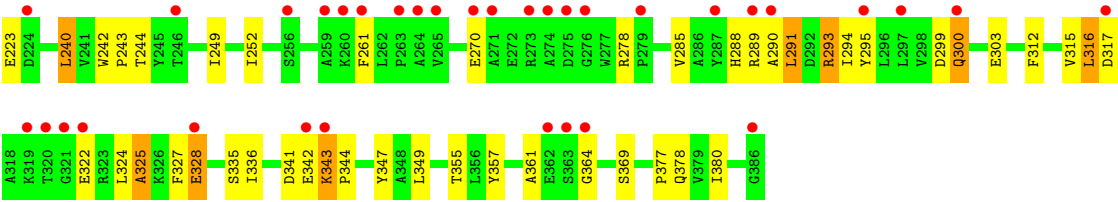


• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN



• Molecule 2: METHYLAMINE DEHYDROGENASE HEAVY CHAIN





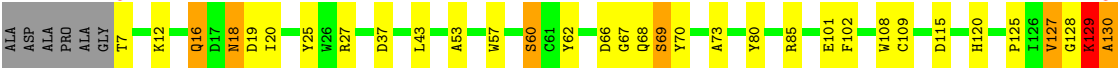
• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain L:



• Molecule 3: METHYLAMINE DEHYDROGENASE LIGHT CHAIN

Chain M:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.73Å 122.73Å 246.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.70 – 2.15 21.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (21.70-2.15) 98.9 (21.70-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.245 0.232 , 0.283	Depositor DCC
R_{free} test set	5081 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 101510 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10411	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

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 14.

All (255) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
3:M:127:VAL:HG22	3:M:128:GLY:N	1.93	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:J:11:GLN:HG2	3:L:21:GLN:OE1	1.99	0.62
3:L:20:ILE:HG22	3:L:25:TYR:CZ	2.34	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:J:44:ALA:HB1	2:J:341:ASP:HB3	1.83	0.61
2:H:273:ARG:HG2	6:H:2293:HOH:O	2.01	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
2:J:19:ALA:HB2	3:L:20:ILE:HG23	1.83	0.59
1:B:99:ARG:NH2	2:J:180[B]:ASP:OD2	2.35	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:J:8:THR:HA	2:J:9:GLN:CG	2.26	0.58
2:H:211:THR:HG23	6:H:2237:HOH:O	2.03	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
5:H:1389:GOL:H32	3:M:37:ASP:OD1	2.03	0.57
2:J:217:THR:CG2	2:J:261:PHE:CZ	2.81	0.57
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:34:PRO:HB3	3:L:44:THR:O	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:20:ILE:HG22	3:L:25:TYR:CE1	2.40	0.56
3:L:57:TRQ:HB2	3:L:108:TRP:HE1	1.68	0.56
2:J:70:ARG:HG3	2:J:70:ARG:HH11	1.70	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
3:L:16:GLN:HE21	3:L:16:GLN:C	2.10	0.55
2:J:249:ILE:HD12	2:J:294:ILE:HG21	1.88	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
3:L:21:GLN:NE2	3:L:37:ASP:OD2	2.38	0.54
2:J:290:ALA:HB3	2:J:291:LEU:HD13	1.89	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
3:L:68:GLN:HE22	3:L:129:LYS:HE2	1.74	0.53
2:H:173:LYS:HE3	6:H:2214:HOH:O	2.08	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
3:L:55:ALA:O	3:L:56:SER:HB3	2.10	0.51
2:H:82:ASN:HB3	2:H:142:THR:HB	1.93	0.51
1:A:17:ALA:CB	1:A:20:ALA:HB2	2.41	0.51
2:J:34:PRO:HG2	3:L:75:ARG:HH12	1.71	0.51
2:H:5:GLU:O	2:H:6:ALA:HB2	2.10	0.51
2:J:312:PHE:HE1	2:J:328:GLU:HG3	1.71	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:GLU:O	6:A:2001:HOH:O	2.18	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:J:13:THR:HG21	6:J:2006:HOH:O	2.13	0.48
2:H:204:VAL:HG22	2:H:214:ILE:HD13	1.95	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
3:L:57:TRQ:CZ3	3:L:108:TRP:HB2	2.45	0.45
2:J:355:THR:HG21	2:J:357:TYR:CE1	2.51	0.45
2:J:328:GLU:O	6:J:2180:HOH:O	2.21	0.45
1:A:95:HIS:HB2	1:A:98:MET:SD	2.56	0.45
1:A:26:ALA:HB3	1:A:31:GLU:OE2	2.16	0.45
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:H:237:ALA:HB2	2:H:289:ARG:HG3	1.98	0.44
2:J:16:GLN:HB3	3:L:18:ASN:O	2.18	0.44
1:B:97:PHE:CZ	2:J:197:ARG:NH1	2.86	0.44
2:J:288:HIS:HE1	2:J:290:ALA:HB3	1.82	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:M:69:SER:HB2	6:M:2051:HOH:O	2.19	0.43
3:L:114:ASP:O	3:L:115:ASP:HB2	2.19	0.43
3:L:20:ILE:HA	3:L:25:TYR:CG	2.54	0.43
1:B:95:HIS:HB3	1:B:97:PHE:CZ	2.53	0.43
2:J:197:ARG:HB2	6:M:2068:HOH:O	2.19	0.43
2:J:290:ALA:HB3	2:J:291:LEU:CD1	2.48	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
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:270[A]:GLU:H	2:H:270[A]:GLU:CD	2.21	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
2:H:249:ILE:HB	2:H:265:VAL:HG12	2.02	0.41
3:L:66:ASP:OD2	3:L:70:TYR:OH	2.30	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
3:L:70:TYR:HB3	3:L:126:ILE:HG23	2.02	0.41
2:H:115:ASP:O	2:H:119:LEU:HA	2.20	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:J:343:LYS:HA	2:J:344:PRO:HD3	1.90	0.41
2:H:280:GLY:HA3	2:H:301:ARG:CZ	2.51	0.41
2:J:16:GLN:CB	3:L:18:ASN:O	2.70	0.40
1:B:57:PHE:N	1:B:57:PHE:CD1	2.89	0.40
2:J:289:ARG:HB3	6:J:2187:HOH:O	2.20	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
2:H:168:GLU:HG3	6:H:2091:HOH:O	2.21	0.40
3:M:27:ARG:HD2	3:M:43:LEU:HD21	2.04	0.40
2:J:335:SER:HB2	2:J:349:LEU:HB3	2.04	0.40
1:A:6:PRO:HB2	1:A:7:SER:H	1.71	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	Distance(Å)	Clash(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%)	2	0
1	B	103/105 (98%)	100 (97%)	2 (2%)	1 (1%)	22	13
2	H	383/386 (99%)	369 (96%)	12 (3%)	2 (0%)	38	31
2	J	380/386 (98%)	350 (92%)	25 (7%)	5 (1%)	18	9
3	L	122/131 (93%)	115 (94%)	6 (5%)	1 (1%)	27	17
3	M	122/131 (93%)	113 (93%)	7 (6%)	2 (2%)	14	6
All	All	1213/1244 (98%)	1137 (94%)	58 (5%)	18 (2%)	16	7

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%)	10	5
1	B	84/85 (99%)	80 (95%)	4 (5%)	35	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	311/311 (100%)	298 (96%)	13 (4%)	40	39
2	J	308/311 (99%)	292 (95%)	16 (5%)	32	29
3	L	104/106 (98%)	101 (97%)	3 (3%)	55	57
3	M	104/106 (98%)	98 (94%)	6 (6%)	28	23
All	All	995/1004 (99%)	944 (95%)	51 (5%)	34	29

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
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

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Mol	Chain	Res	Type
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 chains 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	17,17,18	5.55	7 (41%)	20,24,26	2.71	5 (25%)
3	TRQ	M	57	3	17,17,18	5.45	6 (35%)	20,24,26	2.32	6 (30%)

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	-	0/4/19/21	0/0/2/2
3	TRQ	M	57	3	-	0/4/19/21	0/0/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	57	TRQ	O-C	21.02	1.25	1.11
3	M	57	TRQ	O-C	19.94	1.25	1.11
3	M	57	TRQ	CD2-CG	6.00	1.52	1.41
3	M	57	TRQ	CD2-CE2	5.34	1.48	1.40
3	L	57	TRQ	CD2-CG	4.73	1.49	1.41
3	M	57	TRQ	CZ3-CE3	4.35	1.41	1.34
3	L	57	TRQ	CD2-CE2	4.08	1.46	1.40
3	L	57	TRQ	CZ3-CE3	3.54	1.40	1.34
3	L	57	TRQ	CZ3-CH2	-3.32	1.36	1.45
3	M	57	TRQ	O7-CZ2	3.07	1.30	1.23
3	L	57	TRQ	CE2-CZ2	-2.37	1.48	1.50
3	L	57	TRQ	CA-C	2.13	1.52	1.48
3	M	57	TRQ	CZ3-CH2	-2.09	1.40	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	57	TRQ	C-CA-N	-9.71	104.13	113.83
3	M	57	TRQ	C-CA-N	-7.77	106.07	113.83
3	L	57	TRQ	CD1-CG-CD2	-3.95	103.09	104.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	57	TRQ	CG-CD1-NE1	3.45	113.77	107.94
3	M	57	TRQ	O7-CZ2-CE2	3.19	124.18	118.29
3	M	57	TRQ	CD1-NE1-CE2	3.04	113.18	107.32
3	L	57	TRQ	CB-CG-CD1	-2.45	123.93	128.12
3	M	57	TRQ	CD2-CE3-CZ3	2.40	123.82	120.86
3	M	57	TRQ	CZ3-CH2-CZ2	2.17	121.90	118.83
3	M	57	TRQ	CG-CD2-CE3	2.14	135.18	127.38
3	L	57	TRQ	CG-CD2-CE3	2.04	134.83	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 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	0.52	0	5,5,5	0.90	0
5	GOL	H	1388	-	5,5,5	0.68	0	5,5,5	1.07	0
5	GOL	H	1389	2	5,5,5	0.55	0	5,5,5	1.42	1 (20%)
5	GOL	L	1132	3	5,5,5	0.54	0	5,5,5	0.85	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($^{\circ}$)	Ideal($^{\circ}$)
5	H	1389	GOL	O3-C3-C2	3.11	124.88	109.71

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	105/105 (100%)	1.34	25 (23%) 1 1	62, 79, 91, 97	0
1	B	105/105 (100%)	0.33	5 (4%) 29 33	48, 56, 68, 81	0
2	H	382/386 (98%)	0.15	6 (1%) 68 75	38, 48, 64, 86	0
2	J	381/386 (98%)	0.89	53 (13%) 4 4	46, 71, 89, 97	0
3	L	125/131 (95%)	0.39	4 (3%) 45 49	48, 61, 74, 104	0
3	M	125/131 (95%)	0.32	3 (2%) 56 61	40, 54, 72, 102	0
All	All	1223/1244 (98%)	0.54	96 (7%) 13 16	38, 59, 87, 104	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	274	ALA	6.9
2	J	28	ALA	6.5
3	M	131	SER	6.2
2	J	342	GLU	5.7
2	J	386	GLY	5.5
2	J	6	ALA	5.4
3	M	130	ALA	5.3
1	A	17	ALA	5.1
1	A	9	SER	4.9
1	A	59	ALA	4.7
2	J	27	ALA	4.5
1	A	85	ALA	4.4
1	B	19	GLY	4.3
1	A	64	GLU	4.2
1	A	65	ALA	4.1
1	A	43	VAL	4.0
2	J	24	ALA	4.0
2	J	264	ALA	3.9
1	A	5	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	5	GLU	3.9
1	A	8	GLU	3.9
3	L	131	SER	3.8
1	A	60	GLY	3.8
2	J	276	GLY	3.8
1	B	18	ASP	3.7
2	J	271	ALA	3.6
3	L	130	ALA	3.6
2	J	275	ASP	3.5
2	H	6	ALA	3.5
2	J	259	ALA	3.5
2	J	322	GLU	3.5
3	L	7	THR	3.4
2	J	261	PHE	3.4
2	J	44	ALA	3.3
2	J	209	GLU	3.3
2	J	364	GLY	3.3
2	J	320	THR	3.3
1	A	38	LYS	3.3
2	J	319	LYS	3.2
2	J	362	GLU	3.1
2	J	297	LEU	3.1
2	J	208	THR	3.1
2	J	270	GLU	3.0
2	J	343	LYS	2.9
2	J	30	GLN	2.9
2	J	263	PRO	2.8
2	H	9	GLN	2.8
2	H	209	GLU	2.7
2	J	321	GLY	2.7
1	A	105	GLU	2.7
2	J	260	LYS	2.7
2	J	201	LEU	2.7
1	A	26	ALA	2.6
2	J	9	GLN	2.6
2	H	386	GLY	2.6
2	J	363	SER	2.6
1	A	86	GLY	2.6
1	A	66	ALA	2.5
1	B	80	LEU	2.5
2	J	20	ARG	2.5
1	A	15	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	33	PRO	2.5
2	J	290	ALA	2.5
1	A	45	TRP	2.5
1	B	17	ALA	2.4
2	J	10	ALA	2.4
1	A	27	LYS	2.4
1	A	63	GLY	2.4
2	J	273	ARG	2.4
1	A	11	PHE	2.4
2	J	224	ASP	2.4
2	J	246	THR	2.3
3	M	7	THR	2.3
2	J	300	GLN	2.3
2	J	287	TYR	2.3
2	J	295	TYR	2.3
1	A	7	SER	2.3
1	A	19	GLY	2.3
2	J	151	LEU	2.3
2	J	289	ARG	2.3
3	L	128	GLY	2.3
2	J	102	ILE	2.3
2	H	64	ILE	2.2
1	A	55	VAL	2.2
2	J	256	SER	2.2
2	J	328	GLU	2.2
2	J	317	ASP	2.2
2	J	184	ILE	2.1
2	J	279	PRO	2.1
1	B	102	VAL	2.1
2	J	149	LYS	2.1
2	J	265	VAL	2.0
2	J	7	GLU	2.0
1	A	61	VAL	2.0
2	J	41	ALA	2.0
2	J	207	GLY	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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	TRQ	M	57	16/17	0.17	0.97	54,57,59,59	0
3	TRQ	L	57	16/17	0.14	-0.19	54,57,60,61	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	L	1132	6/6	0.28	9.74	75,76,77,77	0
5	GOL	H	1387	6/6	0.23	8.27	66,71,74,75	0
5	GOL	H	1389	6/6	0.28	4.89	39,46,54,58	0
5	GOL	H	1388	6/6	0.14	1.12	27,42,45,51	0
4	CU	B	1106	1/1	0.11	-1.78	65,65,65,65	0
4	CU	A	1106	1/1	0.07	-3.48	66,66,66,66	0

6.5 Other polymers

There are no such residues in this entry.